Many-Particle Theory

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Preface to the English edition

The world around us consists of interacting many-particle systems. The aim of theoretical atomic, molecular, condensed matter and nuclear physics is to describe the rich variety of phenomena of such systems. Modern many-particle theory is a common denominator of all these, in detail rather different, disciplines of physics and is the subject of this book.

Perhaps the most important fundamental concept of many-particle theory is based on the idea that an interacting many-particle system can be described approximately as a system of non-interacting 'quasi-particles'. However, if we want to mathematically rigorously demonstrate this intuitive idea, a rather complicated formalism is necessary. This formalism rests on three cornerstones. (1) The so-called second quantization, (2) the method of Green's functions, and (3) perturbation-theoretical analysis using Feynman diagrams. These three cornerstones presently form the framework within which many experiments are formulated and understood. Not in the least because of the overwhelming technological importance that many-particle effects in condensed matter physics have attained in recent years, these cornerstones of many-particle physics must be regarded as part of the standard graduate physics curriculum.

Our aim in writing this book is to present the basics of many-particle theory in a closed and easily accessible form. The presentation is primarily aimed at students of theoretical *and* experimental physics, but should also be useful to mathematicians interested in applications, and to theoretically oriented chemists. Only a basic grasp of fundamental quantum mechanics taught in introductory courses is assumed. On this foundation, the material is developed in a systematic and self-contained way. The material in this book consists of well-known results, and great emphasis is placed on performing derivations in detail, without skipping intermediate steps. This makes the material ideal for the use in courses, minimizing the preparations necessary.

The examples are selected to first of all illustrate the relations between the mathematical formalism and physically intuitive concepts. A complete overview of the endless uses of many-particle theory cannot and should not be given within the scope of this book. It is, however, our goal that this book will give the reader the necessary fundamental knowledge of many-particle theory to understand the original literature in condensed matter physics, nuclear physics and quantum chemistry.

There are many people to whom we owe thanks for the preparation of this book. An understandable presentation of Feynman diagrams is impossible without skilled technical artists. Many thanks to Mrs. Buffo for preparing the original artwork, and to the staff at IOP Publishing for very meticulously removing the artwork from the original German manuscript and pasting it into the English manuscript. Many people have helped us with the tedious task of proof-reading the manuscript, and mercilessly pointed out gross or subtle errors, and asked pointed questions about 'what we really mean by' vague and ill-formulated statements. In particular Elisabeth Runge, Mike Johnson, Phil Taylor and Jay Shivamoggi have been extremely helpful. We also thank Leslie McDonald and our editor at IOP Publishing, Lauret Tipping, for helping to transform a strange concoction of German, Swedish and English into something we hope passes for English.

Eberhard Gross
Erich Runge
Olle Heinonen

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Part I

Fundamentals and Examples

Chapter 1

Systems of identical particles

Identical particles are particles which have the same masses, charges, sizes and all other physical properties. In the realm of classical mechanics, identical particles are distinguishable. For example, consider a collision of two identical billiard balls – we can follow the trajectory of each individual ball and thus distinguish them. However, in the physics of microscopic particles where we must use quantum mechanics, the situation is quite different. We can distinguish identical particles which are very far apart from each other; for example, one electron on the moon can be distinguished from one on the earth. On the other hand, when identical particles interact with one another, as in a scattering experiment, the trajectory concept of classical mechanics cannot be applied because of Heisenberg's uncertainty principle. As a consequence, microscopic particles which interact with each other are completely indistinguishable – they cannot be distinguished by any measurement.

The measurable quantities of a stationary quantum mechanical system are the expectation values of operators that represent the observables of the system. If the system consists of identical particles, these expectation values must not change when the coordinates of two particles are interchanged in the wavefunction. (If we could find expectation values which do change when the coordinates of two particles are interchanged, we would have found measurable quantities by which we could distinguish the particles.) Thus, we require that for any possible state Ψ of the system and for all observables B

$$\begin{aligned}&\int \mathrm{d}^N x \Psi^*(x_1,\ldots,x_j,\ldots,x_k,\ldots,x_N)\hat{B}\Psi(x_1,\ldots,x_j,\ldots,x_k,\ldots,x_N)\\&\quad = \int \mathrm{d}^N x \Psi^*(x_1,\ldots,x_k,\ldots,x_j,\ldots,x_N)\hat{B}\Psi(x_1,\ldots,x_k,\ldots,x_j,\ldots,x_N)\end{aligned} \tag{1.1}$$

for all pairs (j, k). (We use a caret to denote operators.)

The coordinates $x \equiv (\mathbf{r}, s)$ contain the space and spin degrees of freedom of the particles. We use the notation

$$\int \mathrm{d}x = \sum_s \int \mathrm{d}^3 r \quad \text{and} \quad \int \mathrm{d}^N x = \int \mathrm{d}x_1 \int \mathrm{d}x_2 \ldots \int \mathrm{d}x_N.$$

To a certain extent, equation (1.1) above defines a system of identical particles. By using this equation, we will derive properties of both the wavefunction and of the operators that describe a system of identical particles. In so doing, we need only require that the expectation values remain unchanged when we interchange *two* particles, since each possible permutation of the particles can be expressed as a sequence of two-particle interchanges. In mathematical terms, each permutation P can be expressed as a product of transpositions P_{jk}

$$P = \prod P_{jk}.$$

The transpositions P_{jk} are expressed as operators with the action

$$\hat{P}_{jk}\Psi(x_1, \ldots, x_j, \ldots, x_k, \ldots, x_N) \equiv \Psi(x_1, \ldots, x_k, \ldots, x_j, \ldots, x_N)$$

on a many-particle wavefunction. Applying the permutation operator $\hat{P}_{jk}$ twice restores the original wavefunction. Hence, it follows that

$$\hat{P}_{jk}\hat{P}_{jk} = \mathrm{Id} = 1, \text{ so } \hat{P}_{jk}^{-1} = \hat{P}_{jk}.$$

By means of these transposition operators, equation (1.1) can be written

$$\langle \Psi \mid \hat{B} \mid \Psi \rangle = \langle \hat{P}_{jk}\Psi \mid \hat{B} \mid \hat{P}_{jk}\Psi \rangle = \langle \Psi \mid \hat{P}_{jk}^{\dagger}\hat{B}\hat{P}_{jk} \mid \Psi \rangle \quad \text{for all } (j,k).$$

This equation must hold for *all* state functions in the Hilbert space under consideration. The equation can then be inserted on the right-hand side of the identity

$$\langle \Phi \mid \hat{B} \mid \Psi \rangle = \frac{1}{4}\Big(\langle \Phi + \Psi \mid \hat{B} \mid \Phi + \Psi \rangle - \langle \Phi - \Psi \mid \hat{B} \mid \Phi - \Psi \rangle$$

$$-i\langle \Phi + i\Psi \mid \hat{B} \mid \Phi + i\Psi \rangle + i\langle \Phi - i\Psi \mid \hat{B} \mid \Phi - i\Psi \rangle \Big)$$

which yields

$$\langle \Phi \mid \hat{B} \mid \Psi \rangle = \langle \Phi \mid \hat{P}_{jk}^{\dagger}\hat{B}\hat{P}_{jk} \mid \Psi \rangle$$

for all (j,k) and for arbitrary wavefunctions Φ and Ψ in the Hilbert space. This implies the operator identity

$$\hat{B} = \hat{P}_{jk}^{\dagger}\hat{B}\hat{P}_{jk} \qquad \text{for all } (j,k). \tag{1.2}$$

In particular, if we take $\hat{B}$ to be the identity operator, *i.e.*, $\hat{B} = 1$, it follows that

$$1 = \hat{P}^{\dagger}_{jk}\hat{P}_{jk}.$$

Multiplication from the right with $\hat{P}_{jk}$ yields

$$\hat{P}_{jk} = \hat{P}^{\dagger}_{jk}$$

so that finally we obtain

$$\hat{P}^{-1}_{jk} = \hat{P}_{jk} = \hat{P}^{\dagger}_{jk}.$$

Thus, the operators that correspond to transpositions of particles are self-adjoint and unitary (so long as they operate on the space of state functions of identical particles).

If we multiply equation (1.2) from the left with $\hat{P}_{jk}$, we obtain

$$\hat{P}_{jk}\hat{B} = \hat{P}_{jk}\hat{P}^{\dagger}_{jk}\hat{B}\hat{P}_{jk} = \hat{B}\hat{P}_{jk}.$$

The operators which represent the observables of a system of identical particles must therefore commute with all permutation operators:

$$\left[\hat{B}, \hat{P}_{jk}\right] = 0 \quad \text{for all } (j,k). \tag{1.3}$$

We will now calculate the eigenvalues of the transposition operators. Let Ψ be an eigenfunction of $\hat{P}_{jk}$ with eigenvalue $a_{(jk)}$:

$$\hat{P}_{jk}\Psi = a_{(jk)}\Psi.$$

It follows that

$$\Psi = \hat{P}^2_{jk}\Psi = a^2_{(jk)}\Psi, \text{ so } a^2_{(jk)} = 1.$$

Since the operators $\hat{P}_{jk}$ are self-adjoint, their eigenvalues are real. Thus

$$a_{(jk)} = \pm 1.$$

In particular, equation (1.3) must hold if $\hat{B}$ is the Hamiltonian $\hat{H}$ of the system under consideration:

$$\left[\hat{H}, \hat{P}_{jk}\right] = 0 \qquad \text{for all } (j,k).$$

Hence, any solution of the Schrödinger equation with proper symmetries under particle-interchange must be a simultaneous eigenfunction of $\hat{H}$ and of all $\hat{P}_{jk}$ (and thus of all possible permutation operators $\hat{P}$).

It seems reasonable to expect that if a function Ψ is an eigenfunction of all $\hat{P}_{jk}$, the eigenvalues of all $\hat{P}_{jk}$ must be identical:

$$\hat{P}_{jk}\Psi = a_{(12)}\Psi \qquad \text{for all } (j,k).$$

Indeed, we can prove this by writing the transposition $\hat{P}_{jk}$ as

$$\hat{P}_{jk} = \hat{P}_{1j}\hat{P}_{2k}\hat{P}_{12}\hat{P}_{2k}\hat{P}_{1j}$$

so that

$$\hat{P}_{jk}\Psi = a^2_{(1j)}a^2_{(2k)}a_{(12)}\Psi = a_{(12)}\Psi$$

for all possible (j,k). We now make the following definitions.

If $\hat{P}_{jk}\Psi = +\Psi$ for all (j,k), we say that Ψ is *symmetric.*

If $\hat{P}_{jk}\Psi = -\Psi$ for all (j,k), we say that Ψ is *antisymmetric.*

Thus, the state function of a system of identical particles must be either symmetric or antisymmetric.

If Ψ_S is symmetric and Ψ_A is antisymmetric, it is clear that for any possible permutation $\hat{P}$ we have

$$\hat{P}\Psi_S = +\Psi_S$$

and

$$\hat{P}\Psi_A = \mathrm{sgn}(P)\cdot\Psi_A$$

where $\mathrm{sgn}(P) = +1$ if $\hat{P}$ contains an even number of transpositions, and $\mathrm{sgn}(P) = -1$ if $\hat{P}$ contains an odd number of transpositions. Symmetric and antisymmetric functions are always orthogonal:

$$\begin{aligned} \langle\Psi_A \mid \Psi_S\rangle &= \langle\Psi_A \mid \hat{P}_{jk} \mid \Psi_S\rangle &= \langle\Psi_A \mid \hat{P}^\dagger_{jk} \mid \Psi_S\rangle \\ &= \langle\hat{P}_{jk}\Psi_A \mid \Psi_S\rangle &= -\langle\Psi_A \mid \Psi_S\rangle \end{aligned}$$

so $\langle\Psi_A \mid \Psi_S\rangle = 0$.

Up to this point we have implicitly assumed that there exist simultaneous eigenfunctions, *i.e.*, symmetric or antisymmetric functions, of all $\hat{P}_{jk}$. Because the transposition operators do not commute, it is not clear that there exists a non-trivial space of functions in which all transposition operators are simultaneously diagonal. We will construct such functions by an explicit procedure below. We start by defining a symmetrization operator $\hat{S}$ by

$$\hat{S} = \sum_{P\in S_N} \hat{P}$$

and an antisymmetrization operator $\hat{A}$ by

$$\hat{A} = \sum_{P \in S_N} \operatorname{sgn}(P)\hat{P}.$$

Each sum runs over all elements P of the permutation group S_N. If $f(x_1, \ldots, x_N)$ is an arbitrary function of N variables, we can use the operation

$$\Psi_S(x_1, \ldots, x_N) \equiv \hat{S}f(x_1, \ldots, x_N)$$

to construct a symmetric function; and through the operation

$$\Psi_A(x_1, \ldots, x_N) \equiv \hat{A}f(x_1, \ldots, x_N)$$

we can construct an antisymmetric function, since for any $\hat{P}_{jk}$ we have

$$\hat{P}_{jk}\hat{S} = \sum_{P \in S_N} \hat{P}_{jk}\hat{P} = \sum_{P \in S_N} \hat{P} = \hat{S}$$

and

$$\begin{aligned} \hat{P}_{jk}\hat{A} &= \sum_{P \in S_N} \operatorname{sgn}(P)\left(\hat{P}_{jk}\hat{P}\right) \\ &= \sum_{P \in N} \left[-\operatorname{sgn}\left(P_{jk}P\right)\right]\left(\hat{P}_{jk}\,\hat{P}\right) \\ &= \sum_{P \in N} \left[-\operatorname{sgn}(P)\right]\hat{P} \\ &= -\hat{A} \end{aligned}$$

and thus

$$\begin{aligned} \hat{P}_{jk}\Psi_S &= \Psi_S \\ \hat{P}_{jk}\Psi_A &= -\Psi_A \end{aligned}$$

for all $(j,\, k)$. Using this procedure, we can construct both symmetric and antisymmetric eigenfunctions of any given many-particle Hamiltonian.

At this point, we introduce a principle of fundamental importance, generally known as the *symmetry postulate*:

> **The Hilbert space of state functions of a system of identical particles contains either *only* symmetric or *only* antisymmetric functions.**

In the first case, the particles are called *bosons*, and in the second case *fermions*. The so-called spin-statistics theorem [1], which we will not prove here, states that bosons only have integer spin and that fermions only have spin equal to half of an odd integer.

To prove the symmetry postulate, we start with an eigenfunction Ψ_0 of the Hamiltonian with definite symmetry, *i.e.*, Ψ_0 is either symmetric or antisymmetric. Any possible state function Φ of the system can be characterized by a non-vanishing overlap with at least one state $\hat{B}\Psi_0$ that can be obtained by operating on Ψ_0 by any possible operator $\hat{B}$. With $\hat{P}_{jk}\Psi_0 = p\Psi_0$, where $p = +1$ or $p = -1$, it follows from equation (1.3) that

$$\langle \hat{P}_{jk}\Phi \mid \hat{B}\Psi_0\rangle = \quad \langle \Phi \mid \hat{B}\hat{P}_{jk}\Psi_0\rangle \quad = p\langle \Phi \mid \hat{B}\Psi_0\rangle$$

i.e., we have

$$\hat{P}_{jk}\Phi = p\Phi$$

for any function Φ which is not in the subspace orthogonal to $\hat{B}\Psi_0$. In other words, any such function Φ must obey the same permutation-symmetry as Ψ_0.

As an example, we consider a system of non-interacting identical particles, which are acted upon by an external potential. The Hamiltonian for this system is

$$\hat{H}_0 = \sum_{i=1}^{N} \hat{h}_i = \sum_{i=1}^{N} [\hat{t}_i + \hat{u}_i] = \sum_{i=1}^{N} \left(-\frac{\hbar^2}{2m}\nabla_i^2 + u(x_i) \right).$$

We assume that we have solved the associated one-particle problem

$$\hat{h}\phi_\nu(x) = \epsilon_\nu \phi_\nu(x).$$

(We will always use Greek indices to denote the quantum states which characterize the single-particle orbitals, for example $\nu = (n, l, m)$.) We can then construct symmetric and antisymmetric solutions $\Phi^{(S)}$ and $\Phi^{(A)}$ to the full problem by simply applying the symmetrization and antisymmetrization operators $\hat{S}$ and $\hat{A}$, which were introduced earlier, to a product of single-particle orbitals:

$$\Phi^{(S)} = \frac{1}{\sqrt{N!}\sqrt{\prod_{k=1}^{K} n_k!}} \sum_{P \in S_N} P\left(\phi_{\nu_1}(x_1) \cdot \phi_{\nu_2}(x_2) \ldots \phi_{\nu_N}(x_N)\right) \tag{1.4}$$

$$\begin{aligned} \Phi^{(A)} &= \frac{1}{\sqrt{N!}} \sum_{P \in S} \operatorname{sgn}(P) P\left[\phi_{\nu_1}(x_1)\phi_{\nu_2}(x_2) \ldots \phi_{\nu_N}(x_N)\right] \\ &= \frac{1}{\sqrt{N!}} \begin{vmatrix} \phi_{\nu_1}(x_1) & \cdots & \phi_{\nu_1}(x_N) \\ \vdots & & \vdots \\ \phi_{\nu_N}(x_1) & \cdots & \phi_{\nu_N}(x_N) \end{vmatrix}. \end{aligned} \tag{1.5}$$

The prefactors are chosen such that $\Phi^{(S)}$ and $\Phi^{(A)}$ are normalized. Here, each k ($< N$) in $\Phi^{(S)}$ denotes a distinct orbital and n_k denotes the number of particles that occupy each state ν_k. A corresponding additional prefactor has no effect on $\Phi^{(A)}$, since the determinant vanishes for $n_k > 1$ in any case.

The functions defined in this way are eigenfunctions of

$$\hat{H}_0\Phi^{(S/A)} = E\Phi^{(S/A)}$$

with eigenvalues

$$E = \sum_{i=1}^{N} \epsilon_{\nu_1}.$$

We will give a brief proof for the case $N = 2$. The proof is quite analogous for arbitrary N.

$$\begin{aligned}
\Phi^{(S/A)}(x_1, x_2) &= \frac{1}{\sqrt{2}}\left[\phi_1(x_1)\phi_2(x_2) \pm \phi_1(x_2)\phi_2(x_1)\right] \\
\hat{H}_0\Phi^{(S/A)}(x_1, x_2) &= \hat{h}_1 \frac{1}{\sqrt{2}}\left[\phi_1(x_1)\phi_2(x_2) \pm \phi_1(x_2)\phi_2(x_1)\right] \\
&\quad + \hat{h}_2 \frac{1}{\sqrt{2}}\left[\phi_1(x_1)\phi_2(x_2) \pm \phi_1(x_2)\phi_2(x_1)\right] \\
&= \frac{1}{\sqrt{2}}\left[\epsilon_1\phi_1(x_1)\phi_2(x_2) \pm \epsilon_2\phi_1(x_2)\phi_2(x_1)\right. \\
&\quad \left. + \epsilon_2\phi_1(x_1)\phi_2(x_2) \pm \epsilon_1\phi_1(x_2)\phi_2(x_1)\right] \\
&= (\epsilon_1 + \epsilon_2)\frac{1}{\sqrt{2}}\left[\phi_1(x_1)\phi_2(x_2) \pm \phi_1(x_2)\phi_2(x_1)\right] \\
&= (\epsilon_1 + \epsilon_2)\,\Phi^{(S/A)}(x_1, x_2).
\end{aligned}$$

The fermion wavefunctions $\Phi^{(A)}$ above are called *Slater determinants*. Upon inspection, we can deduce the following interesting facts about these functions.

(1) If two particles are the same, $\nu_i = \nu_j$ for some $i \neq j$, we have $\Phi^{(A)} = 0$.

(2) If two columns of the determinant are identical, so that $x_i = x_j$ for some $i \neq j$, we have $\Phi^{(A)} = 0$.

The wavefunction vanishes in both cases; and as a result, the probability of finding such a state vanishes as well. This has two consequences.

(1) It is impossible to have two fermions in the same state; one state can be occupied by no more than one particle.

(2) It is impossible to bring two fermions with the same spin projection to the same point.

These two statements comprise the *Pauli principle.* An essential assumption for this principle is that the particles are independent, *i.e.,* that they do not interact with one another, so that the many-particle states can be characterized by occupied and unoccupied single-particle orbitals. Pauli originally formulated the principle for atoms, in which case the assumption that such systems can be realistically regarded as consisting of independent particles (*i.e.,* that the electron–electron interactions can be reasonably well described by an effective external potential), is the basis for the principle. We will justify this assumption in later chapters which discuss the Hartree–Fock approximation.

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It should be emphasized that no such principle exists for bosons. Consequently, we can put an arbitrary number of bosons in one single-particle state.

The symmetric state $\Phi^{(S)}$ is completely determined given the single-particle states that it contains, *e.g.*

$$\Phi^{(S)}_{(\nu_1\nu_4\nu_4)} = \frac{1}{\sqrt{12}} \sum_{P\in S_3} P\left[\phi_{\nu_1}(x_1)\phi_{\nu_4}(x_2)\phi_{\nu_4}(x_3)\right].$$

In contrast, the antisymmetric state $\Phi^{(A)}$ is only determined to within a sign by the single-particle states that it contains. For example, we can define two-particle states from ϕ_{ν_1} and ϕ_{ν_4} by

$$\Phi^{(A)}_{(\nu_1\nu_4)} \equiv \frac{1}{\sqrt{2}} \begin{vmatrix} \phi_{\nu_1}(x_1) & \phi_{\nu_1}(x_2) \\ \phi_{\nu_4}(x_1) & \phi_{\nu_4}(x_2) \end{vmatrix}$$

or by

$$\Phi^{(A)}_{(\nu_1\nu_4)} \equiv \frac{1}{\sqrt{2}} \begin{vmatrix} \phi_{\nu_4}(x_1) & \phi_{\nu_4}(x_2) \\ \phi_{\nu_1}(x_1) & \phi_{\nu_1}(x_2) \end{vmatrix}.$$

We can remove this last ambiguity of the fermion wavefunctions by assigning an arbitrary, but hereafter always the same, enumeration to the ν_i:

$$\begin{array}{cccc} \nu_1 & \nu_2 & \nu_3 & \dots \\ \downarrow & \downarrow & \downarrow & \dots \\ \phi_1(x) & \phi_2(x) & \phi_3(x) & \dots \end{array}$$

and, according to the same principle, by enumerating the single-particle orbitals that belong to these quantum numbers. Given an *ordered* N-tuple of indices

$$c = (c_1, c_2, \dots, c_N)$$

with $c_i \in \mathcal{N}$, where $\mathcal{N}$ is the set of natural numbers, and $c_1 < c_2 < \dots < c_N$ the Slater determinant

$$\Phi^{(A)}_c(x_1, x_2, \dots, x_N) \equiv \frac{1}{\sqrt{N!}} \sum_{P\in S_N} \mathrm{sgn}(P) \cdot P\left[\phi_{c_1}(x_1)\phi_{c_2}(x_2)\dots\phi_{c_N}(x_N)\right]$$

is then unambiguously defined; for by giving the sequence, each product of single-particle orbitals distinguished by increasing indices and consequently corresponding to identical permutations, is defined by a positive sign. Hence, the signs of all other permutations are also determined. As a result, the example above becomes

$$\begin{aligned} c = (1,4) \Rightarrow \quad \Phi_c^{(A)}(x_1, x_2) &= \frac{1}{\sqrt{2}} \sum_{P \in S_N} \operatorname{sgn}(P) \cdot P\left[\phi_1(x_1)\phi_4(x_2)\right] \\ &= \frac{1}{\sqrt{2}} \left[\phi_1(x_1)\phi_4(x_2) - \phi_1(x_2)\phi_4(x_1)\right] \\ &= \frac{1}{\sqrt{2}} \begin{vmatrix} \phi_1(x_1) & \phi_1(x_2) \\ \phi_4(x_1) & \phi_4(x_2) \end{vmatrix} \\ &= \frac{1}{\sqrt{2}} \begin{vmatrix} \phi_1(x_1) & \phi_4(x_1) \\ \phi_1(x_2) & \phi_4(x_2) \end{vmatrix} . \end{aligned}$$

The value of the determinant is invariant under interchange of all rows and columns so long as the enumeration is retained. We use

$$P(1, 2, ..., N) = (P(1), P(2), \ldots, P(N))$$

to denote symbolically a permutation of N elements. For example

$$P(1,2,3) = (3,2,1) \Rightarrow P(1) = 3,\ P(2) = 2,\ P(3) = 1.$$

Thus, the Slater determinant can be written in either of two ways:

$$\begin{aligned} \Phi_c^{(A)}(x_1, \ldots, x_N) &= \frac{1}{\sqrt{N!}} \sum_{P \in S_N} \operatorname{sgn}(P) \phi_{c_1}(x_{P(1)}) \ldots \phi_{c_N}(x_{P(N)}) \\ &= \frac{1}{\sqrt{N!}} \sum_{P \in S_N} \operatorname{sgn}(P) \phi_{c_{P(1)}}(x_1) \ldots \phi_{c_{P(N)}}(x_N). \end{aligned}$$

These two possibilities correspond to the row–column interchanges in the determinant. Both exist for the completely symmetrized wavefunction $\Phi_c^{(S)}$ as well. We will also characterize the symmetric functions by ordered N-tuples of indices, but for symmetric functions the ordering is unimportant.

In the remainder of this chapter will we prove one more important property of the many-particle wavefunctions $\Phi^{(S)}$ and $\Phi^{(A)}$. For each observable B of a system of identical particles, we have

$$\int \mathrm{d}^N x \, \Phi_b^* \hat{B} \Phi_c = \frac{\sqrt{N!}}{\sqrt{\prod_{k=1}^{K} n_k^{(c)}!}} \int \mathrm{d}^N x \, \Phi_b^* \hat{B} \phi_{c_1}(x_1) \ldots \phi_{c_N}(x_N) \qquad (1.6)$$

both for $\Phi = \Phi^{(S)}$ and for $\Phi = \Phi^{(A)}$ (in the latter case, $\prod_{k=1}^{K} n_k^{(c)}! = 1$). We will prove this only for the Slater determinant $\Phi^{(A)}$ – the proof for $\Phi^{(S)}$ is similar. By definition

$$\int \mathrm{d}^N x\, \Phi_b^* \hat{B} \Phi_c = \int \mathrm{d}^N \Phi_b^* \hat{B} \frac{1}{\sqrt{N!}} \sum_P \mathrm{sgn}(P) \cdot P \left[\phi_{c_1}(x_1) \ldots \phi_{c_N}(x_N)\right].$$

Since we have $\hat{B}\hat{P} = \hat{P}\hat{B}$ for observables of the system, this expression becomes

$$\begin{aligned} &\frac{1}{\sqrt{N!}} \int \mathrm{d}^N x\, \Phi_b^* \sum_P \mathrm{sgn}(P) \cdot P \left[\hat{B}\phi_{c_1}(x_1) \ldots \phi_{c_N}(x_N)\right] \\ &= \frac{1}{\sqrt{N!}} \int \mathrm{d}^N x \sum_P \mathrm{sgn}(P) \cdot P \left(P^{-1}\Phi_b^*\right) \hat{B}\phi_{c_1}(x_1) \ldots \phi_{c_N}(x_N). \end{aligned}$$

As $P^{-1}\Phi_b^* = \mathrm{sgn}(P^{-1}) \cdot \Phi_b^* = \mathrm{sgn}(P)\Phi_b^*$, we may write this as

$$\frac{1}{\sqrt{N!}} \sum_P \mathrm{sgn}^2(P) \cdot P \int \mathrm{d}^N x\, \Phi_b^* \hat{B}\phi_{c_1}(x_1) \ldots \phi_{c_N}(x_N).$$

Since the value of the integral remains unchanged if we interchange the integration variables $x_i \to x_{P(i)}$, we therefore obtain the same value for each permutation (altogether $N!$ times), and thus arrive at the expression

$$\sqrt{N!} \int \mathrm{d}^N x \Phi_b^*(x_1, \ldots, x_N) \hat{B}\phi_{c_1}(x_1) \ldots \phi_{c_N}(x_N).$$

With these results, we can prove that the orthonormality of the families of many-particle functions $\{\Phi_c^{(S)}\}$ and $\{\Phi_c^{(A)}\}$ follows from the orthonormality of the single-particle orbitals $\{\phi_\nu(x)\}$. Explicitly, we must show that

$$\int \mathrm{d}^N x\, \Phi_b^* \Phi_c = \delta_{b,c}. \tag{1.7}$$

For $\Phi^{(A)}$, equation (1.7) with $b = c$ becomes

$$\begin{aligned}\int \Phi_c^* \Phi_c \mathrm{d}^N x &= \sqrt{N!} \int \mathrm{d}^N x \Phi_c^* \phi_{c_1}(x_1) \ldots \phi_{c_n}(x_N) \\ &= \sqrt{N!} \int \mathrm{d}^N x \frac{1}{\sqrt{N!}} \sum_P \mathrm{sgn}(P) \phi^*_{c_{P(1)}}(x_1) \ldots \phi^*_{c_{P(N)}}(x_N) \\ &\quad \times \phi_{c_1}(x_1) \ldots \phi_{c_N}(x_N) \\ &= \sum_P \mathrm{sgn}(P) \int \mathrm{d}x_1 \phi^*_{c_{P(1)}}(x_1) \phi_{c_1}(x_1) \int \mathrm{d}x_2 \ldots \\ &\quad \times \underbrace{\int \mathrm{d}x_n \, \phi^*_{c_{P(N)}}(x_N) \phi_{c_N}(x_N)}_{=\delta_{P(N),N}} \\ &= 1.\end{aligned}$$

Since we have assumed that the $\{\phi_i\}$ are orthogonal, the product of integrals will be non-zero only for the identity permutation

$$P(1) = 1, P(2) = 2, \ldots, P(N) = N$$

in which case the result is unity because sgn(Id)=1 and because the single-particle orbitals are normalized. If $b \neq c$, there exists at least one index b_j, which is not contained in c. It follows that at least one factor in the product of integrals shown above always vanishes – therefore the entire expression also vanishes. The proof is similar for symmetric functions $\Phi^{(S)}$. If, in this case, a particular single-particle state is multiply occupied, the sum over all permutations contains several non-vanishing terms whose contribution is reduced precisely by a factor $\prod_{k=1}^{K} n_k^{(c)}!$.

We conclude this chapter by proving the extremely important *completeness theorem*:

> **If the family $\{\phi_\nu(x)\}$ is complete, so too are the families $\{\Phi_c^{(A)}\}$ and $\{\Phi_c^{(S)}\}$ of many-particle functions in the corresponding Hilbert spaces of antisymmetric and symmetric many-particle functions, respectively.**

As an example, consider localized spinless particles. The theorem assures that if $\{\phi_\nu(\mathbf{r})\}$ is complete in $\mathcal{L}_2^{(A)}$, then $\{\Phi_c^{(A)}(\mathbf{r}_1, \ldots, \mathbf{r}_N)\}$ is complete in

$$\mathcal{L}_2^{(A)}(\underbrace{\mathcal{R}^3 \times \mathcal{R}^3 \times \ldots \times \mathcal{R}^3}_{N \text{ times}})$$

and $\{\Phi_c^{(S)}(\mathbf{r}_1, \ldots, \mathbf{r}_N)\}$ is complete in

$$\mathcal{L}_2^{(S)}(\underbrace{\mathcal{R}^3 \times \mathcal{R}^3 \times \ldots \times \mathcal{R}^3}_{N \text{ times}})$$

where $\mathcal{L}_2^{(S/A)}(\mathcal{R}^3 \times \ldots \times \mathcal{R}^3)$ denote the Hilbert spaces of symmetric/antisymmetric square-integrable functions on $\mathcal{R}^3 \times \ldots \times \mathcal{R}^3$ with $\mathcal{R}^3$ the three-dimensional Euclidean space.

To prove the theorem, we begin by showing that an arbitrary many-particle wavefunction can be expanded in products of single-particle functions. We fix the last $N-1$ coordinates at $x_i^{(0)}$, $i = 2, 3, \ldots, N$, and expand the wavefunction with respect to the first one:

$$\Psi(x_1, x_2^{(0)}, \ldots, x_N^{(0)}) = \sum_{\nu_1} a_{\nu_1} \phi_{\nu_1}(x_1).$$

The expansion coefficients are functions of the fixed coordinates:

$$a_{\nu_1} = a_{\nu_1}\left(x_2^{(0)}, x_3^{(0)}, \ldots, x_N^{(0)}\right)$$

so that

$$\Psi(x_1, x_2, \ldots, x_N) = \sum a_{\nu_1}(x_2, \ldots, x_N)\phi_{\nu_1}(x_1).$$

If we expand further with respect to the next coordinates

$$a_{\nu_1}(x_2, \ldots, x_N) = \sum_{\nu_2} a_{\nu_1,\nu_2}(x_3, \ldots, x_N)\phi_{\nu_2}(x_2)$$

and so on, we obtain

$$\begin{aligned} \Psi(x_1, x_2, \ldots, x_N) &= \sum_{\nu_1}\sum_{\nu_2} a_{\nu_1,\nu_2}\phi_{\nu_1}(x_1)\phi_{\nu_2}(x_2) \\ &= \sum_{\nu_1,\ldots,\nu_N} a_{\nu_1,\ldots,\nu_N}\phi_{\nu_1}(x_1)\ldots\phi_{\nu_N}(x_N). \end{aligned}$$

If the functions Ψ have definite symmetries $\hat{P}_{jk}\Psi = \pm\Psi$ with '+' for bosons, and minus for fermions, we can conclude that the expansion coefficients $a_{\nu_1,\nu_2,\ldots,\nu_N}$ have the same symmetry:

$$\begin{aligned} \sum_{\nu_1,\ldots,\nu_N} \pm a_{\nu_1,\ldots,\nu_j,\ldots,\nu_k,\ldots,\nu_N}\phi_{\nu_1}(x_1) \;\ldots\; & \phi_{\nu_j}(x_j)\ldots\phi_{\nu_k}(x_k)\ldots\phi_{\nu_N}(x_N) \\ &= \pm\Psi(x_1, \ldots, x_j, \ldots, x_k, \ldots, x_N) \\ &= \hat{P}_{jk}\Psi(x_1, \ldots, x_j, \ldots, x_k, \ldots, x_N) \\ &= \Psi(x_1, \ldots, x_k, \ldots, x_j, \ldots, x_N) \\ = \sum_{\nu_1,\ldots,\nu_N} a_{\nu_1,\ldots,\nu_j,\ldots,\nu_k,\ldots\nu_N}\phi_{\nu_1}(x_1) \;\ldots\; & \phi_{\nu_j}(x_k)\ldots\phi_{\nu_k}(x_j)\ldots\phi_{\nu_N}(x_N) \\ = \sum_{\nu_1,\ldots,\nu_N} a_{\nu_1,\ldots,\nu_k,\ldots,\nu_j,\ldots,\nu_N}\phi_{\nu_1}(x_1) \;\ldots\; & \phi_{\nu_k}(x_k)\ldots\phi_{\nu_j}(x_j)\ldots\phi_{\nu_N}(x_N). \end{aligned}$$

On the last line, the indices were simply renamed, $\nu_k \leftrightarrow \nu_j$. If we compare the last line with the first, it follows from the linear independence of the product functions that

$$\pm a_{\nu_1,\ldots,\nu_j,\ldots,\nu_k,\ldots,\nu_N} = a_{\nu_1,\ldots,\nu_k,\ldots\nu_j,\ldots,\nu_N} = P_{jk} a_{\nu_1,\ldots,\nu_j,\ldots,\nu_k,\ldots,\nu_N}.$$

Thus, it follows that the coefficients belonging to permuted index combinations

$$(\nu_1', \nu_2', \ldots, \nu_N') = P(\nu_1, \nu_2, \ldots, \nu_N)$$

differ at the most by a multiplicative sign, so that

$$a_{\nu_1',\ldots,\nu_N'} = \begin{pmatrix} + \\ \mathrm{sgn}(P) \end{pmatrix} a_{\nu_1,\ldots,\nu_N}$$

with '+' for bosons and sgn(P) for fermions. In the last step of the proof, we also replace the multiple sums over all indices in

$$\Psi(x_1, \ldots, x_N) = \sum_{\nu_1,\ldots,\nu_N} \phi_{\nu_1}(x_1) \ldots \phi_{\nu_N}(x_N) a_{\nu_1,\ldots,\nu_N}$$

by an (infinite) sum over all ordered combinations $c = (\nu_1, \ldots, \nu_N)$, connecting a (finite) sum over all permutations $P(\nu_1, \ldots, \nu_N)$ of these combinations, with the result

$$\begin{aligned} &\Psi(x_1, \ldots, x_N) \\ &= \sum_{c=(\nu_1,\ldots,\nu_N)} \sum_{P(c)=P(\nu_1,\ldots,\nu_N)} P\left[a_{\nu_1,\ldots,\nu_N} \phi_{\nu_1}(x_1) \ldots \phi_{\nu_N}(x_N)\right]. \end{aligned}$$

By using the above result

$$a_{P(\nu_1,\ldots,\nu_N)} = a_{P(c)} = \begin{pmatrix} + \\ \mathrm{sgn}(P) \end{pmatrix} a_c$$

it follows finally that

$$\begin{aligned} \Psi(x_1, \ldots, x_N) &= \sum_c a_c \sum_{P \in S_N} \begin{pmatrix} + \\ \mathrm{sgn}(P) \end{pmatrix} P\left[\phi_{\nu_1}(x_1) \ldots \phi_{\nu_2}(x_2)\right] \\ &\equiv \sum_c f_c \Phi_c^{(S/A)}(x_1, \ldots, x_N). \end{aligned}$$

We have shown then that we can expand arbitrary symmetric or antisymmetric functions in $\Phi_c^{(S)}$ and $\Phi_c^{(A)}$, respectively. The coefficients a_c differ from the coefficients f_c due to the normalization of the function $\Phi^{(S/A)}$.

Chapter 2

Second quantization for fermions

In this chapter, we will define annihilation and creation operators. These operators are mappings between the many-particle Hilbert spaces of different particle numbers:

$$\hat{c}_k \; : \; \mathcal{H}(N) \quad \rightarrow \mathcal{H}(N-1) \tag{2.1}$$

$$\hat{c}_k^\dagger \; : \; \mathcal{H}(N-1) \rightarrow \mathcal{H}(N) \qquad k \in \mathcal{N} \tag{2.2}$$

For example, for localized systems, we can think of $\mathcal{H}(N)$ as

$$L_2^{(A)}(\underbrace{\mathcal{R}^3 \times \mathcal{R}^3 \times \ldots \times \mathcal{R}^3}_{N \text{ times}})$$

the Hilbert space of square-integrable antisymmetric functions on $\mathcal{R}^3 \times \ldots \times \mathcal{R}^3$.

We proved in the previous chapter that the Slater determinants $\Phi_c(x_1, \ldots, x_N)$ form a basis in the N-fermion Hilbert space. We define the action of the annihilation operators $\hat{c}_k$ on this basis by

$$\hat{c}_k \Phi_{(c_1,\ldots,c_N)}(x_1, \ldots, x_N) \equiv 0, \text{ if } k \notin \{c_1, \ldots, c_N)$$

and if $k = c_j$, by

$$\hat{c}_k \Phi_{(c_1,\ldots,c_N)}(x_1, \ldots, x_N) \equiv (-1)^{j-1} \Phi_{(c_1,\ldots,c_{j-1},c_{j+1},\ldots,c_N)}(x_1, \ldots, x_{N-1})$$

$$= \frac{(-1)^{j-1}}{\sqrt{(N-1)!}} \sum_{P \in S_{N-1}} \operatorname{sgn}(P) P \left(\phi_{c_1}(x_1) \ldots \phi_{c_{j-1}}(x_{j-1}) \phi_{c_{j+1}}(x_{j+1}) \ldots \right). \tag{2.3}$$

The variables x_i are only written out for the sake of clarity — the $\hat{c}_k$ are operators on Hilbert spaces and act on abstract functions. The notation introduced here is commonly used and its meaning is clear even though the numbers of the arguments on either side of the equivalence differ.

Essentially what happens when $\hat{c}_k$ acts on a Slater determinant is that the orbital with index k is crossed out from the determinant. Pictorially speaking, the particle which occupied this orbital is 'annihilated'. From the fixed sign it is important to remember the the Slater determinant is only *unambiguously* determined by a given *ordered* N-tuple $c = (c_1, c_2, \ldots, c_N)$, with $c_1 < c_2 \ldots < c_N, \quad c_i \in \mathcal{N}$. The orbital ϕ_k, which is crossed out by the action of $\hat{c}_k$, thus has a 'fixed place' inside the Slater determinant. According to the definition given in equation (2), the orbital to be crossed out must first be moved to the top of the determinant, which gives rise to the sign $(-1)^{j-1}$. The meaning of this sign-convention will be made clear in the following example. If we assume that $k = c_j$, we can illustrate the action of $\hat{c}_k$ as follows:

$$\hat{c}_k \frac{1}{\sqrt{N}} \begin{vmatrix} \varphi_{c_1}(x_1) & \ldots & \varphi_{c_1}(x_N) \\ \vdots & & \vdots \\ \varphi_{c_j}(x_1) & \ldots & \varphi_{c_j}(x_N) \\ \vdots & & \vdots \\ \varphi_{c_N}(x_1) & \ldots & \varphi_{c_N}(x_N) \end{vmatrix} .$$

This corresponds to the following operations:

(1) interchange the row with $c_j = k$ with each row above it until it is at the top of the determinant, which gives a prefactor $(-1)^{j-1}$;

(2) cross out the first row and the last column of the determinant;

(3) normalize the new determinant.

Thus,

$$\hat{c}_k \frac{1}{\sqrt{N}} \begin{vmatrix} \varphi_{c_1}(x_1) & \ldots & \varphi_{c_1}(x_N) \\ \vdots & & \vdots \\ \varphi_{c_j}(x_1) & \ldots & \varphi_{c_j}(x_N) \\ \vdots & & \vdots \\ \varphi_{c_N}(x_1) & \ldots & \varphi_{c_N}(x_N) \end{vmatrix}$$

$$= \frac{(-1)^{j-1}}{\sqrt{(N-1)!}} \begin{vmatrix} \cancel{\varphi_{c_j}(x_1)} & \cancel{\cdots} & \cancel{\varphi_{c_j}(x_N)} \\ \varphi_{c_1}(x_1) & \cdots & \varphi_{c_1}(x_N) \\ \varphi_{c_2}(x_1) & \cdots & \varphi_{c_2}(x_N) \\ \vdots & & \vdots \\ \varphi_{c_{j-1}}(x_1) & \cdots & \varphi_{c_{j-1}}(x_N) \\ \varphi_{c_{j+1}}(x_1) & \cdots & \varphi_{c_{j+1}}(x_N) \\ \vdots & & \vdots \\ \varphi_{c_N}(x_1) & \cdots & \varphi_{c_N}(x_N) \end{vmatrix}$$

$$= \frac{(-1)^{j-1}}{\sqrt{(N-1)!}} \begin{vmatrix} \varphi_{c_1}(x_1) & \cdots & \varphi_{c_1}(x_{N-1}) \\ \vdots & & \vdots \\ \varphi_{c_{j-1}}(x_1) & \cdots & \varphi_{c_{j-1}}(x_{N-1}) \\ \varphi_{c_{j+1}}(x_1) & \cdots & \varphi_{c_{j+1}}(x_{N-1}) \\ \vdots & & \vdots \\ \varphi_{c_N}(x_1) & \cdots & \varphi_{c_N}(x_{N-1}) \end{vmatrix} .$$

The operators $\hat{c}_k$ are defined as *linear* operators on the Hilbert space $\mathcal{H}(N)$. The action of $\hat{c}_k$ on a general many-particle wavefunction Ψ is then completely determined by the expansion of Ψ in Slater determinants, $\Psi = \sum_c f_c \Phi_c$:

$$\hat{c}_k \Psi = \hat{c}_k \left(\sum_c f_c \Phi_c \right) \equiv \sum_c f_c \left(\hat{c}_k \Phi_c \right) .$$

We define the creation operator $\hat{c}_k^\dagger$ as the adjoint of $\hat{c}_k$. Hence, the action of $\hat{c}_k^\dagger$ on a Slater determinant follows from the definition of adjoint operators. If $\Phi_c \in \mathcal{H}(N-1)$ and $\Phi_b \in \mathcal{H}(N)$, we have

$$\begin{aligned} \langle \hat{c}_k^\dagger \Phi_c \mid \Phi_b \rangle &= \langle \Phi_c \mid \hat{c}_k \Phi_b \rangle \\ &= \begin{cases} (-1)^{j-1} \langle \Phi_c \mid \Phi_{b-\{k\}} \rangle & \text{if there is a } j \text{ with } k = b_j \\ 0 & \text{otherwise} \end{cases} \end{aligned}$$

and from equation (1.7), this is

$$\begin{aligned} & \begin{cases} (-1)^{j-1} \delta_{c,b-\{k\}} & \text{if there is a } j \text{ such that } k = b_j \\ 0 & \text{otherwise} \end{cases} \\ = & \sum_{i=1}^{N} (-1)^{i-1} \delta_{c_1 b_1} \delta_{c_2 b_2} \ldots \delta_{c_{i-1} b_{i-1}} \delta_{k b_i} \delta_{c_i b_{i+1}} \ldots \delta_{c_{N-1} b_N} \\ = & \begin{cases} (-1)^{j-1} \delta_{\tilde{c},b} & \text{if there is a } j \text{ such that } c_{j-1} < k < c_j \\ 0 & \text{otherwise} \end{cases} \end{aligned}$$

where $\tilde{c}$ denotes the N-tuple which is the result of inserting k between c_{j-1} and c_j in c. Furthermore, this is equal to

$$\begin{cases} (-1)^{j-1}\langle \Phi_{\tilde{c}} \mid \Phi_b\rangle & \text{if there is a } j \text{ for which } c_{j-1} < k < c_j \\ 0 & \text{otherwise.} \end{cases}$$

We have thus shown that

$$\hat{c}_k^{\dagger}\Phi_c = \begin{cases} (-1)^{j-1}\Phi_{\tilde{c}} & \text{if there is a } j \text{ with } c_{j-1} < k < c_j \\ 0 & \text{otherwise.} \end{cases}$$

This result clearly means (if $c_\ell < k < c_{\ell+1}$)

$$\hat{c}_k^{\dagger}\frac{1}{\sqrt{N!}}\begin{vmatrix} \varphi_{c_1}(x_1) & \dots & \varphi_{c_1}(x_N) \\ \vdots & & \vdots \\ \varphi_{c_N}(x_1) & \dots & \varphi_{c_N}(x_N) \end{vmatrix}$$

$$\equiv \frac{1}{\sqrt{(N+1)!}}\begin{vmatrix} \varphi_k(x_1) & \dots & \varphi_k(x_{N+1}) \\ \varphi_{c_1}(x_1) & \dots & \varphi_{c_1}(x_{N+1}) \\ \vdots & & \vdots \\ \varphi_{c_N}(x_1) & \dots & \varphi_{c_N}(x_{N+1}) \end{vmatrix}$$

$$= \frac{(-1)^\ell}{\sqrt{(N+1)!}}\begin{vmatrix} \varphi_{c_1}(x_1) & \dots & \varphi_{c_1}(x_{N+1}) \\ \vdots & & \vdots \\ \varphi_{c_\ell}(x_1) & \dots & \varphi_{c_\ell}(x_{N+1}) \\ \varphi_k(x_1) & \dots & \varphi_k(x_{N+1}) \\ \varphi_{c_{\ell+1}}(x_1) & \dots & \\ \vdots & & \vdots \\ \varphi_{c_N}(x_1) & \dots & \varphi_{c_N}(x_{N+1}) \end{vmatrix}$$

The action of $\hat{c}_k^{\dagger}$ thus 'creates' an additional particle in the state ϕ_k. As with $\hat{c}_k$, the action of $\hat{c}_k^{\dagger}$ on an arbitrary many-particle state $\Psi = \sum_c f_c\Phi_c$ is clear from the linearity of the adjoint operators:

$$\hat{c}_k^{\dagger}\Psi = \hat{c}_k^{\dagger}\left[\sum_c f_c\Phi_c\right] = \sum_c f_c\left(\hat{c}_k^{\dagger}\Phi_c\right).$$

According to equations (2.1) and (2.2) the creation and annihilation operators map Hilbert spaces of *fixed* particle numbers onto each other. However, the formalism of second quantization is especially suited for problems with variable particle numbers. Therefore, it is more appropriate to form the product Hilbert space $\mathcal{F} \equiv \bigotimes_{N=0}^{\infty} \mathcal{H}(N)$ from the Hilbert spaces $(\mathcal{H}(N), \langle \mid \rangle_N)$ of antisymmetric wavefunctions of N particles. We define the scalar product on $\mathcal{F}$ to be the natural scalar product

$$\langle \bigotimes_{N=0}^{\infty} \phi_N \mid \bigotimes_{N=0}^{\infty} \tilde{\phi}_N \rangle \equiv \sum_{N=0}^{\infty} \langle \phi_N \mid \tilde{\phi}_N \rangle_N .$$

We can then regard $\hat{c}_k$ and $\hat{c}_k^\dagger$ as operators on the space $\mathcal{F}$, the so-called *Fock-space*, instead of as collections of operators which map different Hilbert spaces $\mathcal{H}(N)$ onto one another.

In single-particle quantum mechanics the states are usually represented by the quantum numbers in the Dirac notation, *e.g.*, the state $\mid n\ell m\rangle$ with position representation $\langle \mathbf{r} \mid n\ell m\rangle = \phi_{n\ell m}$. We can characterize the Slater determinants in an analogous way by their associated N-tuples of indices: $\mid c\rangle$ with the position–spin representation $\langle x_1, \ldots, x_N \mid c\rangle = \Phi_c(x_1, \ldots, x_N)$.

Another equivalent possibility is the so-called *occupation-number representation*:

$$\mid c\rangle \equiv \mid n_1, n_2, n_3, \ldots\rangle$$

with $n_i = 0$ if $i \notin \{c_1, \ldots, c_N\}$

and $n_i = 1$ if $i \in \{c_1, \ldots, c_N\}$.

For example, suppose ϕ_1, ϕ_3 and ϕ_4 are occupied, so $c = (1, 3, 4)$. This gives

$$\mid 1, 3, 4\rangle = \mid 1_1, 0_2, 1_3, 1_4, 0_5, 0_6, \ldots\rangle .$$

We should keep in mind that the position-spin representation of such an abstract state vector is simply a normal Slater determinant, just as before. By using the occupation-number representation, however, we can write the the action of the creation and annihilation operators somewhat more compactly:

$$\begin{aligned} \hat{c}_k \mid n_1, \ldots, 1_k, \ldots\rangle &= (-1)^{\left[\sum_{j<k} n_j\right]} \mid n_1, \ldots, 0_k, \ldots\rangle \\ \hat{c}_k \mid n_1, \ldots, 0_k, \ldots\rangle &= 0 \end{aligned}$$

or, in summary

$$\hat{c}_k \mid n_1, \ldots, n_k, \ldots\rangle = \theta_k n_k \mid n_1, \ldots, 0_k, \ldots\rangle$$

with

$$\theta_k \equiv (-1)^{\left[\sum_{j<k} n_j\right]} .$$

Likewise, we have

$$\begin{aligned} \hat{c}_k^\dagger \mid n_1, \ldots, 0_k, \ldots\rangle &= \theta_k \mid n_1, \ldots, 1_k, \ldots\rangle \\ \hat{c}_k^\dagger \mid n_1, \ldots, 1_k, \ldots\rangle &= 0 \end{aligned}$$

and hence

$$\hat{c}_k^\dagger \mid n_1, \ldots, n_k, \ldots\rangle \;=\; \theta_k(1-n_k) \mid n_1, \ldots, 1_k, \ldots\rangle.$$

If we act with an annihilation operator $\hat{c}_k$ on a 'determinant' which only has the state ϕ_k occupied, a 'zero-row' determinant remains. In this determinant, there are no longer any occupied states. We define this state as the *vacuum.*

$$\hat{c}_k \mid 0_1, \ldots, 0_{k-1}, 1_k, 0_{k+1}, \ldots\rangle \equiv\mid \mathrm{vac}\rangle =\mid 0\,\rangle.$$

Obviously, we have

$$\hat{c}_k \mid 0\,\rangle = 0 \qquad \text{for all k in } \mathcal{N}.$$

By applying the creation operators to the vacuum state, we can generate every possible N-particle state. We obtain the basis functions through

$$\mid c_1, c_2, \ldots, c_N\rangle = \hat{c}_{c_1}^\dagger \hat{c}_{c_2}^\dagger \ldots \hat{c}_N^\dagger \mid 0\rangle = \prod_{k=1}^{\infty} \left(\hat{c}_k^\dagger\right)^{n_k} \mid 0\rangle.$$

This correspondence between $\hat{c}_{c_1}^\dagger \hat{c}_{c_2}^\dagger \ldots \hat{c}_{c_N}^\dagger \mid 0\rangle$ and the determinant containing the elements $\phi_{c_i}(x_j)$ contains minus signs, since the factor $(-1)^{j-1}$ was not included directly in the definition of the operators $\hat{c}_k$.

We now arrive at the most important property of the fermion creation and annihilation operators: their anticommutation relations

$$\begin{aligned} \{\hat{c}_\ell, \hat{c}_k\} &= 0 \\ \{\hat{c}_\ell^\dagger, \hat{c}_k^\dagger\} &= 0 \\ \{\hat{c}_\ell^\dagger, \hat{c}_k\} &= \delta_{\ell,k}. \end{aligned} \tag{2.4}$$

The proof of the anticommutation relations runs as follows:

$$\begin{aligned} \hat{c}_k\hat{c}_\ell \mid n_1, \ldots, n_k, \ldots, n_\ell, \ldots\rangle &= \theta_\ell n_\ell \hat{c}_k \mid n_1, \ldots, n_k, \ldots, 0_\ell, \ldots\rangle \\ &= \theta_\ell \theta_k n_\ell n_k \mid n_1, \ldots, 0_k, \ldots, 0_\ell, \ldots\rangle \\ \hat{c}_\ell\hat{c}_k \mid n_1, \ldots, n_k, \ldots, n_\ell, \ldots\rangle &= \theta_k n_k \hat{c}_\ell \mid n_1, \ldots, 0_k, \ldots, n_\ell, \ldots\rangle \\ &= \theta_k \tilde{\theta}_\ell n_k n_\ell \mid n_1, \ldots, 0_k, \ldots, 0_\ell, \ldots\rangle. \end{aligned}$$

The factor $\tilde{\theta}_\ell$ is just $-\theta_\ell$, unless we have $n_k = 0$, in which case the entire expression vanishes. Hence, we can write the last expression as

$$-\theta_k\theta_\ell n_k n_\ell \mid n_1, \ldots, 0_k, \ldots, 0_\ell, \rangle.$$

Thus, we have $(\hat{c}_k\hat{c}_\ell + \hat{c}_\ell\hat{c}_k) \mid n_1, \ldots, n_k, \ldots\rangle = 0$ for any arbitrary Slater determinant, and the first of the anticommutation relations above follows.

The proof of the remaining relations runs analogously. As an example, we will also show the proof of the last one for the case $\ell = k$:

$$\begin{aligned}
\hat{c}_k\hat{c}_k^\dagger \mid n_1,\ldots,n_k,\ldots\rangle &= \hat{c}_k\theta_k(1-n_k) \mid n_1,\ldots,1_k,\ldots\rangle \\
&= \theta_k\theta_k(1-n_k) \mid n_1,\ldots,0_k,\ldots\rangle \\
&= (1-n_k) \mid n_1,\ldots,0_k,\ldots\rangle. \\
\hat{c}_k^\dagger\hat{c}_k \mid n_1,\ldots,n_k,\ldots\rangle &= \hat{c}_k^\dagger\theta_k n_k \mid n_1,\ldots,0_k,\ldots\rangle \\
&= \theta_k\theta_k n_k(1-0) \mid n_1,\ldots,1_k,\ldots\rangle \\
&= n_k \mid n_1,\ldots,1_k,\ldots\rangle.
\end{aligned}$$

Thus,

$$\begin{aligned}
\left(\hat{c}_k^\dagger\hat{c}_k + \hat{c}_k\hat{c}_k^\dagger\right) \mid n_1,\ldots,n_k,\ldots\rangle &= \begin{cases} \mid n_1,\ldots,1_k,\ldots\rangle & \text{if } n_k = 1 \\ \mid n_1,\ldots,0_k,\ldots\rangle & \text{if } n_k = 0 \end{cases} \\
&= \mid n_1,\ldots,n_k,\ldots\rangle
\end{aligned}$$

i.e.

$$\{\hat{c}_k^\dagger, \hat{c}_k\} = 1.$$

Because of the property $\hat{c}_k^\dagger\hat{c}_k \mid n_1,n_2,\ldots\rangle = n_k \mid n_1,n_2,\ldots\rangle$, we can introduce the *number operator* $\hat{N}$ through

$$\hat{N} \equiv \sum_{k=1}^{\infty} \hat{c}_k^\dagger\hat{c}_k. \tag{2.5}$$

From this definition, it follows that

$$\hat{N} \mid n_1,n_2,\ldots\rangle = \left(\sum_{k=1}^{\infty} n_k\right) \mid n_1,n_2,\ldots\rangle = N \mid n_1,n_2,\ldots\rangle$$

for Slater determinants.

If we expand an arbitrary many-particle state in Slater determinants (or completely symmetrized functions in the case of bosons), we obtain:

$$\mid \Psi\rangle = \sum_c f_c \mid \Phi_c\rangle \Rightarrow \hat{c}_\ell^\dagger\hat{c}_\ell \mid \Psi\rangle = \sum_c f_c\hat{c}_\ell^\dagger\hat{c}_\ell \mid \Phi_c\rangle = \sum_c f_c n_\ell^{(c)} \mid \Phi_c\rangle.$$

Thus, the expectation value of the number of particles in the single-particle state ℓ in the state $\mid \Psi\rangle$ is

$$\langle n_\ell\rangle \equiv \langle \Psi \mid \hat{c}_\ell^\dagger\hat{c}_\ell \mid \Psi\rangle = \sum_c\sum_{c'} f_{c'} f_c n_\ell^{(c)} \langle \Phi_{c'} \mid \Phi_c\rangle = \sum_c \mid f_c \mid^2 n_\ell^{(c)}.$$

Since $\sum_c |f_c|^2 = 1$, it follows that

$$0 \leq \langle n_\ell\rangle \leq 1$$

for fermions ($n_\ell^{(c)} = 0$ or 1).

In the remainder of this chapter, we will express 'normal' operators (*i.e.*, the operators that we are familiar with from first quantization) in terms of the creation and annihilation operators. The result is known as the *second quantization representation* of the operators. We will show that we have:

(1) for single-particle operators

$$\hat{H}_0 = \sum_{i=1}^{N} \hat{h}(x_i) = \sum_{i,j=1}^{\infty} \langle i \mid \hat{h} \mid j\rangle \hat{c}_i^\dagger \hat{c}_j \tag{2.6}$$

with $\langle i|\hat{h}|j\rangle = \int \phi_i^*(x)\hat{h}(x)\phi_j(x)\mathrm{d}x$; and

(2) for local two-particle operators

$$\hat{V} = \frac{1}{2}\sum_{\substack{i,j=1\\ i\neq j}}^{N} \hat{v}(x_i, x_j) = \frac{1}{2}\sum_{ijk\ell=1}^{\infty} \langle ij \mid \hat{v} \mid k\ell\rangle \hat{c}_i^\dagger \hat{c}_j^\dagger \hat{c}_\ell \hat{c}_k \tag{2.7}$$

with $\langle ij|\hat{v}|k\ell\rangle = \int\int \phi_i^*(x)\phi_j^*(x')v(x,x')\phi_k(x)\phi_\ell(x')\,\mathrm{d}x\,\mathrm{d}x'$.

The action of the operators in second quantization defined by equations (2.6) and (2.7) is defined only on Slater determinants. Hence, to determine the action on an arbitrary many-fermion wavefunction, that wavefunction must first be expanded in Slater determinants. In contrast, the operators in first quantization act directly on the coordinates of the many-particle wavefunction. It is important to emphasize that equations (2.6) and (2.7) imply that the operators in first and second quantization are equal, *i.e.*, their actions on an arbitrary many-fermion wavefunction lead to the same result.

To prove this identity, we must show that the actions of the operators are identical on the complete set of Slater determinants; *i.e.*

$$\sum_{i=1}^{N} \hat{h}(x_i) \mid \Phi_c\rangle = \sum_{i,j=1}^{\infty} \langle i \mid \hat{h} \mid j\rangle \hat{c}_i^\dagger \hat{c}_j \mid \Phi_c\rangle \text{ for all } \Phi_c$$

and

$$\frac{1}{2}\sum_{\substack{i\neq j\\ i,j=1}}^{N} \hat{v}(x_i, x_j) \mid \Phi_c\rangle = \frac{1}{2}\sum_{ijk\ell=1}^{\infty} \langle ij \mid \hat{v} \mid k\ell\rangle \hat{c}_i^\dagger \hat{c}_j^\dagger \hat{c}_\ell \hat{c}_k \mid \Phi_c\rangle \text{ for all } \Phi_c.$$

To prove these identities, we once again expand the states on the left and on the right in the complete set $\{\Phi_b\}$ and show that the expansion coefficients are identical, *i.e.*, that the matrix elements satisfy

$$\sum_{i=1}^{N} \langle \Phi_b \mid \hat{h}(x_i) \mid \Phi_c \rangle = \sum_{i,j=1}^{\infty} \langle i \mid \hat{h} \mid j \rangle \langle \Phi_b \mid \hat{c}_i^\dagger \hat{c}_j \mid \Phi_c \rangle$$

for all Φ_c and Φ_b; and that

$$\sum_{\substack{i,j=1 \\ i \neq j}}^{N} \langle \Phi_b \mid \hat{v}(x_i, x_j) \mid \Phi_c \rangle = \sum_{ijk\ell=1}^{\infty} \langle ij \mid \hat{v} \mid k\ell \rangle \langle \Phi_b \mid \hat{c}_i^\dagger \hat{c}_j^\dagger \hat{c}_\ell \hat{c}_k \mid \Phi_c \rangle$$

for all Φ_b and Φ_c. We begin with the single-particle operator in the first quantization. From equation (1.6) we have

$$\begin{aligned}
&\sum_{i=1}^{N} \langle \Phi_b \mid \hat{h}(x_i) \mid \Phi_c \rangle \\
&\quad = \sum_{i=1}^{N} \sqrt{N!} \int \mathrm{d}^N x \, \Phi_b^*(x_1, \ldots, x_N) \hat{h}(x_i) \phi_{c_1}(x_1), \ldots, \phi_{c_N}(x_N) \\
&\quad = \sum_{i=1}^{N} \sum_{P \in S_N} \operatorname{sgn}(P) \left(\int \phi_{b_{P(1)}}^*(x_1) \phi_{c_1}(x_1) \mathrm{d}x_1 \right) \ldots \\
&\quad\quad \times \ldots \left(\int \phi_{b_{P(i)}}^*(x_i) \hat{h}(x_i) \phi_{c_i}(x_i) \mathrm{d}x_i \right) \ldots \left(\int \ldots \mathrm{d}x_N \right) .
\end{aligned}$$

The $(N-1)$-fold product of integrals in which $\hat{h}(x_i)$ does not appear, contains at least one factor in which the indices of the single-particle orbitals are interchanged. As a result, this factor vanishes. It follows that the matrix element vanishes if two or more indices in the N-tuples b and c are interchanged. Thus, there are only two cases to consider:

(1) $b = c$

$$\begin{aligned}
\langle \Phi_c \mid \hat{H}_0 \mid \Phi_c \rangle &= \sum_{i=1}^{N} \sum_{P \in S_N} \operatorname{sgn}(P) \left(\int \phi_{c_{P(1)}}^*(x_1) \phi_{c_1}(x_1) \mathrm{d}x_1 \right) \ldots \\
&\quad \times \left(\int \phi_{c_{P(i)}}^*(x_i) \hat{h}(x_i) \phi_{c_i}(x_i) \mathrm{d}x_i \right) \ldots
\end{aligned}$$

The $(N-1)$-fold product of integrals which do not contain $\hat{h}(x_i)$ vanishes unless

$$c_{P(1)} = c_1 \ , \ c_{P(2)} = c_2 \ , \ldots , \ c_{P(i-1)} = c_{i-1} \ , \ c_{P(i+1)} = c_{i+1} \ , \ldots .$$

Hence, we must also have $c_{P(i)} = c_i$, so that we obtain a non-zero expression only for the identical permutations:

$$\langle \Phi_c \mid \hat{H}_0 \mid \Phi_c \rangle = \sum_{i=1}^{N} \int \phi^*_{c_i}(x_i)\hat{h}(x_i)\, \mathrm{d}x_i = \sum_{i=1}^{N} \langle c_i \mid \hat{h} \mid c_i \rangle . \tag{2.8}$$

(2) b and c differ in *one* index; *e.g.*, $b_k \notin c$ and $c_\ell \notin b$, or in detail

$$\begin{array}{rcl}
b_1 & = & c_1 \\
\vdots & = & \vdots \\
b_{k-1} & = & c_{k-1} \\
b_k & & \\
b_{k+1} & = & c_k \\
\vdots & = & \vdots \\
b_\ell & = & c_{\ell-1} \\
 & & c_\ell \\
b_{\ell+1} & = & c_{\ell+1} \\
\vdots & & \vdots \\
b_N & = & c_N .
\end{array}$$

In this case we can only obtain a non-zero value when the integral with $\hat{h}(x_i)$ contains the two different orbitals ϕ_{c_ℓ} and ϕ_{b_k}. Thus, the sum over i only gives one contribution for the case $i = \ell$, whereas the sum over all permutations gives a non-zero contribution only for one particular permutation P_0. This permutation is given by

$$\begin{array}{rccc}
P_0(1) = 1 & \ldots & & P_0(k-1) = k-1 \\
P_0(k) = k+1 & \ldots & & P_0(\ell-1) = \ell \\
P_0(\ell) = k & P_0(\ell+1) = \ell+1 & \ldots & \\
\ldots & P_0(N-1) = N-1 & P_0(N) = N. &
\end{array}$$

In this case we obtain

$$\langle \Phi_b \mid \hat{H}_0 \mid \Phi_c \rangle = \mathrm{sgn}(P_0) \langle b_k \mid \hat{h} \mid c_\ell \rangle .$$

We must now show that the second-quantization representation of $\hat{H}_0$ leads to the same matrix elements:

$$\sum_{i,j=1}^{\infty} \langle i \mid \hat{h} \mid j \rangle \langle \Phi_b \mid \hat{c}_i^\dagger \hat{c}_j \mid \Phi_c \rangle = \sum_{i,j=1}^{\infty} \langle i \mid \hat{h} \mid j \rangle \langle \hat{c}_i \Phi_b \mid \hat{c}_j \Phi_c \rangle .$$

If there are some $i = b_r$ and $j = c_s$, we have

$$\langle \hat{c}_i \Phi_b \mid \hat{c}_j \Phi_c \rangle = \pm \langle b_i \ldots \not{b}_r \ldots b_N \mid c_1 \ldots \not{c}_s \ldots c_N \rangle$$

where $\not{b}_r$ and $\not{c}_s$ indicate that the states b_r and c_s have been annihilated. The matrix element apparently vanishes if b and c differ in more than one index. We must then further consider the following two cases:

(1) $b = c$

$$\langle \hat{c}_i \Phi_c \mid \hat{c}_j \Phi_c \rangle = \begin{cases} 0 & \text{for } i \neq j \\ \langle \Phi_c \mid \hat{c}_i^\dagger \hat{c}_j \mid \Phi_c \rangle = n_i \langle \Phi_c \mid \Phi_c \rangle = n_i & \text{for } i = j. \end{cases}$$

Thus

$$\langle \Phi_c \mid \hat{H}_0 \mid \Phi_c \rangle = \sum_{i=1}^{\infty} n_i \langle i \mid \hat{h} \mid i \rangle = \sum_{i=1}^{N} \langle c_i \mid \hat{h} \mid c_i \rangle.$$

(2) $b_k \notin c$ and $c_\ell \notin b$. In this case, we have

$$\langle \hat{c}_i \Phi_b \mid \hat{c}_j \Phi_c \rangle = \begin{cases} \pm 1 & \text{if } i = b_k \text{ and } j = c_\ell \\ 0 & \text{otherwise} \end{cases}$$

where the respective signs correspond to the $\mathrm{sgn}(P_0)$ above, so that we obtain

$$\langle \Phi_b \mid \hat{H}_0 \mid \Phi_c \rangle = \mathrm{sgn}(P_0) \langle b_k \mid \hat{h} \mid c_\ell \rangle.$$

Thus, the statement is proven for single-particle operators.

The calculations become rather lengthy for two-particle operators (particularly in first quantization). In summary, one obtains

(1) $b = c$:

$$\langle \Phi_c \mid \hat{V} \mid \Phi_c \rangle = \frac{1}{2} \sum_{i,j=1}^{N} \left(\langle c_i c_j \mid \hat{v} \mid c_i c_j \rangle - \langle c_i c_j \mid \hat{v} \mid c_j c_i \rangle \right) \qquad (2.9)$$

(2) $b_k \neq c_k$ for one k, but $b_s = c_s$ for $s \neq k$:

$$\langle \Phi_b \mid \hat{V} \mid \Phi_c \rangle = \sum_{i=1}^{N} \left(\langle c_i b_k \mid \hat{v} \mid c_i c_k \rangle - \langle b_k c_i \mid \hat{v} \mid c_i c_k \rangle \right)$$

(3) $b_k \neq c_k$ and $b_\ell \neq c_\ell$ for one k and one ℓ, but $b_s = c_s$ for $s \neq k, \ell$:

$$\langle \Phi_b \mid \hat{V} \mid \Phi_c \rangle = \left(\langle b_k b_\ell \mid \hat{v} \mid c_k c_\ell \rangle - \langle b_\ell b_k \mid \hat{v} \mid c_k c_\ell \rangle \right).$$

(4) If the Slater determinants Φ_b and Φ_c differ in three or more indices, the matrix elements vanish;

$$\langle \Phi_b \mid \hat{V} \mid \Phi_c \rangle = 0.$$

It should be noted from the cases (2) and (3) that, at most, the overall sign changes if the different orbitals are not in the same rows of the determinants.

The proof that the matrix elements of the two-particle operators are identical in first and second quantization will not be pursued any further. The calculations are similar to the case of single-particle operators. As an example, we will show equation (2.9) above for second quantization, since we will use this equation later:

$$\langle \Phi_c \mid \hat{V} \mid \Phi_c \rangle = \frac{1}{2} \sum_{ijk\ell=1}^{\infty} \langle ij \mid \hat{v} \mid k\ell \rangle \langle \Phi_c \mid \hat{c}_i^\dagger \hat{c}_j^\dagger \hat{c}_\ell \hat{c}_k \mid \Phi_c \rangle.$$

The second matrix element is only non-zero when we have

$$\hat{c}_i^\dagger \hat{c}_j^\dagger \hat{c}_\ell \hat{c}_k \mid \Phi_c \rangle = \pm \mid \Phi_c \rangle.$$

From this it follows that we must have either

(1) $k = j$ and $\ell = i$, or

(2) $k = i$ and $\ell = j$.

In these cases we obtain with the help of the anticommutation relation equation (2.4):

(1)

$$\begin{aligned} \hat{c}_i^\dagger \hat{c}_j^\dagger \hat{c}_\ell \hat{c}_k \mid \Phi_c \rangle &= \hat{c}_i^\dagger \hat{c}_j^\dagger \hat{c}_i \hat{c}_j \mid \Phi_c \rangle \\ &= \delta_{ij} \cdot \hat{c}_i^\dagger \hat{c}_i \mid \Phi_c \rangle - \hat{c}_i^\dagger \hat{c}_i \hat{c}_j^\dagger \hat{c}_j \mid \Phi_c \rangle \\ &= \delta_{ij} n_i \mid \Phi_c \rangle - n_i n_j \mid \Phi_c \rangle \end{aligned}$$

(2)

$$\begin{aligned} \hat{c}_i^\dagger \hat{c}_j^\dagger \hat{c}_\ell \hat{c}_k \mid \Phi_c \rangle &= \hat{c}_i^\dagger \hat{c}_j^\dagger \hat{c}_j \hat{c}_i \mid \Phi_c \rangle = -\hat{c}_i^\dagger \hat{c}_j^\dagger \hat{c}_i \hat{c}_j \mid \Phi_c \rangle \\ &= -\delta_{ij} \hat{c}_i^\dagger \hat{c}_i \mid \Phi_c \rangle + \hat{c}_i^\dagger \hat{c}_i \hat{c}_j^\dagger \hat{c}_j \mid \Phi_c \rangle \\ &= -\delta_{ij} n_i \mid \Phi_c \rangle + n_i n_j \mid \Phi_c \rangle \end{aligned}$$

so, combining the two cases we obtain

$$\begin{aligned}\langle \Phi_c \mid \hat{v} \mid \Phi_c \rangle &= \frac{1}{2} \sum_{i,j=1}^{\infty} n_i n_j \left(\langle ij \mid \hat{v} \mid ij \rangle - \langle ij \mid \hat{v} \mid ji \rangle \right) \\ &= \frac{1}{2} \sum_{i,j=1}^{N} \left(\langle c_i c_j \mid \hat{v} \mid c_i c_j \rangle - \langle c_i c_j \mid \hat{v} \mid c_j c_i \rangle \right) .\end{aligned}$$

Thus, we have seen that the so-called second quantization, within the present framework, is no more than an alternative formulation of quantum mechanics, and that this formulation is completely equivalent to the usual one. However, the second quantization provides a tool that permits a description of processes such as creation and annihilation of particles. Such processes cannot be discussed from the basis of the Schrödinger equation, but only from within the framework of quantum field theory.

Chapter 3

Second quantization for bosons

Second quantization for bosons is analogous to second quantization for fermions: the action of the creation and annihilation operators is defined on the complete system of symmetrized functions

$$\Phi_c(x_1,\ldots,x_N)=\frac{1}{\sqrt{N!}}\frac{1}{\sqrt{\prod_{k=1}^{\infty}n_k^{(c)}!}}\sum_{P\in S_N}P\left[\varphi_{c_1}(x_1)\ldots\varphi_{c_N}(x_N)\right]. \quad (3.1)$$

Again, we represent these states by the occupation numbers n_i in the Dirac notation. The occupation numbers declare that the single-particle state i appears n_i times in $(c_1,\ldots,c_N)$:

$$\mid c\rangle=\mid c_1,\ldots,c_N\rangle\equiv\mid n_1,n_2,n_3,\ldots\rangle$$

with the position–spin representation

$$\langle x_1,\ldots,x_N\mid n_1\ldots\rangle=\Phi_c(x_1,\ldots,x_N).$$

In contrast to the case of the fermion wavefunctions, the occupation numbers are not restricted to only the values 0 and 1.

We then remind ourselves once more of the definition of the fermion creation and annihilation operators:

$$\hat{c}_k\mid\ldots,n_k\ldots\rangle\equiv\theta_k n_k\mid\ldots,(n_k-1),\ldots\rangle$$

$$\hat{c}_k^{\dagger}\mid\ldots,n_k,\ldots\rangle=\begin{cases}\theta_k(n_k+1)\mid\ldots,(n_k+1),\ldots\rangle & \text{if } n_k=0\\ 0 & \text{if } n_k=1.\end{cases}$$

If we remove the prefactor θ_k and the restrictions that the occupation numbers are less than or equal to unity from these definitions, we obtain almost immediately the definitions of the boson operators. Explicitly

$$\begin{aligned}\hat{b}_k\mid\ldots,n_k,\ldots\rangle &\equiv \sqrt{n_k}\mid\ldots,(n_k-1),\ldots\rangle\\ \hat{b}_k^{\dagger}\mid\ldots,n_k,\ldots\rangle &\equiv \sqrt{n_k+1}\mid\ldots,(n_k+1),\ldots\rangle.\end{aligned}$$

The square roots in these definitions (which are the only additions we had to make to the action of the fermion operators $\hat{c}_k$ and $\hat{c}_k^\dagger$) are chosen so that we can introduce the number operator just as in the case of the fermions

$$\hat{N} \equiv \sum_{k=1}^{\infty} \hat{b}_k^\dagger \hat{b}_k$$

since we then have

$$\hat{b}_k^\dagger \hat{b}_k \mid \ldots, n_k, \ldots \rangle = \sqrt{n_k}\, \hat{b}_k^\dagger \mid \ldots, (n_k - 1), \ldots \rangle = n_k \mid \ldots, n_k, \ldots \rangle.$$

By applying the creation operators on the vacuum, we can generate all the basis functions of the type in equation (3.1):

$$\mid n_1, n_2, n_3, \ldots \rangle = \prod_{k=1}^{\infty} \frac{\left(\hat{b}_k^\dagger\right)^{n_k}}{\sqrt{n_k!}} \mid 0 \rangle.$$

Furthermore, $\hat{b}_k$ and $\hat{b}_k^\dagger$ are the adjoints of one another, and the following commutation relations hold:

$$\begin{aligned} \left[\hat{b}_\ell, \hat{b}_k\right] &= 0 \\ \left[\hat{b}_\ell^\dagger, \hat{b}_k^\dagger\right] &= 0 \\ \left[\hat{b}_\ell, \hat{b}_k^\dagger\right] &= \delta_{\ell,k}. \end{aligned} \tag{3.2}$$

The representations of single-particle and two-particle operators for bosons are identical to the representations of the fermion operators:

$$\hat{H}_0 = \sum_{i=1}^{N} \hat{h}(x_i) = \sum_{i,j=1}^{\infty} \langle i \mid \hat{h} \mid j \rangle \hat{b}_i^\dagger \hat{b}_j \tag{3.3}$$

and

$$\hat{V} = \xcancel{\frac{1}{2} \sum_{\substack{i,j=1 \\ i \neq j}}^{N}} \hat{v}(x_i, x_j) = \frac{1}{2} \sum_{ijk\ell=1}^{\infty} \langle ij \mid \hat{v} \mid k\ell \rangle \hat{b}_i^\dagger \hat{b}_j^\dagger \hat{b}_\ell \hat{b}_k. \tag{3.4}$$

Chapter 4

Unitary transformations and field operators

The considerations up to this point have been based on a a *fixed* orthonormal basis of single-particle functions $\{\varphi_k(x)\}$. We will now discuss what happens when we transform to another orthonormal basis $\{\chi_k(x)\}$.

We begin by expanding the old orthonormal basis in terms of the new one:

$$\varphi_k(x) = \sum_j D_{kj}\chi_j(x). \tag{4.1}$$

We are dealing with an orthonormal basis; hence, the transformation D must be unitary:

$$D^\dagger D = 1 = D\,D^\dagger$$

The inverse transformations are

$$\chi_k(x) = \sum_j \left(D^\dagger\right)_{kj} \varphi_j(x) = \sum_j D^*_{jk}\,\varphi_j(x). \tag{4.2}$$

The wavefunction $\varphi_k(x)$ is the x-representation of the abstract Hilbert space vector $\hat{c}_k^\dagger \mid 0\,\rangle$, so

$$\begin{aligned}\langle\, x \mid \hat{c}_k^\dagger \mid 0\,\rangle &= \varphi_k(x) = \sum_j D_{kj}\,\chi_j(x) \\ &\equiv \sum_j D_{kj}\langle\, x \mid a_j^\dagger \mid 0\,\rangle = \langle\, x \mid \sum_j D_{kj} a_j^\dagger \mid 0\,\rangle.\end{aligned}$$

Thus, if we interpret the new basis functions $\chi_j(x)$ as the x-representation of the Hilbert space vector $\hat{a}_j^\dagger \mid 0\,\rangle$, *i.e.*, the operators $\hat{a}_j^\dagger$ act relative to the basis $\{\chi_j(x)\}$ in the same way as the operators $\hat{c}_k^\dagger$ act relative to the basis $\{\varphi_k(x)\}$, the new creation operators must satisfy

$$\hat{c}_k^\dagger = \sum_j D_{jk} \hat{a}_j^\dagger. \tag{4.3}$$

The corresponding inverse relations are

$$\hat{a}_k^\dagger = \sum_j D_{jk}^* \hat{c}_j^\dagger. \tag{4.4}$$

The transformation to a new single-particle basis thus corresponds to a unitary transformation of the creation operators. Such unitary transformations will play an extremely important role in later chapters.

If we define the annihilation operators corresponding to $\hat{a}_j^\dagger$ as the adjoint operator of $\hat{a}_j^\dagger$

$$\hat{a}_j \equiv \left(\hat{a}_j^\dagger\right)^\dagger$$

we can immediately derive a relation between these and the annihilation operators $\hat{c}_k$:

$$\begin{aligned}
\langle \Psi \mid \hat{c}_k \mid \Phi \rangle &= \langle \Phi \mid \hat{c}_k^\dagger \mid \Psi \rangle^* = \langle \Phi \mid \sum_j D_{kj} \hat{a}_j^\dagger \mid \Psi \rangle^* = \langle \sum_j D_{kj} \hat{a}_j^\dagger \Psi \mid \Phi \rangle \\
&= \sum_j D_{kj}^* \langle \hat{a}_j^\dagger \Psi \mid \Phi \rangle = \sum_j D_{kj}^* \langle \Psi \mid \hat{a}_j \mid \Phi \rangle \\
&= \langle \Psi \mid \sum_j D_{kj}^* \hat{a}_j \mid \Phi \rangle.
\end{aligned}$$

Hence

$$\hat{c}_k = \sum_j D_{kj}^* \hat{a}_j. \tag{4.5}$$

The inverse transformation of equation (4.5) is

$$\sum_k D_{ki} \hat{c}_k = \sum_j \underbrace{\sum_k D_{ki}\, D_{kj}^*}_{=\delta_{ij}} \hat{a}_j = \hat{a}_i. \tag{4.6}$$

From equation (4.6) we see that the transformation between the annihilation operators $\hat{c}_k$ and $\hat{c}_k$ is unitary; it is the transpose of the transformation of creation operators. The fact that the new creation and annihilation operators obtained by a unitary transformation satisfy the same commutation relations as the original operators is of crucial importance. For example, it follows from

$$\left[\hat{c}_\ell, \hat{c}_k^\dagger\right] = \delta_{\ell,k}$$

that we also have

$$\left[\hat{a}_\ell, \hat{a}_k^\dagger\right] = \sum_i \sum_j D_{i\ell} D_{jk}^* \underbrace{\left[\hat{c}_i, \hat{c}_j^\dagger\right]}_{=\delta_{ij}} = \sum_j D_{j\ell} D_{jk}^* = \delta_{\ell,k}.$$

Furthermore, the representations of operators in terms of these sets of creation and annihilation operators are formally identical; for example

$$\begin{aligned}
\hat{H}_0 &= \sum_i \sum_j \langle i \mid \hat{h} \mid j\rangle \hat{c}_i^\dagger \hat{c}_j \\
&= \sum_i \sum_j \langle i \mid \hat{h} \mid j\rangle \sum_k D_{ik} \hat{a}_k^\dagger \sum_\ell D_{j\ell}^* \hat{a}_\ell \\
&= \sum_k \sum_\ell \underbrace{\sum_i D_{ik} \langle i \mid}_{=\langle k|} \hat{h} \quad \underbrace{\sum_j D_{j\ell}^* \mid j\rangle}_{=|\ell\rangle \text{ by equation (4.2)}} \quad \hat{a}_k^\dagger \hat{a}_\ell \\
&= \sum_k \sum_\ell \langle k \mid \hat{h} \mid \ell\rangle \hat{a}_k^\dagger \hat{a}_\ell.
\end{aligned}$$

We will now consider a particular example of such a basis transformation: as our new basis we choose the eigenfunctions of the x-operators in the x-representation [remember that $x = (\mathbf{r}, s) =$ (position, spin)], which are δ-functions:

$$\chi_k(y) \ \text{corresponds to} \ \delta(x-y).$$

The index k thus corresponds to the continuous variable x. The functions $\delta(x-y)$ form a system of single-particle orbitals, which describe particles that are localized at the position–spin-point x. This means that the probability of finding the particle at any other point $y \neq x$ vanishes. Since the system of δ-functions forms a basis, we can expand any possible single-particle function in δ-functions:

$$f(y) = \int f(x)\delta(x-y)\,\mathrm{d}x.$$

Moreover, the δ-functions are orthogonal:

$$\int \delta(x-y)\delta(z-y)\,\mathrm{d}y = \delta(x-z).$$

However, the δ-functions cannot normalized in the usual sense but this will not cause any problems in the present context.

The transformation of basis introduced earlier

$$\varphi_j(y) = \sum_k D_{jk}\chi_k(y)$$

then becomes

$$\varphi_j(y) = \int \mathrm{d}x\, \varphi_j(x)\delta(x-y).$$

Again, the variable x takes on the role of the index k.

The corresponding transformation to the new creation operators

$$\hat{a}_k^\dagger = \sum_j D_{jk}^* \hat{c}_j^\dagger$$

becomes

$$\hat{\psi}^\dagger(x) = \sum_j \varphi_j^*(x)\hat{c}_j^\dagger \tag{4.7}$$

and for the new annihilation operators we obtain

$$\hat{\psi}(x) = \sum_j \varphi_j(x)\hat{c}_j. \tag{4.8}$$

The operators $\hat{\psi}^\dagger(x)$ and $\hat{\psi}(x)$ are traditionally called *field operators.* It is an important fact that these operators satisfy the same commutation relations as the original operators $\hat{c}_i^\dagger$, $\hat{c}_i$ and $\hat{b}_i^\dagger$, $\hat{b}_i$, respectively, *i.e.,* for fermions

$$\begin{aligned}
\{\hat{\psi}(x), \hat{\psi}(x')\} &= 0 \\
\{\hat{\psi}^\dagger(x), \hat{\psi}^\dagger(x')\} &= 0 \\
\{\hat{\psi}(x), \hat{\psi}^\dagger(x')\} &= \delta(x-x')
\end{aligned} \tag{4.9}$$

and for bosons

$$\begin{aligned}
\left[\hat{\psi}(x), \hat{\psi}(x')\right] &= 0 \\
\left[\hat{\psi}^\dagger(x), \hat{\psi}^\dagger(x')\right] &= 0 \\
\left[\hat{\psi}(x), \hat{\psi}^\dagger(x')\right] &= \delta(x-x').
\end{aligned} \tag{4.10}$$

The representation of single-particle and two-particle operators by the field operators proceeds according to equations for fermions (2.6) and (2.7), and equations (3.3) and (3.4) for bosons, respectively:

$$\hat{H}_0 = \int \mathrm{d}x\, \hat{\psi}^\dagger(x)h(x)\hat{\psi}(x) \tag{4.11}$$

$$\hat{V} = \frac{1}{2}\int\int \mathrm{d}x\,\mathrm{d}x'\, \hat{\psi}^\dagger(x)\hat{\psi}^\dagger(x')v(x,x')\hat{\psi}(x')\hat{\psi}(x). \tag{4.12}$$

We end this chapter by discussing a pictorial interpretation of the field operators. The operator $\hat{c}_i^\dagger$ creates a particle in the state φ_i, which is characterized by the quantum number i. Similarly, the operator $\hat{\psi}^\dagger(x)$ creates a particle which is localized at the point x. Thus, for the formalism to be consistent, the position–spin representation of the state $\hat{\psi}^\dagger \mid 0\rangle$ must be a δ-function centered at x. We give a brief verification that this is the case:

$$\hat{\psi}^\dagger(x) \mid 0\rangle = \sum_i \varphi_i^*(x)\hat{c}_i^\dagger \mid 0\rangle = \sum_i \varphi_i^*(x) \mid 0_1, \ldots, 1_i, 0_{i+1}, \ldots\rangle$$

which yields

$$\begin{aligned}\langle y \mid \hat{\psi}^\dagger \mid 0\rangle &= \sum_i \varphi_i^*(x)\langle y \mid 0_1, \ldots, 1_i, 0_{i+1}, \ldots\rangle \\ &= \sum_i \varphi_i^*(x)\varphi_i(y) = \delta(x-y).\end{aligned}$$

Chapter 5

Example: the Hamiltonian of translationally invariant systems in second quantization

The Hamiltonian of an interacting many-particle system is in first quantization

$$\begin{aligned} \hat{H} &= \hat{T} + \hat{U} + \hat{V} \\ &= \sum_{i=1}^{N} \frac{\hat{p}_i^2}{2m} + \sum_{i=1}^{N} u(\mathbf{r}_i) + \frac{1}{2} \sum_{\substack{i,j=1 \\ i \neq j}}^{N} v(\mathbf{r}_i, \mathbf{r}_j). \end{aligned}$$

For simplicity, we have assumed that the potentials are spin-independent. For a tranlsationally invariant system, the external potential must be constant

$$u(\mathbf{r}) = u = \text{constant}$$

and the particle–particle interactions can only depend on the relative positions of the particles

$$v(\mathbf{r}, \mathbf{r}') = v(\mathbf{r} - \mathbf{r}').$$

Translationally invariant systems are necessarily infinite. This idealization implies that we are considering systems where we can ignore surface effects.

The first question we encounter when we want to express the Hamiltonian of a translationally invariant system in second quantization, is the choice of a suitable single-particle basis. To obtain this, we consider the system of a large cube with sides L and volume $\Omega = L^3$. At the end of the calculation we go to the so-called thermodynamic limit $N \to \infty$, $\Omega \to \infty$ while keeping N/Ω constant. To make the calculations translationally invariant, we impose periodic boundary conditions on the edges of the cube. If we solve the single-particle Schrödinger equation without an external potential with such boundary conditions, the eigenfunctions will provide a suitable system of functions. The eigenfunctions are the plane waves

$$\phi_{\mathbf{k}\sigma}(x) = \frac{1}{\sqrt{\Omega}} e^{i\mathbf{k}\cdot\mathbf{r}} \chi_\sigma(s). \tag{5.1}$$

These functions are momentum eigenfunctions with the discrete momenta $\mathbf{k} = (2\pi/L)\left(n_x\mathbf{e}_x + n_y\mathbf{e}_y + n_z\mathbf{e}_z\right)$, where n_x, n_y, n_z are any integers and $\mathbf{e}_x$, $\mathbf{e}_y$, $\mathbf{e}_z$ are unit vectors in the x-, y- and z-directions. For spin-1/2 fermions, which we will hereafter restrict ourselves to, the $\chi_\sigma(s)$ denote the usual Pauli-spinors:

$$\chi_+(s) = \begin{cases} 1 & \text{for } s = +1/2 \\ 0 & \text{for } s = -1/2 \end{cases}$$

$$\chi_-(s) = \begin{cases} 0 & \text{for } s = +1/2 \\ 1 & \text{for } s = -1/2. \end{cases} \tag{5.2}$$

(The representation of $\chi_\sigma(s)$ as functions of the double-valued variable $s = \pm 1/2$ is equivalent to the traditional notation in the form of two-vectors $\chi_+ = \binom{1}{0}$, $\chi_- = \binom{0}{1}$.)

The countably infinite number of functions given by equation (5.1) form an orthonormal system:

$$\begin{aligned} \int_\Omega \phi^*_{\mathbf{k}'\sigma'}(x)\phi_{\mathbf{k}\sigma}(x)\mathrm{d}x &= \frac{1}{\Omega}\int_\Omega e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}}\mathrm{d}^3r \sum_s \chi^*_\sigma(s)\chi_{\sigma'}(s) \\ &= \delta_{\mathbf{k},\mathbf{k}'}\,\delta_{\sigma,\sigma'} = \delta_{n_x,n'_x}\delta_{n_y,n'_y}\delta_{n_z,n'_z}\delta_{\sigma,\sigma'}. \end{aligned}$$

By a theorem from the theory of Fourier series, the system $\{\phi_{\mathbf{k}\sigma}\}$ is complete in the space of square-integrable functions which are periodic with period Ω. We will here only be interested in functions that are defined only on the volume Ω itself, but the completeness will of course apply here.

From equation (2.6), we obtain the second-quantized representation of the kinetic energy-operator in the single-particle basis equation (5.1):

$$\hat{T} = \sum_{\mathbf{k},\sigma}\sum_{\mathbf{k}',\sigma} \langle \mathbf{k}'\sigma' \mid \frac{\hat{p}^2}{2m} \mid \mathbf{k}\sigma\rangle \hat{c}^\dagger_{\mathbf{k}'\sigma'}\hat{c}_{\mathbf{k}\sigma}.$$

Evaluation of the matrix elements yields

$$\begin{aligned}
&\langle \mathbf{k}'\sigma' \mid \frac{\hat{p}^2}{2m} \mid \mathbf{k}\sigma\rangle \\
&= \sum_s \int_\Omega \mathrm{d}^3 r \, \frac{1}{\sqrt{\Omega}} \mathrm{e}^{-i\mathbf{k}'\cdot\mathbf{r}} \chi^*_{\sigma'}(s) \left[-\frac{\hbar^2\nabla^2}{2m}\right] \frac{1}{\sqrt{\Omega}} \mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}} \chi_\sigma(s) \\
&= \frac{\hbar^2 k^2}{2m} \frac{1}{\Omega} \int_\Omega \mathrm{d}^3 r \, \mathrm{e}^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}} \sum_s \chi^*_{\sigma'}(s)\chi_\sigma(s) \\
&= \frac{\hbar^2 k^2}{2m} \delta_{\mathbf{k},\mathbf{k}'} \delta_{\sigma,\sigma'}.
\end{aligned}$$

Thus, we obtain in all

$$\hat{T} = \sum_{\mathbf{k}\sigma} \frac{\hbar^2 k^2}{2m} \hat{c}^\dagger_{\mathbf{k}\sigma} \hat{c}_{\mathbf{k}\sigma}. \tag{5.3}$$

Similarly, we obtain for the external (constant) potential the representation

$$\hat{U} = \sum_{\mathbf{k}\sigma} u \hat{c}^\dagger_{\mathbf{k}\sigma} \hat{c}_{\mathbf{k}\sigma} = u\hat{N}.$$

In order to calculate the interaction term, we expand the particle–particle potential in a Fourier series

$$v(\mathbf{r}-\mathbf{r}') = \frac{1}{\Omega} \sum_{\mathbf{q}} v_{\mathbf{q}} \mathrm{e}^{i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')} \tag{5.4}$$

with the components given by

$$v_{\mathbf{q}} = \int_\Omega \mathrm{d}^3 r \, v(\mathbf{r}) \mathrm{e}^{-i\mathbf{q}\cdot\mathbf{r}}. \tag{5.5}$$

We can write the interaction in terms of this Fourier series as

$$\hat{V} = \frac{1}{2} \sum_{\substack{i,j=1 \\ i\neq j}}^{N} v(\mathbf{r}_i - \mathbf{r}_j) = \frac{1}{2\Omega} \sum_{\mathbf{q}} v_{\mathbf{q}} \sum_{\substack{i,j=1 \\ i\neq j}}^{N} \mathrm{e}^{i\mathbf{q}\cdot(\mathbf{r}_i-\mathbf{r}_j)},$$

and, by using equation (2.7), the second-quantized representation becomes

$$\begin{aligned}
\hat{V} \;=\; & \frac{1}{2\Omega} \sum_{\mathbf{q}} v_{\mathbf{q}} \sum_{\mathbf{k}_1\sigma_1} \sum_{\mathbf{k}_2\sigma_2} \sum_{\mathbf{k}_3\sigma_3} \sum_{\mathbf{k}_4\sigma_4} \langle \mathbf{k}_1\sigma_1, \mathbf{k}_2\sigma_2 \mid \mathrm{e}^{i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')} \mid \mathbf{k}_3\sigma_3, \mathbf{k}_4\sigma_4\rangle \\
& \times \hat{c}^\dagger_{\mathbf{k}_1\sigma_1} \hat{c}^\dagger_{\mathbf{k}_2\sigma_2} \hat{c}_{\mathbf{k}_4\sigma_4} \hat{c}_{\mathbf{k}_3\sigma_3}.
\end{aligned}$$

The matrix elements are

$$
\begin{aligned}
&\langle \mathbf{k}_1\sigma_1, \mathbf{k}_2\sigma_2 \mid e^{i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')} \mid \mathbf{k}_3\sigma_3, \mathbf{k}_4\sigma_4\rangle \\
&= \frac{1}{\Omega^2}\int_\Omega\int_\Omega d^3r\, d^3r' \sum_s \chi^*_{\sigma_1}(s)\chi_{\sigma_3}(s) e^{i\mathbf{r}\cdot(\mathbf{k}_3-\mathbf{k}_1)} e^{i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')} \\
&\quad \times e^{i\mathbf{r}'\cdot(\mathbf{k}_4-\mathbf{k}_2)} \sum_{s'} \chi^*_{\sigma_2}(s')\chi_{\sigma_4}(s') \\
&= \delta_{\sigma_1\sigma_3}\delta_{\sigma_2\sigma_4}\frac{1}{\Omega}\int d^3r\, e^{i[(\mathbf{k}_3+\mathbf{q})-\mathbf{k}_1]\cdot\mathbf{r}}\frac{1}{\Omega}\int d^3r'\, e^{i[(\mathbf{k}_4-\mathbf{q})-\mathbf{k}_2]\cdot\mathbf{r}'} \\
&= \delta_{\sigma_1\sigma_3}\delta_{\sigma_2\sigma_4}\delta_{(\mathbf{k}_3+\mathbf{q}),\mathbf{k}_1}\delta_{(\mathbf{k}_4-\mathbf{q}),\mathbf{k}_2}\,.
\end{aligned}
$$

Finally, when we insert this expression for the matrix elements into the representation of the interaction potential and rename the summation indices according to

$$\sigma \equiv \sigma_1 \qquad \sigma' \equiv \sigma_2 \qquad \mathbf{k} \equiv \mathbf{k}_3 \qquad \mathbf{k}' \equiv \mathbf{k}_4$$

we obtain the result

$$
\begin{aligned}
\hat{H} &= \sum_{\mathbf{k}\sigma}\left(\frac{\hbar^2k^2}{2m} + u\right)\hat{c}^\dagger_{\mathbf{k}\sigma}\hat{c}_{\mathbf{k}\sigma} \\
&\quad + \frac{1}{2\Omega}\sum_{\mathbf{q}}\sum_{\substack{\mathbf{k}\sigma\\ \mathbf{k}'\sigma'}} v_{\mathbf{q}}\hat{c}^\dagger_{(\mathbf{k}+q)\sigma}\hat{c}^\dagger_{(\mathbf{k}'-\mathbf{q})\sigma'}\hat{c}_{\mathbf{k}'\sigma'}\hat{c}_{\mathbf{k}\sigma}\,. \qquad (5.6)
\end{aligned}
$$

From equation (5.6), we see that there are two advantages in using the plane waves as a single-particle basis.

(1) The kinetic energy is diagonal in this representation.

(2) The translational invariance of the interaction potential makes it possible to use a Fourier transformation with respect to the relative coordinate $(\mathbf{r} - \mathbf{r}')$ only, that is, it is not necessary to use two separate Fourier series with respect to both $\mathbf{r}$ and $\mathbf{r}'$. This means that the number of independent sums in the second quantization representation of the interaction potential can be reduced by three.

We will use the result equation (5.6) later in the discussion of the homogeneous electron gas.

Chapter 6

Density operators

In this chapter we will discuss operators which have expectation values that correspond to the particle density. Consider first a single particle. The probability of finding this particle at x in state ν is given by

$$\rho_\nu(x) = \varphi_\nu^*(x)\varphi_\nu(x) = \langle \nu \mid x\rangle\langle x \mid \nu\rangle.$$

In this case, we then apparently have two possible ways of defining a density operator.

(1) $\hat{\rho}(x) \equiv | x\rangle\langle x |$. The probability density $\rho_\nu(x)$ is then just the expectation value of the operator $\hat{\rho}(x)$ in the state $\mid \nu\rangle$:

$$\langle \nu \mid \hat{\rho}(x) \mid \nu\rangle = \langle \nu \mid x\rangle\langle x \mid \nu\rangle = \rho_\nu(x).$$

(2) $\hat{n}_\nu \equiv \mid \nu\rangle\langle \nu \mid$. According to this second definition of a density operator we obtain ρ_ν as the expectation value of $\hat{n}_\nu$ in the $\hat{x}$-eigenfunctions $\mid x\rangle$:

$$\langle x \mid \hat{n}_\nu \mid x\rangle = \langle x \mid \nu\rangle\langle \nu \mid x\rangle = \rho_\nu(x).$$

Even though these two density operators lead to identical expectation values, the operators themselves are not at all identical. The operator $\hat{\rho}(x)$ is the projector on $\mid x\rangle$ and $\hat{n}_\nu$ is the projector on $\mid \nu\rangle$.

For later purposes we will now once again calculate the x-representation (position–spin representation) of the operator $\hat{\rho}(x)$:

$$\begin{aligned}\langle x_1' \mid \hat{\rho}(x) \mid x_1\rangle &= \langle x_1' \mid x\rangle\langle x \mid x_1\rangle \\ &= \delta(x_1' - x)\delta(x - x_1) \\ &= \delta(x - x_1)\delta(x_1' - x_1).\end{aligned}$$

Thus, in this representation the operator $\hat{\rho}(x)$ is a local multiplicative operator. Just as for local potentials,where we only need to write the diagonal elements and can imply a δ-function; for example, we write

$$\hat{v} = v(x_1)$$

instead of

$$\hat{v} = v(x_1)\delta(x_1 - x_2).$$

Similarly, we will only write

$$\hat{\rho}(x) = \delta(x - x_1)$$

for the density operator.

We now turn the discussion to many-particle systems. If a system is in a (symmetric or antisymmetric) state $\Psi(x_1, x_2, \ldots, x_N)$, the probability density of finding one particle at x is given by

$$\rho_\Psi(x) = N \int \mathrm{d}^{N-1}x\, \Psi^*(x, x_2, \ldots, x_N)\Psi(x, x_2, \ldots, x_N). \tag{6.1}$$

In equation (6.1), the density is normalized on the particle number N. Again, there are two possible ways of defining a density operator.

(1) The natural many-particle generalization of the single-particle density operator $\hat{\rho}$ discussed above is (in the x-representation)

$$\hat{\rho}(x) = \sum_{i=1}^{N} \delta(x - x_i)$$

so that we have again a local multiplicative operator in the x-representation. From this definition it follows that

$$\begin{aligned} &\langle \Psi \mid \hat{\rho}(x) \mid \Psi\rangle \\ &= \int \mathrm{d}^N x\, \Psi^*(x_1, \ldots, x_N) \left[\sum_{i=1}^{N} \delta(x - x_i)\right] \Psi(x_1, \ldots, x_N) \end{aligned}$$

and because of the assumed symmetry or antisymmetry of Ψ, this expression is

$$N \int \mathrm{d}^{N-1}x \Psi^*(x, x_2, \ldots, x_N)\Psi(x, x_2, \ldots, x_N) = \rho_\Psi(x).$$

We also write down the second-quantized representation of this operator:

$$\hat{\rho}(x) = \sum_{i=1}^{N} \delta(x - x_i) \equiv \sum_{i=1}^{N} \hat{\sigma}_x(x_i)$$

so that the second-quantized representation can be written

$$\hat{\rho}(x) = \sum_{i,j=1}^{\infty} \langle i \mid \hat{\sigma}_x \mid j \rangle \hat{c}_i^{\dagger} \hat{c}_j$$

where

$$\begin{aligned}
\langle i \mid \hat{\sigma}_x \mid j \rangle &= \int \mathrm{d}y \, \varphi_i^*(y) \hat{\sigma}_x(y) \varphi_j(y) \\
&= \int \mathrm{d}y \, \varphi_i^*(y) \delta(x-y) \varphi_j(y) \\
&= \varphi_i^*(x) \varphi_j(x).
\end{aligned}$$

Hence, we arrive at

$$\hat{\rho}(x) = \sum_{i,j=1}^{\infty} \varphi_i^*(x) \varphi_j(x) \hat{c}_i^{\dagger} \hat{c}_j = \hat{\psi}^{\dagger}(x) \hat{\psi}(x). \tag{6.2}$$

This result is, perhaps, not too surprising, since we demonstrated in Chapters 4 and 5 that the operator $(\hat{c}_k^{\dagger} \hat{c}_k)$ in general counts the particles in state k. Because of the unique correspondence between these creation and annihilation operators and the field operators, the operator $\hat{\psi}^{\dagger}(x)\hat{\psi}(x)$ then counts the number of particles in state x, *i.e.*, the number of particles at position $\mathbf{x}$ with spin s. We should then expect that if we integrate $\hat{\rho}$ over all x we will obtain the total particle number operator, equation (2.5), defined earlier:

$$\begin{aligned}
\int \hat{\rho}(x) \mathrm{d}x &= \int \hat{\psi}^{\dagger}(x) \hat{\psi}(x) \, \mathrm{d}x = \sum_{i,j=1}^{\infty} \hat{c}_i^{\dagger} \hat{c}_j \underbrace{\int \varphi_i^*(x) \varphi_j(x) \, \mathrm{d}x}_{\delta_{i,j}} \\
&= \sum_{i,j=1}^{\infty} \hat{c}_i^{\dagger} \hat{c}_j = \hat{N}.
\end{aligned}$$

(2) The second possible way of defining a density operator is through

$$\hat{n}_{\Psi} = \sum_{k,\ell=1}^{\infty} \mid k \rangle n_{k\ell} \langle \ell \mid$$

where $n_{k\ell} = \langle \Psi \mid \hat{c}_{\ell}^{\dagger} \hat{c}_k \mid \Psi \rangle$. This definition yields

$$\begin{aligned}\langle x \mid \hat{n}_\Psi \mid x\rangle &= \sum_{k,\ell=1}^{\infty} \langle x \mid k\rangle n_{k\ell}\langle \ell \mid x\rangle \\ &= \sum_{k,\ell=1}^{\infty} \varphi_\ell^*(x)\varphi_k(x)\langle \Psi \mid \hat{c}_\ell^\dagger \hat{c}_k \mid \Psi\rangle \\ &= \langle \Psi \mid \hat{\rho}(x) \mid \Psi\rangle = \rho_\Psi(x).\end{aligned}$$

Whereas the ν- and x-representations were constructed in a formally similar way in the single-particle case, the correspondence between $\hat{\rho}(x)$ and $\hat{n}_\Psi$ is not that obvious in the many-particle problem. In particular, the operator $\hat{\rho}(x)$ is an operator that acts on the many-particle Hilbert space, whereas $\hat{n}_\Psi$ acts on the single-particle Hilbert space. However, the trace of $\hat{n}_\Psi$ is equal to the particle number. This is easily verified in the x-representation:

$$\mathrm{Tr}\,(\hat{n}_\Psi) = \int \mathrm{d}x\,\langle x \mid \hat{n}_\Psi \mid x\rangle = \int \mathrm{d}x\,\rho_\Psi(x) = N.$$

On the other hand, the numbers $n_{k\ell}$ above are precisely the matrix elements of the operator $\hat{n}_\Psi$ in the underlying single-particle basis:

$$\langle i \mid \hat{n}_\Psi \mid j\rangle = \sum_{k,\ell=1}^{\infty} \underbrace{\langle i \mid k\rangle}_{=\delta_{ik}} n_{k\ell} \underbrace{\langle \ell \mid j\rangle}_{=\delta_{\ell j}} = n_{ij}.$$

Furthermore, the matrix $n_{k\ell}$ is Hermitian, since

$$\begin{aligned} n_{k\ell}^* &= \langle \Psi \mid \hat{c}_\ell^\dagger \hat{c}_k \mid \Psi\rangle^* \\ &= \langle \Psi \mid \left(\hat{c}_\ell^\dagger \hat{c}_k\right)^\dagger \mid \Psi\rangle \\ &= \langle \Psi \mid \hat{c}_k^\dagger \hat{c}_\ell \mid \Psi\rangle = n_{\ell k}.\end{aligned}$$

It follows that we can find a unitary transformation D which diagonalizes $n_{k\ell}$:

$$\left(D^\dagger\, n\, D\right)_{k\ell} = n_\ell \delta_{k\ell}.$$

The matrix elements on the diagonal are obtained from

$$\begin{aligned} n_\ell &= \sum_{kj} \left(D^\dagger\right)_{\ell k} n_{kj} D_{j\ell} \\ &= \sum_{kj} D_{k\ell}^* D_{j\ell} \langle \Psi \mid \hat{c}_j^\dagger \hat{c}_k \mid \Psi\rangle \\ &= \langle \Psi \mid \left(\sum_j D_{j\ell}\hat{c}_j^\dagger\right)\left(\sum_k D_{k\ell}^* \hat{c}_k\right) \mid \Psi\rangle.\end{aligned}$$

If we define

$$\hat{a}_\ell \equiv \sum_k D^*_{k\ell}\hat{c}_k$$

and

$$\hat{a}^\dagger_\ell \equiv \sum_j D_{j\ell}\hat{c}^\dagger_j$$

the operators $\hat{a}^\dagger_\ell$ and $\hat{a}_\ell$ are adjoint, and we have

$$n_\ell = \langle \Psi \mid \hat{a}^\dagger_\ell \hat{a}_\ell \mid \Psi \rangle .$$

Thus, if we had started with $\langle x \mid \hat{a}^\dagger_\ell \mid 0\rangle$ as the underlying single-particle basis, the matrix $n_{k\ell}$ would have been diagonal, and the operator $\hat{n}_\Psi$ would have had the following form:

$$\hat{n}_\Psi = \sum_{k=1}^{\infty} n_k \mid k\rangle\langle k \mid . \tag{6.3}$$

The numbers n_k have in this diagonal form a clear meaning: n_k is the occupation number of the orbital $\mid k\rangle$ in the many-particle state Ψ.

We can write the expectation value of an arbitrary single-particle operator $\hat{F}$, given by

$$\hat{F} = \sum_{i,j=1}^{\infty} \langle i \mid \hat{f} \mid j\rangle \hat{c}^\dagger_i \hat{c}_j$$

in the many-particle state Ψ, in a more compact form as a trace with the help of the operators $\hat{n}_\Psi$:

$$\begin{aligned} \langle \Psi \mid \hat{F} \mid \Psi\rangle &= \sum_{i,j=1}^{\infty} \langle i \mid \hat{f} \mid j\rangle \underbrace{\langle \Psi \mid \hat{c}^\dagger_i \hat{c}_j \mid \Psi\rangle}_{=n_{ji}} \\ &= \sum_{i,j=1}^{\infty} \langle i \mid \hat{f} \mid j\rangle\langle j \mid \hat{n}_\Psi \mid i\rangle = \mathrm{Tr}\left(\hat{f}\hat{n}_\Psi\right). \end{aligned}$$

We conclude this chapter by considering the so-called *density matrix*. This quantity is defined by

$$\rho_\Psi(x,x') \equiv N \int \Psi^*(x',x_2,\ldots,x_N)\Psi(x,x_2,\ldots,x_N)\mathrm{d}^{N-1}x. \tag{6.4}$$

Also in the case of the density matrix, we can define two different operators which have matrix elements given by equation (6.4):

(1) $\hat{\rho}(x,x') \equiv \sum_{i=1}^{N} \delta(x'-x_i')\delta(x-x_i)$. The so-called 'density matrix operator' defined in this way is non-local in the x-representation; explicitly, this means that

$$\begin{aligned}
&\langle x_1 \ldots x_N \mid \hat{\rho}(x,x') \mid x_1', \ldots x_N' \rangle \\
&= \sum_{i=1}^{N} \delta(x_1 - x_1')\delta(x_2 - x_2') \ldots \\
&\quad \times \ldots \left[\delta(x' - x_i')\delta(x - x_i)\right] \ldots \delta(x_N - x_N').
\end{aligned}$$

We can use this result to show that the density matrix is the expectation value of the operator $\hat{\rho}(x,x')$ in the many-particle state Ψ:

$$\begin{aligned}
&\langle \Psi \mid \hat{\rho}(x,x') \mid \Psi \rangle \\
&= \int \mathrm{d}^N x \int \mathrm{d}^N x' \, \langle \Psi \mid x_1', \ldots, x_N' \rangle \\
&\quad \times \langle x_1', \ldots, x_N' \mid \hat{\rho}(x,x') \mid x_1, \ldots, x_N \rangle \langle x_1, \ldots, x_N \mid \Psi \rangle \\
&= \int \mathrm{d}^N x \int \mathrm{d}^N x' \, \Psi^*(x_1', \ldots, x_N') \sum_{i=1}^{N} \delta(x_1 - x_1') \times \ldots \\
&\quad \times \ldots \delta(x' - x_i')\delta(x - x_i) \ldots \delta(x_N - x_N')\Psi(x_1, \ldots, x_N) \\
&= \sum_{i=1}^{N} \int \mathrm{d}^N x \, \Psi^*(x_1, \ldots, x', x_{i+1}, \ldots, x_N)\delta(x - x_i) \\
&\quad \times \Psi(x_1, \ldots, x_i, \ldots, x_N) \\
&= N \int \mathrm{d}^{N-1} x \, \Psi^*(x', x_2, \ldots, x_N)\Psi(x, x_2, \ldots, x_N) \\
&= \rho_\Psi(x,x').
\end{aligned}$$

We also write down the representation of the density matrix in second quantization:

$$\begin{aligned}
\hat{\rho}(x,x') &= \sum_{i=1}^{N} \delta(x' - x_i')\delta(x - x_i) \equiv \sum_{i=1}^{N} \langle x_i' \mid \hat{\sigma}_{x,x'} \mid x_i \rangle \\
&= \sum_{i,j=1}^{\infty} \hat{c}_i^\dagger \hat{c}_j \langle i \mid \hat{\sigma}_{x,x'} \mid j \rangle
\end{aligned}$$

where

$$\begin{aligned}
\langle i \mid \hat{\sigma}_{x,x'} \mid j \rangle &= \int \mathrm{d}y \int \mathrm{d}y' \, \langle i \mid y' \rangle \langle y' \mid \hat{\sigma}_{x,x'} \mid y \rangle \langle y \mid j \rangle \\
&= \int \mathrm{d}y \int \mathrm{d}y' \, \varphi_i^*(y')\delta(x' - y')\delta(x - y)\varphi_j(y) \\
&= \varphi_i^*(x')\varphi_j(x).
\end{aligned}$$

Thus

$$\hat{\rho}(x,x') = \sum_{i,j=1}^{\infty} \hat{c}_i^\dagger \hat{c}_j \varphi_i^*(x')\varphi_j(x) = \hat{\psi}^\dagger(x')\hat{\psi}(x). \tag{6.5}$$

(2) In the second possible representation of the density matrix, we use the operator $\hat{n}_\Psi$ defined earlier to form a non-diagonal matrix element in the x-representation:

$$\begin{aligned} \langle x \mid \hat{n}_\Psi \mid x' \rangle &= \sum_{k,\ell=1}^{\infty} \langle x \mid k \rangle n_{k\ell} \langle \ell \mid x' \rangle \\ &= \sum_{k,\ell=1}^{\infty} \varphi_\ell^*(x')\varphi_k(x) \langle \Psi \mid \hat{c}_\ell^\dagger \hat{c}_k \mid \Psi \rangle \\ &= \langle \Psi \mid \hat{\rho}(x,x') \mid \Psi \rangle = \rho_\Psi(x,x'). \end{aligned}$$

We will now also prove an important statement about the density operator $\hat{n}_\Psi$: Let Ψ be a fermion wavefunction. Then

$$\hat{n}_\Psi^2 = \hat{n}_\Psi \quad \Leftrightarrow \quad \Psi \text{ is a Slater determinant.}$$

Proof:

'$\Rightarrow$' We start with a single-particle basis in which the matrix $(n_{k\ell})$ is diagonal. Then

$$\begin{aligned} \hat{n}_\Psi^2 &= \sum_{k=1}^{\infty}\sum_{\ell=1}^{\infty} n_\ell \mid \ell \rangle \underbrace{\langle \ell \mid k \rangle}_{=\delta_{\ell k}} \langle k \mid n_k \\ &= \sum_{k=1}^{\infty} n_k^2 \mid k \rangle\langle k \mid = \sum_{k=1}^{\infty} n_k \mid k \rangle\langle k \mid \end{aligned}$$

so $n_k^2 = n_k$, which means that n_k is either 0 or 1. This implies that Ψ is a Slater determinant.

'$\Leftarrow$' Let $\mid \Psi \rangle = \hat{c}_1^\dagger \hat{c}_2^\dagger \ldots \hat{c}_N^\dagger \mid 0 \rangle$, so that

$$n_{k\ell} = \langle \Psi \mid \hat{c}_\ell^\dagger \hat{c}_k \mid \Psi \rangle = \begin{cases} 0 & \text{if } k \neq \ell \\ n_k & \text{if } k = \ell \end{cases}$$

with

$$n_k = \begin{cases} 1 & k \leq N \\ 0 & k > N. \end{cases}$$

Thus

$$\hat{n}_\Psi = \sum_{k=1}^{\infty} n_k \mid k \rangle\langle k \mid = \sum_{k=1}^{N} \mid k \rangle\langle k \mid$$

and $\hat{n}_\Psi^2 = \hat{n}_\Psi$.

For a Slater determinant, the density matrix then has the form

$$\rho(x, x') = \langle x \mid \hat{n}_\Psi \mid x' \rangle = \sum_{k=1}^{N} \langle x \mid k \rangle \langle k \mid x' \rangle = \sum_{k=1}^{N} \varphi_k^*(x') \varphi_k(x). \tag{6.6}$$

Chapter 7

The Hartree–Fock approximation

The Hartree–Fock approximation (HF) is based on the hope that we can approximately describe an interacting fermion system in terms of an effective single-particle problem. The starting point is the idea that each particle moves in a mean-field potential, which is produced by all other particles and, in case there is one, by an external potential.

For the sake of simplicity, we will assume that the potential is local in the x-representation. Thus, the exact Hamiltonian of the system

$$\hat{H} = \sum_{i=1}^{N} (\hat{t}_i + \hat{u}_i) + \frac{1}{2} \sum_{\substack{i,j=1 \\ i \neq j}}^{N} \hat{v}_{ij}$$

becomes in this representation

$$\hat{H} = \sum_{i=1}^{N} \left[-\frac{\hbar^2}{2m} \nabla_i^2 + u(x_i) \right] + \frac{1}{2} \sum_{\substack{i,j=1 \\ i \neq j}}^{N} v(x_i, x_j).$$

Our goal is to approximate this two-particle operator by an effective single-particle potential

$$\hat{H}_{\mathrm{HF}} = \sum_{i=1}^{N} \hat{h}_{\mathrm{HF}}^{(i)} = \sum_{i=1}^{N} \left(\hat{t}_i + \hat{v}_{\mathrm{HF}}^{(i)} \right)$$

where the effective single-particle potential $\hat{v}_{\mathrm{HF}}$, the 'Hartree–Fock' potential, is unknown at the present. The solutions with the correct symmetry of the corresponding eigenvalue equation

$$\hat{H}_{\mathrm{HF}} \Phi = E \Phi$$

are then simply Slater determinants

$$\Phi = \frac{1}{\sqrt{N!}} \det \left[\varphi_i(x_j)\right].$$

The single-particle orbitals in these Slater determinants are formally obtained from the equation

$$\hat{h}_{\mathrm{HF}}\varphi_j = \tilde{\epsilon}\varphi_j.$$

However, so long as we do not know the Hartree–Fock potential, we, of course, cannot calculate the single-particle orbitals from this equation. To arrive at a way of determining these we make the *ansatz* of a Slater determinant of single-particle orbitals for the exact many-body wavefunction. By Ritz' variational theorem, there is a rational way to optimize this *ansatz* by minimizing the total energy of the system. Minimizing the total energy with respect to the single-particle orbitals will then yield the Hartree–Fock equation for these.

Thus, we vary the expectation value of the *exact* Hamiltonian in a Slater determinant of single-particle orbitals: ~ мэч - магал 4 С .

$$\frac{\delta}{\delta\varphi_\alpha^*(x)} \left[\langle\Phi \mid \hat{H} \mid \Phi\rangle - \sum_{i=1}^{N} \epsilon_i \int \mathrm{d}y\, \varphi_i(y)\varphi_i^*(y)\right] = 0. \qquad (7.1)$$

The Lagrangian multipliers ϵ_i in equation (7.1) arise from the constraint that the single-particle orbitals be normalized. For the total energy of the system to be a minimum with respect to the Slater determinant trial functions, it is necessary that the expression in brackets is stationary, *i.e.*, that the first variation of this expression with respect to the trial functions vanishes. (We should at this point recall that it is possible to vary $(\mathrm{Re}\varphi_\alpha)$ and $(\mathrm{Im}\varphi_\alpha)$ independently. This possibility can however be rewritten as formally independent variations of φ_α and φ_α^*. From the real-valued functional equation (7.1) above we then obtain, as usual, pairwise adjoint equations. It is sufficient to consider only one of these.)

We calculate the expectation value of $\hat{H}$ in a Slater determinant by introducing second quantization (*cf.* equations (2.8) and (2.9)):

$$\langle\Phi \mid \hat{H} \mid \Phi\rangle = \sum_{i=1}^{N}\langle i \mid \hat{h} \mid j\rangle + \frac{1}{2}\left(\sum_{i,j=1}^{N}\langle ij \mid \hat{v} \mid ij\rangle - \sum_{i,j=1}^{N}\langle ij \mid \hat{v} \mid ji\rangle\right). \qquad (7.2)$$

The expectation value of the interaction potential consists of two terms; the first term is traditionally called the *direct term*, and the second the *exchange term*.

Explicitly, the variational equation (7.1) becomes [illegible] component

$$\begin{aligned}
0 \;=\;& \frac{\delta}{\delta\varphi_\alpha^*(x)}\Bigg\{\sum_{i=1}^{N}\int \mathrm{d}y\varphi_i^*(y)\left[-\frac{\hbar^2\nabla^2}{2m}+u(y)\right]\varphi_i(y)\\
&+\frac{1}{2}\sum_{i,j=1}^{N}\int\int \mathrm{d}y\,\mathrm{d}y'\,\varphi_i^*(y)\varphi_j^*(y')v(y,y')\varphi_i(y)\varphi_j(y')\\
&-\frac{1}{2}\sum_{i,j=1}^{N}\int\int \mathrm{d}y\,\mathrm{d}y'\,\varphi_i^*(y)\varphi_j^*(y')v(y,y')\varphi_j(y)\varphi_i(y')\\
&-\sum_{i=1}^{N}\epsilon_i\int \mathrm{d}y\,\varphi_i^*(y)\varphi_i(y)\Bigg\}\\
=\;& \left[-\frac{\hbar^2}{2m}\nabla^2+u(x)\right]\varphi_\alpha(x)+\frac{1}{2}\sum_{j=1}^{N}\int \mathrm{d}y'\,\varphi_j^*(y')v(x,y')\varphi_\alpha(x)\varphi_j(y')\\
&+\frac{1}{2}\sum_{i=1}^{N}\int \mathrm{d}y\,\varphi_i^*(y)v(y,x)\varphi_i(y)\varphi_\alpha(x)\\
&-\frac{1}{2}\sum_{j=1}^{N}\int \mathrm{d}y'\,\varphi_j^*(y')v(x,y')\varphi_j(x)\varphi_\alpha(y')\\
&-\frac{1}{2}\sum_{i=1}^{N}\int \mathrm{d}y\,\varphi_i^*(y)v(y,x)\varphi_\alpha(y)\varphi_i(x)-\epsilon_\alpha\varphi_\alpha(x).
\end{aligned}$$

Sloppy math

From this calculation we see that the second and the third, and the fourth and the fifth terms are equal. We then use the representation given in equation (6.6) for the density and the density matrix for Slater determinants

$$\rho(y)=\sum_{i=1}^{N}\varphi_i^*(y)\varphi_i(y)\quad\text{and}\quad\rho(x,y)=\sum_{i=1}^{N}\varphi_i^*(y)\varphi_i(x)$$

to finally obtain

$$\begin{aligned}
&\left[-\frac{\hbar^2}{2m}\nabla^2+u(x)+\int \mathrm{d}y\,\rho(y)v(x,y)\right]\varphi_\alpha(x)\\
&\qquad-\int\rho(x,y)v(x,y)\varphi_\alpha(y)\mathrm{d}y \;=\; \epsilon_\alpha\varphi_\alpha(x).
\end{aligned}\tag{7.3}$$

Equation (7.3) is the *Hartree-Fock equation.* The minimization of the total energy has with this equation provided us with a prescription for the construction of an optimal effective single-particle potential, $\hat{v}_{\mathrm{HF}}$. This prescription is

$$\hat{v}_{\mathrm{HF}}\varphi_i=u(x)\varphi_i(x)+\int \mathrm{d}y\,\rho(y)v(x,y)\varphi_i(x)-\int\rho(x,y)v(x,y)\varphi_i(y)\mathrm{d}y.$$

In addition to the external potential $u(x)$ and the classical potential energy $\int \mathrm{d}y\, \rho(y)v(x,y)$, the Hartree–Fock potential contains a non-local part, the so-called exchange operator. As we would expect, the Hartree–Fock potential is identical for all single-particle orbitals – this corresponds to our notion of 'identical particles'. It is easy to verify that $\hat{v}_{\mathrm{HF}}$ is Hermitian. To do that, we first note that we have $\rho^*(x,y) = \rho(y,x)$ (*cf.* equation (6.6)). We then obtain

$$\begin{aligned}
\langle f \mid \hat{v}_{\mathrm{HF}} \mid g\rangle &= \int f^*(x) \int \rho(y)v(x,y)g(x)\,\mathrm{d}y\,\mathrm{d}x \\
&\quad - \int f^*(x) \int \rho(x,y)v(x,y)g(y)\,\mathrm{d}y\,\mathrm{d}x + \langle f \mid \hat{u} \mid g\rangle \\
&= \left[\int f(x) \int \rho(y)v(x,y)\,\mathrm{d}y\, g^*(x)\,\mathrm{d}x\right]^* \\
&\quad - \left[\int f(x) \int \rho^*(x,y)v(x,y)g^*(y)\,\mathrm{d}y\,\mathrm{d}x\right]^* + \langle f \mid \hat{u} \mid g\rangle \\
&= \left[\int g^*(x) \int \rho(y)v(x,y)\mathrm{d}y\, f(x)\,\mathrm{d}x\right]^* + (\langle g \mid \hat{u} \mid f\rangle)^* \\
&\quad - \left[\int g^*(y) \int \rho(x,y)v(y,x)f(x)\,\mathrm{d}x\,\mathrm{d}y\right]^* \\
&= (\langle g \mid \hat{v}_{\mathrm{HF}} \mid f\rangle)^* .
\end{aligned}$$

Since $\hat{v}_{\mathrm{HF}}$ and $\hat{h}_{\mathrm{HF}}$ are Hermitian operators, the Lagrangian parameter ϵ_α, which entered in equation (7.3) as an eigenvalue, must be real, and the eigenfunctions φ_α must be mutually orthogonal. In retrospect, it is clear that it was not necessary to enforce the orthogonality of the single-particle orbitals with an additional term $\sum_{i,j=1}^{N} \epsilon_{ij} \int \varphi_i^*(x)\varphi_j(x)\mathrm{d}x$ in the variational principle.

The direct term and the exchange term both contain the density matrix. Thus, both terms depend on the single-particle orbitals which we still have to determine. It is clear that we cannot solve the Hartree–Fock equation like a normal eigenvalue problem. Instead, we must use a so-called *self-consistent procedure*.

We start with

(0) an initial approximation $\varphi_i(x)$, $i = 1, \ldots, N$

and then calculate the

(1) Hartree–Fock potential $\hat{v}_{\mathrm{HF}}$ from the density matrix

$$\rho(x,y) = \sum_{i=1}^{N} \varphi_i^*(y)\varphi_i(x)$$

with which we solve the eigenvalue equation

(2) $(\hat{t} + \hat{v}_{\mathrm{HF}})\varphi_\alpha = \epsilon_\alpha \varphi_\alpha$.

In general, this equation has infinitely many solutions. The last step then consists of

(3) selecting N orbitals $\varphi_\alpha^{(\mathrm{new})}$ with the N lowest eigenvalues ϵ_α.

Using these orbitals, we calculate a new Hartree–Fock potential by repeating step (1). We can then iterate the scheme above until 'self-consistency' is achieved, that is, until the procedure converges so that the new orbitals obtained in step (3) are the same as the ones used in previous step (1).

In general, we obtain from the solution of the eigenvalue problem not only the occupied single-particle orbitals, which are necessary to determine $\rho(x, y)$ and $\hat{v}_{\mathrm{HF}}$, but, in principle, also an infinite set of unoccupied single-particle orbitals. All these orbitals together form the basis of the single-particle Hilbert space.

We now proceed and assume that we have solved the Hartree–Fock equations for a single-particle problem. We then obtain the Hartree–Fock approximation of the total energy of the system by inserting the Slater determinant of the occupied orbitals in the expression equation (7.2) that we derived earlier:

$$E_{\mathrm{HF}} = \sum_{i=1}^{N} \langle i \mid \hat{t} + \hat{u} \mid i \rangle + \frac{1}{2} \sum_{i,j=1}^{N} \left[\langle ij \mid \hat{v} \mid ij \rangle - \langle ij \mid \hat{v} \mid ji \rangle \right].$$

Adding and subtracting the double sum once in this expression yields

$$\begin{aligned} E_{\mathrm{HF}} &= \sum_{i=1}^{N} \int \mathrm{d}x\, \varphi_i^*(x) \Bigg[\Bigg(-\frac{\hbar^2 \nabla^2}{2m} + u(x) \\ &\quad + \sum_{j=1}^{N} \int \mathrm{d}y\, \varphi_j^*(y) v(x,y) \varphi_j(y) \Bigg) \varphi_i(x) \\ &\quad - \sum_{j=1}^{N} \int \mathrm{d}y\, \varphi_j^*(y) v(x,y) \varphi_i(y) \varphi_j(x) \Bigg] \\ &\quad - \frac{1}{2} \sum_{i,j=1}^{N} \left(\langle ij \mid \hat{v} \mid ij \rangle - \langle ij \mid \hat{v} \mid ji \rangle \right). \end{aligned}$$

If we insert the Hartree–Fock equation (7.3) in this expression, we obtain

$$\sum_{i=1}^{N} \underline{\int \mathrm{d}x\, \varphi_i^*(x) \epsilon_i \varphi_i(x)} - \frac{1}{2} \sum_{i,j=1}^{N} \left(\langle ij \mid \hat{v} \mid ij \rangle - \langle ij \mid \hat{v} \mid ji \rangle \right).$$

$$\sum_{i,j}^{N} \langle i | \hat{h} | j \rangle = \sum_{i,j}^{N} \epsilon_i -$$

From the normalization of the single-particle orbitals, it finally follows that

$$\begin{aligned} E_{\mathrm{HF}} &= \sum_{i=1}^{N} \epsilon_i - \frac{1}{2} \sum_{i,j=1}^{N} \left(\langle ij \mid \hat{v} \mid ij \rangle - \langle ij \mid \hat{v} \mid ji \rangle \right) \\ &= \frac{1}{2} \sum_{i=1}^{N} \left(\epsilon_i + \langle i \mid \hat{t} + \hat{u} \mid i \rangle \right). \end{aligned} \tag{7.4}$$

The last equality is obtained by a completely analogous calculation, but with the simple sum split in two equal pieces instead of the double sum. We also write out explicitly the expression

$$\epsilon_\alpha = \langle \alpha \mid \hat{t} + \hat{u} \mid \alpha \rangle + \sum_{j=1}^{N} \left(\langle \alpha j \mid \hat{v} \mid \alpha j \rangle - \langle \alpha j \mid \hat{v} \mid j\alpha \rangle \right) \tag{7.5}$$

which we used to derive equation (7.4). Equation (7.5) follows from the Hartree–Fock equation by multiplying by $\varphi_\alpha^*(x)$ and integrating over x.

At this point the question emerges as to why the Hartree–Fock energy does not equal the sum of the single-particle energies ϵ_i. If we were to stay within the initial assumption that we can approximate the exact Hamiltonian by an effective single-particle operator (*i.e.*, $\hat{H}_{\mathrm{HF}}$), we would have obtained the sum $\sum_{i=1}^{N} \epsilon_i$ as an approximation of the total energy. However, this initial assumption was used later in the derivation as the basis for the Slater-determinant *ansatz*, which we used in the variational principle. The total energy obtained from this *ansatz* should then be better than $\sum_i \epsilon_i$. It is easy to show with a perturbation calculation that this is indeed the case. To do this, we assume that we have solved the Hartree–Fock equations and thus have determined the self-consistent potential. If we then abbreviate the interaction term in the Hartree–Fock potential as the single-particle operator $\hat{f}$, we can then write the exact Hamiltonian in the form

$$\begin{aligned} \hat{H} &= \sum_{i=1}^{N} \left(\hat{t}_i + \hat{u}_i + \hat{f}_i \right) + \left(\frac{1}{2} \sum_{\substack{i,j=1 \\ i \neq j}}^{N} \hat{v}_{ij} - \sum_{i=1}^{N} \hat{f}_i \right) \\ &= \hat{H}_{\mathrm{HF}} + \hat{H}'. \end{aligned}$$

If we then treat $\hat{H}'$ as a perturbation, we obtain in zeroth order perturbation theory

$$E^{(0)} = \langle \Phi \mid \hat{H}_{\mathrm{HF}} \mid \Phi \rangle = \sum_{i=1}^{N} \epsilon_i$$

and in first order

$$\begin{aligned} E^{(1)} &= \langle \Phi \mid \hat{H}' \mid \Phi \rangle = \langle \Phi \mid \frac{1}{2} \sum_{\substack{i \neq j \\ i,j=1}}^{N} \hat{v}_{ij} \mid \Phi \rangle - \langle \Phi \mid \sum_{i=1}^{N} \hat{f}_i \mid \Phi \rangle \\ &= \frac{1}{2} \sum_{i,j=1}^{N} \left(\langle ij \mid \hat{v} \mid ij \rangle - \langle ij \mid \hat{v} \mid ji \rangle \right) \\ &\quad - \sum_{i,j=1}^{N} \left(\langle ij \mid \hat{v} \mid ij \rangle - \langle ij \mid \hat{v} \mid ji \rangle \right). \end{aligned}$$

From these expressions we see that

$$E_{\text{HF}} = E^{(0)} + E^{(1)}.$$

Thus, the energy E_{HF} which is optimized by using the variational principle agrees with the energy obtained from first order perturbation theory, whereas the sum over the single-particle energies ϵ_i only agrees with zeroth order perturbation theory. The fact that the entire interaction energy is subtracted again from the sum of orbital energies in the expression for E_{HF} has furthermore a clear interpretation. According to equation (7.5), each individual ϵ_i contains

$$\begin{aligned} \epsilon_i &= \langle i \mid \hat{t} + \hat{u} \mid i \rangle + \sum_{j=1}^{N} \left(\langle ij \mid \hat{v} \mid ij \rangle - \langle ij \mid \hat{v} \mid ji \rangle \right) \\ &= \langle i \mid \hat{t} + \hat{u} \mid i \rangle + \sum_{\substack{j=1 \\ j \neq i}}^{N} \left(\langle ij \mid \hat{v} \mid ij \rangle - \langle ij \mid \hat{v} \mid ji \rangle \right) \end{aligned}$$

i.e., ϵ_i contains the energies of the interactions with all other occupied orbitals. For example, ϵ_1 contains the interaction with particle 2, particle 3 and so on, up to particle N; ϵ_2 contains once again the energy of the interaction between particle 2 and particle 1, and so on. Thus, all the interaction energies will be counted twice in the sum over ϵ_i:

$$\frac{1}{2} \sum_{i,j=1}^{N} \left(\langle ij \mid \hat{v} \mid ij \rangle - \langle ij \mid \hat{v} \mid ji \rangle \right).$$

This double counting is then compensated for in the expression for E_{HF}, equation (7.4).

We will here now also give a second derivation of the Hartree–Fock equations. This derivation will give emphasis to another property of the

Hartree–Fock operator. We begin this derivation by writing the variation of the energy functional as

$$0 = \left. \frac{\partial}{\partial \eta} \frac{\langle \Phi + \eta\chi \mid \hat{H} \mid \Phi\rangle}{\langle \Phi + \eta\chi \mid \Phi\rangle} \right|_{\eta=0}$$

and restrict ourselves to variations such that

(1) $\Phi + \eta\Phi$ is, just as Φ, a Slater determinant, and

(2) only *one* orbital will be varied:

$$\begin{aligned} \Phi + \eta\chi &= \begin{vmatrix} \varphi_1(x_1) & \varphi_2(x_2) & \cdots \\ \vdots & \vdots & \vdots \\ (\varphi_p + \eta\psi)(x_1) & (\varphi_p + \eta\psi)(x_2) & \cdots \\ \vdots & \vdots & \vdots \\ \varphi_N(x_1) & \varphi_N(x_2) & \cdots \end{vmatrix} \\ &= \det|\varphi_1, \ldots, \varphi_p, \ldots| + \eta \det|\varphi_1, \ldots, \psi, \ldots|. \end{aligned}$$

For ψ we will now take the elements of the (yet to be determined) complete orthonormal family consisting of the occupied orbitals $\varphi_1, \ldots, \varphi_N$ and the unoccupied orbitals $\varphi_{N+1}, \ldots$. The variation obviously vanishes for the first ones. We then replace φ_p, where $p \leq N$, with $\varphi_p + \eta\varphi_q$, where $q > N$. This means that we consider a state $\mid \chi\rangle$ which is in some sense an excitation of the state $\mid \Phi\rangle$:

$$\mid \chi\rangle = \hat{c}_q^\dagger \hat{c}_p \mid \Phi\rangle \equiv \mid \Phi_{qp}\rangle \quad \text{with} \quad \begin{cases} p \leq N \\ q > N \end{cases} .$$

The variational equation then becomes

$$\begin{aligned} 0 &= \left. \frac{\partial}{\partial \eta} \frac{\langle \Phi \mid \hat{H} \mid \Phi\rangle + \eta\langle \Phi_{qp} \mid \hat{H} \mid \Phi\rangle}{\underbrace{\langle \Phi \mid \Phi\rangle}_{=1} + \eta \underbrace{\langle \Phi_{qp} | \Phi\rangle}_{=0}} \right|_{\eta=0} = \langle \Phi_{qp} | \hat{H} | \Phi\rangle \\ &= \langle \Phi_{qp} \mid \sum_{i=1}^{N} (\hat{t}_i + \hat{u}_i) \mid \Phi\rangle + \langle \Phi_{qp} \mid \frac{1}{2} \sum_{\substack{i \neq j \\ i,j=1}} \hat{v}_{ij} \mid \Phi\rangle \end{aligned}$$

where we have used the orthonormality of the functions $\{\varphi_i\}$. The result we obtain from the variation is

$$0 = \langle q | \hat{t} + \hat{u} | p\rangle + \sum_{j=1}^{N} \left(\langle qj | \hat{v} | pj\rangle - \langle qj | \hat{v} | jp\rangle \right) \quad \text{for all } q > N, \, p \leq N.$$

The Hartree–Fock equation follows indeed from this expression, for if we define the Hartree–Fock operator $\hat{h}_{\mathrm{HF}}$ as before, this equation yields

$$\langle q|\hat{h}_{\mathrm{HF}}|p\rangle = 0 \quad \text{for all } q > N,\, p \leq N.$$

Thus, the Hartree–Fock operator has no non-zero matrix elements between occupied and unoccupied states. Hence, we can diagonalize the Hermitian operator $\hat{h}_{\mathrm{HF}}$ with a unitary transformation $\hat{D}$, which has the property that it only transforms occupied states into occupied ones, and unoccupied states into unoccupied ones:

$$\begin{pmatrix} \epsilon_1 & \cdots & & & \\ \vdots & \ddots & & & \\ & & \epsilon_N & & \\ & & & \epsilon_{N+1} & \\ & & & & \ddots \end{pmatrix}$$
$$= \begin{pmatrix} \hat{D}_b^\dagger & 0 \\ 0 & \hat{D}_u^\dagger \end{pmatrix} \begin{pmatrix} \text{occupied} & 0 \\ 0 & \text{unoccupied} \end{pmatrix} \begin{pmatrix} D_b & 0 \\ 0 & D_u \end{pmatrix}.$$

It is important to understand that the form of $\hat{h}_{\mathrm{HF}}$ is invariant under this diagonalization precisely because of this block-form of the transformation matrix. However, with this form invariance, the matrix equation above means that

$$\epsilon_i = \langle i|\hat{h}_{\mathrm{HF}}|i\rangle = \langle i|\hat{t} + \hat{u}|i\rangle + \sum_{j=1}^{N} \left(\langle ij|\hat{v}|ij\rangle - \langle ij|\hat{v}|ji\rangle\right)$$

in a suitable bases. This is in principle the Hartree–Fock equation.

The property that the matrix elements of $\hat{H}$ between the Hartree–Fock wavefunction and the excited state Φ_{qp} vanish

$$\langle \Phi_{qp}|\hat{H}|\Phi\rangle = 0$$

is very important in applications of the Hartree–Fock wavefunction and is frequently referred to as *Brillouin's theorem.*

As an example, we will now consider the Hartree–Fock equation for atomic systems:

$$\begin{aligned}\left(-\frac{\hbar\nabla^2}{2m} - \frac{Ze^2}{r} + e^2 \int \frac{\rho(r')}{|\mathbf{r}-\mathbf{r}'|}\mathrm{d}^3r'\right) \varphi_\alpha(\mathbf{r}, s) & \\ -e^2 \sum_{s'} \int \frac{\rho(\mathbf{r}s, \mathbf{r}'s')}{|\mathbf{r}-\mathbf{r}'|} \varphi_\alpha(\mathbf{r}'s')\mathrm{d}^3r' &= \epsilon_\alpha \varphi_\alpha(\mathbf{r}s). \quad (7.6)\end{aligned}$$

We have set $\rho(\mathbf{r}) = \sum_s \rho(x) = \sum_s \rho(\mathbf{r}s)$ in the direct term. It is impossible to perform an analogous spin-elimination in the exchange term. This means that the Hartree–Fock potential is spin-dependent, even if the exact Hamiltonian of the system does not depend on spin.

The direct part of the Hartree–Fock potential is clearly nothing but the electrostatic potential due to the charge density of all electrons. This fact seems at first to be nonsensical, since the effective potential that acts on an orbital should not contain the electrostatic potential of this particular orbital, but only that of all the *other* electrons. Fortunately, this 'self-interaction' is canceled by a corresponding expression in the exchange potential:

$$\begin{aligned}
\epsilon_\alpha \varphi_\alpha(x) &= \left(-\frac{\hbar^2\nabla^2}{2m} - \frac{Ze^2}{r}\right)\varphi_\alpha(x) + \sum_{i=1}^{N}\int \mathrm{d}x'\,\frac{\varphi_i^*(x')\varphi_i(x')}{|\mathbf{r}-\mathbf{r}'|}\varphi_\alpha(x) \\
&\quad - \sum_{i=1}^{N}\int \mathrm{d}x'\,\frac{\varphi_i^*(x')\varphi_i(x)}{|\mathbf{r}-\mathbf{r}'|}\varphi_\alpha(x') \\
&= \left(-\frac{\hbar^2\nabla^2}{2m} - \frac{Ze^2}{r}\right)\varphi_\alpha(x) + \sum_{\substack{i=1\\ i\neq\alpha}}^{N}\int \mathrm{d}x'\,\frac{\varphi_i^*(x')\varphi_i(x')}{|\mathbf{r}-\mathbf{r}'|}\varphi_\alpha(x) \\
&\quad - \sum_{\substack{i=1\\ i\neq\alpha}}^{N}\int \mathrm{d}x'\,\frac{\varphi_i^*(x')\varphi_i(x)}{|\mathbf{r}-\mathbf{r}'|}\varphi_\alpha(x')
\end{aligned}$$

(for $\alpha < N$). We emphasize that this term is canceled only when $\varphi_\alpha(x)$ is an occupied orbital. Hence, the unoccupied orbitals formally interact with N particles.

We will now also briefly discuss to what extent one can treat ionized states and excited states within the Hartree–Fock approximation. It should first be emphasized that because of the nature of the approximation, one cannot attach any exact physical meaning to the orbital energies. However, in the case of atoms one can approximately relate the orbital energies to the ionization energies. This is because one can describe a singly ionized atomic state by a Slater determinant, which contains all ground state orbitals except for the most weakly bound one. Thus, one starts with the assumption that the rest of the orbitals do not change when these electrons are removed. The expectation value of the energy in a determinant that contains all ground state orbitals except for φ_k is obtained from equation (7.2):

$$
\begin{aligned}
E_{\mathrm{HF}}(N-1_k) &= \sum_{\substack{i=1\\ i\neq k}}^{N} \langle i \mid \hat{t}+\hat{u} \mid i\rangle \\
&\quad + \frac{1}{2} \sum_{\substack{i,j=1\\ i\neq j\neq k}}^{N} \left(\langle ij \mid \hat{v} \mid ij\rangle - \langle ij \mid \hat{v} \mid ji\rangle\right) \\
&= E_{\mathrm{HF}}(N) - \langle k \mid \hat{t}+\hat{u} \mid k\rangle \\
&\quad - \frac{1}{2}\sum_{i=1}^{N} \left(\langle ik \mid \hat{v} \mid ik\rangle - \langle ik \mid \hat{v} \mid ki\rangle\right) \\
&\quad - \frac{1}{2}\sum_{j=1}^{N} \left(\langle kj \mid \hat{v} \mid kj\rangle - \langle kj \mid \hat{v} \mid jk\rangle\right)
\end{aligned}
$$

and since $\langle ij \mid \hat{v} \mid k\ell\rangle = \langle ji \mid \hat{v} \mid \ell k\rangle$, the expression above becomes

$$
\begin{aligned}
& E_{\mathrm{HF}}(N) - \left[\langle k|\hat{t}+\hat{u}|k\rangle + \sum_{j=1}^{N} \left(\langle kj|\hat{v}|kj\rangle - \langle kj|\hat{v}|jk\rangle\right)\right] \\
&= E_{\mathrm{HF}}(N) - \epsilon_k .
\end{aligned}
$$

We thus obtain *Koopman's theorem* for the ionization energies I_k:

$$
I_k = E_{\mathrm{HF}}(N-1_k) - E_{\mathrm{HF}}(N) = -\epsilon_k . \tag{7.7}
$$

The ionization energies that are calculated in this way agree rather well with the experimentally determined values. The same holds for the photoabsorption thresholds for knocking electrons out of deep-lying shells.

The suggestion to describe excited many-particle states by a wavefunction $\hat{c}_k^{\dagger}\hat{c}_\ell|\Phi_0\rangle$ presents itself. In this wavefunction, a state which is occupied in the Hartree–Fock ground state is replaced by an unoccupied one:

$$
\begin{aligned}
E_{\mathrm{HF}}(N-1_\ell+1_k) &= \langle \hat{c}_k^{\dagger}\hat{c}_\ell\Phi_0 \mid \hat{H} \mid \hat{c}_k^{\dagger}\hat{c}_\ell\Phi_0\rangle \\
&= \sum_{\substack{i=1\\ i\neq \ell}}^{N} \langle i \mid \hat{t}+\hat{u} \mid i\rangle + \langle k \mid \hat{t}+\hat{u} \mid k\rangle \\
&\quad \underbrace{+\frac{1}{2} \sum_{\substack{i,j=1\\ i\neq j\neq \ell}}^{N} \left(\langle ij \mid \hat{v} \mid ij\rangle - \langle ij \mid \hat{v} \mid ji\rangle\right)}_{=\frac{1}{2}\sum_{i,j=1}^{N}(\ldots)-\sum_{j=1}^{N}(\langle \ell j|\hat{v}|\ell j\rangle-\langle \ell j|\hat{v}|j\ell\rangle)}
\end{aligned}
$$

$$\begin{aligned}
&\underbrace{+\frac{1}{2}\left[\sum_{\substack{i=1\\ i\neq\ell}}^{N}\left(\langle ik\,|\hat{v}|\,ik\rangle-\langle ik\,|\hat{v}|\,ki\rangle\right)+\sum_{\substack{j=1\\ j\neq\ell}}^{N}\left(\langle jk\,|\hat{v}|\,jk\rangle-\langle kj\,|\hat{v}|\,jk\rangle\right)\right]}_{=\sum_{\substack{j=1\\ j\neq\ell}}^{N}\left(\langle kj|\hat{v}|kj\rangle-\langle kj|\hat{v}|jk\rangle\right)}\\
= \; & \sum_{i=1}^{N}\langle i\mid \hat{t}+\hat{u}\mid i\rangle+\frac{1}{2}\sum_{i,j=1}^{N}\left(\langle ij\mid\hat{v}\mid ij\rangle-\langle ij\mid\hat{v}\mid ji\rangle\right)\\
& -\langle \ell\mid \hat{t}+\hat{u}\mid \ell\rangle-\sum_{j=1}^{N}\left(\langle \ell j\mid\hat{v}\mid \ell j\rangle-\langle \ell j\mid\hat{v}\mid j\ell\rangle\right)\\
& +\langle k\mid \hat{t}+\hat{u}\mid k\rangle+\sum_{\substack{j=1\\ j\neq\ell}}^{N}\left(\langle kj\mid\hat{v}\mid kj\rangle-\langle kj\mid\hat{v}\mid jk\rangle\right)\\
= \; & E_{\mathrm{HF}}(N)-\epsilon_{\ell}+\epsilon_{k}-\left(\langle k\ell|\hat{v}|k\ell\rangle-\langle k\ell|\hat{v}|\ell k\rangle\right).
\end{aligned}$$

The excitation energy

$$(\Delta E)_{\ell k}=E_{\mathrm{HF}}(N-1_{\ell}+1_{k})-E_{\mathrm{HF}}(N)$$

becomes

$$(\Delta E)_{\ell k}=\epsilon_{k}-\epsilon_{\ell}-\left(\langle k\ell|\hat{v}|k\ell\rangle-\langle k\ell|\hat{v}|\ell k\rangle\right). \tag{7.8}$$

At this point it should be emphasized that the excitation energies calculated in this way are not generally any upper bounds to the exact energies, in contrast to the Hartree–Fock ground state energy. Furthermore, as we have just discussed, the unoccupied orbitals of the ground state interact formally with N particles, and not with $N-1$, which would have been correct for excited states. For very large systems, this difference between $(N-1)$ particles and N particles does not make much difference. For atomic systems, however, this difference has drastic consequences: consider first a *neutral* atom. An unoccupied orbital is in this case essentially affected by the total electrostatic potential of the nucleus and the electrons. This potential vanishes exponentially asymptotically, since the $-Z/r$-potential of the nucleus and the contributions from the electrons cancel asymptotically. A true, excited electron should thus asymptotically feel the potential of the nucleus and of only $N-1$ electrons, which together behave as $-1/r$. Since the excited electrons is so to speak outside the atom, pictorially speaking, its energy is essentially determined by the asymptotic behavior of the potential. It follows that the unoccupied orbitals determined through the Hartree–Fock procedure are bound far too weakly. As a result, we cannot expect that the excitation energies for atoms calculated by this procedure should agree particularly well with experimental values.

The formula above is also interesting from another point of view: the variational principle, which we evoked in the derivation of the Hartree–Fock equations, only guarantees that E_{HF} is *stationary* with respect to small variations in the single-particle orbitals. Hence, it would be very useful to find a criterion which would enable us to state whether the solutions we have found correspond to the *minimum* energy. A necessary condition for this is certainly

$$E_{\text{HF}}(N) < E_{\text{HF}}(N - 1_\ell + 1_k)$$

i.e., $(\Delta E)_{\ell k} > 0$, or

$$\epsilon_k > \epsilon_\ell + \left(\langle k\ell|\hat{v}|k\ell\rangle - \langle k\ell|\hat{v}|\ell k\rangle\right), \quad \text{for all} \begin{cases} \ell \le N \\ k > N \end{cases} .$$

For systems with extended states we can neglect the matrix elements in the potential, so that in this case the criterion is reduced to $\epsilon_k > \epsilon_\ell$. In other words, the orbital energies of the occupied states must lie deeper than the unoccupied ones. We will now give a crude estimate to show that the matrix elements of the interaction potential is, on the average, a factor of $(1/N)$ smaller than the single particle energies. (In examples from solid state theory, N is of the order of 10^{23}.)

We consider only cases without external potentials and restrict ourselves to interactions which are homogeneous of degree (-1) in the position coordinates. An example of such a potential is the Coulomb potential. The virial theorem holds under these assumptions. This theorem states the following: let Φ be a solution of a minimization problem of the type

$$0 = \delta\langle\Phi|\hat{T} + \hat{V}_{\text{int}}|\Phi\rangle$$

which can be obtained by *free* variations of the problem, so that Φ is not obtained by just fitting parameters. We then consider the normalized functions

$$\Phi_\alpha(\mathbf{r}_1 s_1, \ldots, \mathbf{r}_N s_N) \equiv \alpha^{3N/2}\Phi(\alpha\mathbf{r}_1 s_1, \ldots, \alpha\mathbf{r}_N s_N)$$

which are obtained by a scale transformation of Φ. These functions satisfy

$$\begin{aligned}
0 &= \frac{\partial}{\partial\alpha}|_{\alpha=1} \langle\Phi_\alpha \mid \hat{T} + \hat{V}_{\text{int}} \mid \Phi_\alpha\rangle \\
&= \frac{\partial}{\partial\alpha}\bigg|_{\alpha=1} \Big[\langle\Phi \mid \hat{T} \mid \Phi_\alpha\rangle + \langle\Phi \mid \hat{V}_{\text{int}} \mid \Phi_\alpha\rangle\Big] \\
&= \frac{\partial}{\partial\alpha}\bigg|_{\alpha=1} \Big[\alpha^2\langle\Phi_{\alpha=1} \mid \hat{T} \mid \Phi_{\alpha=1}\rangle + \alpha\langle\Phi_{\alpha=1} \mid \hat{V}_{\text{int}} \mid \Phi_{\alpha=1}\rangle\Big] \\
&= 2\langle\Phi_{\alpha=1} \mid \hat{T} \mid \Phi_{\alpha=1}\rangle + \langle\Phi_{\alpha=1} \mid \hat{V}_{\text{int}} \mid \Phi_{\alpha=1}\rangle
\end{aligned}$$

so that

$$2\langle\Phi|\hat{T}|\Phi\rangle = -\langle\Phi|\hat{V}_{\text{int}}|\Phi\rangle$$

which is the virial theorem.

The Hartree–Fock solution is *not* obtained by free variations according to the Rayleigh-Ritz principle, but by restricting the variations to Slater determinants. However, since the scale transformation maps Slater determinants back onto Slater determinants, we have again

$$2\langle\hat{T}\rangle_{\mathrm{HF}} = -\langle\hat{V}\rangle_{\mathrm{HF}}. \tag{7.9}$$

By using the relation equation (7.4) between the total energy and the single particle energies, we see that

$$\begin{aligned}\sum_{i=1}^{N}\epsilon_i - \langle V\rangle_{\mathrm{HF}} = E_{\mathrm{HF}} &= \langle T\rangle + \langle V\rangle_{\mathrm{HF}}\\ &= -\frac{1}{2}\langle V\rangle_{\mathrm{HF}} + \langle V\rangle_{\mathrm{HF}},\end{aligned}$$

which means that

$$\sum_{i=1}^{N}\epsilon_i = \frac{3}{2}\langle V\rangle_{\mathrm{HF}} = \frac{3\cdot 1}{2\cdot 2}\sum_{ij}\left(\langle ij|\hat{v}|ij\rangle - \langle ij|\hat{v}|ji\rangle\right).$$

We introduce average quantities

$$N\cdot\bar{\epsilon} = \frac{3}{4}N^2\overline{(\langle ij|\hat{v}|ij\rangle - \langle ij|\hat{v}|ji\rangle)}.$$

We have then shown that the difference between the matrix elements is proportional to $\bar{\epsilon}/N$.

We will close this section with a brief discussion of the so-called Hartree approximation, which is the historic predecessor of the Hartree–Fock approximation. In the Hartree approximation, one makes the *ansatz* of a product of different single particle orbitals for the wavefunction of the system:

$$\Phi_{\mathrm{H}}(x_1,\ldots,x_N) = \varphi_1(x_1)\cdot\ldots\cdot\varphi_N(x_N).$$

In this case one also begins with a model of non-interacting particles, but in the Hartree approximation one does not take into consideration the required antisymmetry of the wavefunction. If one varies the total energy obtained from this product-*ansatz* under the constraint that the single particle orbitals be normalized, the Hartree-equations are obtained:

$$\left(-\frac{\hbar^2\nabla^2}{2m} + u(x) + \sum_{\substack{\nu=1\\ \nu\neq\alpha}}^{N}\int \mathrm{d}y\varphi_\nu^*(y)\varphi_\nu(y)v(x,y)\right)\varphi_\alpha(x) = \epsilon_\alpha\varphi_\alpha(x). \tag{7.10}$$

The total energy corresponding to a self-consistent solution of this system of equations is

$$E_{\mathrm{H}} = \sum_{i=1}^{N} \epsilon_i - \frac{1}{2} \sum_{\substack{i,j=1 \\ i \neq j}}^{N} \langle ij|\hat{v}|ij\rangle .$$

The interaction energies, which are counted twice in the sum over the orbital energies, are subtracted out, just as in the Hartree–Fock energy (*cf.* equation (7.4)).

The effective Hartree potential differs from the Hartree–Fock potential in that it does not contain the exchange terms. Consequently, the Hartree potential is a *local* operator, which significantly facilitates solving equation (7.10) self-consistently compared to solving the Hartree–Fock equations (7.3). Moreover, the Hartree potential is different for each state. This property is not only physically wrong (it contradicts the indistinguishability of identical microscopic particles), but also complicates numerical solutions, since one must solve a different eigenvalue equation for each orbital. As a consequence, one cannot in general choose the Hartree orbitals to be orthogonal, since they originate from different eigenvalue problems.

In contrast to Φ_{H}, the Hartree–Fock wavefunction satisfies

$$\lim_{x_i \to x_j} \Phi_{\mathrm{HF}}(x_1, \ldots, x_i, \ldots, x_j, \ldots, x_N) = 0$$

since it is a Slater determinant. This is precisely the content of the Pauli principle, according to which two fermions with equal spin $s_i = s_j$ cannot be at the same position $\mathbf{r}_i = \mathbf{r}_j$. Hence, the motions of fermions with equal spin are correlated in the Hartree–Fock model, in contrast to the Hartree model. There is certainly no such restriction for two particles with different spin; their motions are largely uncorrelated. A repulsive particle–particle interaction, such as the Coulomb interaction, should make it unlikely that two particles come close to each other (even when they have opposite spin). On the basis of this fact, and because the Hartree–Fock energies are obtained from a variational principle they are too high . The difference between the exact ground state energy and the Hartree–Fock ground state energy has been given the name *correlation energy.* An important goal of this book is to develop systematic ways to calculate the correlation energy. However, we will first acquaint ourselves with another variation of the Hartree–Fock approximation, which is important for practical calculations.

Chapter 8

Restricted Hartree–Fock approximation and the symmetry dilemma

The Hamiltonian of a non-relativistic atom commutes with the operators for the square and z-component of both the total angular momentum and total spin of the system:

$$\left[\hat{H},\hat{L}^2\right] = \left[\hat{H},\hat{L}_z\right] = 0 = \left[\hat{H},\hat{S}^2\right] = \left[\hat{H},\hat{S}_z\right].$$

As a result, the exact solution of the many-particle Schrödinger equation must be simultaneous eigenfuctions of all these operators. The Hartree–Fock Hamiltonian, however, does not commute with any of these operators. Consequently, the solutions of the Hartree–Fock equations do not have proper symmetry.

The unrestricted variation of the Hartree–Fock *ansatz* led to single-particle orbitals of the form

$$\varphi_\nu(x) = \varphi_\nu^{(+)}(\mathbf{r}) \cdot \chi_+(s) + \varphi_\nu^{(-)}(\mathbf{r})\chi_-(s) \tag{8.1}$$

where χ_σ denote the Pauli spinors, equation (5.3). The simplest way to construct Hartree–Fock wavefunctions with better symmetry properties is to restrict the form of the single-particle orbitals from the beginning; for example

$$\begin{aligned} \varphi_\nu^{\mathrm{UHF}}(x) &= \varphi_\nu^{(+)}(\mathbf{r}) \cdot \chi_+(s) \quad \text{for } \nu = 1,\ldots,N_+ \\ \varphi_{(N_++\nu)}^{\mathrm{UHF}}(x) &= \varphi_{N_++\nu}^{(-)}(\mathbf{r}) \cdot \chi_-(s) \quad \text{for } \nu = 1,\ldots,N_- \end{aligned} \tag{8.2}$$

where $N_+ + N_- = N$ is the total number of particles. The orbitals selected in this way are eigenfunctions of the spin projection operators

$$\hat{s}_z \varphi_\nu^{\mathrm{UHF}}(x) = \begin{cases} +\frac{\hbar}{2}\varphi_\nu^{\mathrm{UHF}}(x) & \text{for } \nu = 1, \ldots, N_+ \\ -\frac{\hbar}{2}\varphi_\nu^{\mathrm{UHF}}(x) & \text{for } \nu = N_+ + 1, \ldots, N \end{cases}$$

so that we have for the corresponding Slater determinants Φ^{UHF}

$$\hat{S}_z \Phi^{\mathrm{UHF}}(x_1 \ldots x_N) = (N_+ - N_-)\frac{\hbar}{2}\Phi^{\mathrm{UHF}}(x_1 \ldots x_N).$$

If we vary the expectation value $\langle \Phi^{\mathrm{UHF}} \mid \hat{H} \mid \Phi^{\mathrm{UHF}} \rangle$ with respect to the single particle orbitals equation (8.2), we obtain a simplified self-consistent procedure. This commonly used, restricted procedure, is often referred to as *the* Hartree–Fock approximation. When necessary, the difference between this and other, further restricted procedures can be emphasized by calling it the 'unrestricted Hartree–Fock' (UHF). This terminology is somewhat misleading — the *ansatz* equation (8.2) is in fact already a restriction of the general Hartree–Fock orbitals in equation (8.1).

Since the UHF-equations are of such practical importance in calculations, we will now derive them for the case of spin-independent potentials. From equation (7.2) we have the expectation value of the energy:

$$\begin{aligned}
\langle \Phi^{\mathrm{UHF}} \mid \hat{H} \mid \Phi^{\mathrm{UHF}} \rangle &= \sum_{i=1}^{N} \int \mathrm{d}x\, \varphi_i^*(x) \left[-\frac{\hbar^2 \nabla^2}{2m} + u(\mathbf{r}) \right] \varphi_i(x) \\
&+ \frac{1}{2} \sum_{i,j=1}^{N} \int\!\!\int \mathrm{d}x \mathrm{d}x'\, \varphi_i^*(x)\varphi_j^*(x') v(\mathbf{r},\mathbf{r}')\varphi_i(x)\varphi_j(x') \\
&- \frac{1}{2} \sum_{i,j=1}^{N} \int\!\!\int \mathrm{d}x \mathrm{d}x'\, \varphi_i^*(x)\varphi_j^*(x') v(\mathbf{r},\mathbf{r}')\varphi_j(x)\varphi_i(x') \\
= &\int \mathrm{d}^3r \sum_s \sum_{i=1}^{N} \varphi_i^*(x) \left[-\frac{\hbar^2 \nabla^2}{2m} + u(\mathbf{r}) \right] \varphi_i(x) \\
&+ \frac{1}{2} \int \mathrm{d}^3r \int \mathrm{d}^3r' \left[\sum_s \sum_{i=1}^{N} \varphi_i^*(x)\varphi_i(x) \right] v(\mathbf{r},\mathbf{r}') \left[\sum_{s'} \sum_{j=1}^{N} \varphi_j^*(x')\varphi_j(x') \right] \\
&- \frac{1}{2} \int \mathrm{d}^3r \int \mathrm{d}^3r' \sum_{s,s'} \left[\sum_{i=1}^{N} \varphi_i^*(x)\varphi_i(x') \right] v(\mathbf{r},\mathbf{r}') \left[\sum_{j=1}^{N} \varphi_j^*(x')\varphi_j(x) \right].
\end{aligned}$$

If we insert the UHF *ansatz*, equation (8.2), into $\sum_{j=1}^{N} \varphi_j^*(x')\varphi_j(x)$ we obtain

$$\sum_{j=1}^{N_+} \varphi_j^{(+)}(\mathbf{r}')^* \varphi_j^{(+)}(\mathbf{r}) \chi_+^*(s')\chi_+(s)$$
$$+\sum_{j=1}^{N_-} \varphi_j^{(-)}(\mathbf{r}')^* \varphi_j^{(-)}(\mathbf{r}) \chi_-^*(s')\chi_-(s).$$

We define the spin-independent density matrix by

$$\rho^{(\pm)}(\mathbf{r},\mathbf{r}') \equiv \sum_{j=1}^{N_\pm} \varphi_j^{(\pm)}(\mathbf{r}')^* \varphi_j^{(\pm)}(\mathbf{r})$$

with diagonal elements

$$\rho^{(\pm)}(\mathbf{r}) \equiv \rho^{(\pm)}(\mathbf{r},\mathbf{r}')$$

the total density is, in terms of the density matrix,

$$\rho(\mathbf{r}) = \rho^{(+)}(\mathbf{r}) + \rho^{(-)}(\mathbf{r}).$$

If we also use $\sum_s \chi_\sigma(s)\chi_{\sigma'}(s) = \delta_{\sigma\sigma'}$, we finally arrive at

$$\begin{aligned}
\langle\Phi^{\mathrm{UHF}}|\hat{H}|\Phi^{\mathrm{UHF}}\rangle &= \sum_{j=1}^{N_+} \int \mathrm{d}^3r\, \varphi_j^{(+)}(\mathbf{r})^* \left[-\frac{\hbar^2\nabla^2}{2m}\right] \varphi_j^{(+)}(\mathbf{r}) \\
&+\sum_{j=1}^{N_-} \int \mathrm{d}^3r\, \varphi_j^{(-)}(\mathbf{r})^* \left[-\frac{\hbar^2\nabla^2}{2m}\right] \varphi_j^{(-)}(\mathbf{r}) \\
&+\int \mathrm{d}^3r\, \rho(\mathbf{r})u(\mathbf{r}) + \frac{1}{2}\int \mathrm{d}^3r \int \mathrm{d}^3r'\, \rho(\mathbf{r})v(\mathbf{r},\mathbf{r}')\rho(\mathbf{r}') \\
&-\frac{1}{2}\int \mathrm{d}^3r \int \mathrm{d}^3r' \Big[\rho^{(+)}(\mathbf{r},\mathbf{r}')v(\mathbf{r},\mathbf{r}')\rho^{(+)}(\mathbf{r}',\mathbf{r}) \\
&+ \rho^{(-)}(\mathbf{r},\mathbf{r}')v(\mathbf{r},\mathbf{r}')\rho^{(-)}(\mathbf{r}',\mathbf{r})\Big].
\end{aligned} \tag{8.3}$$

The structure of equation (8.3) shows that only interactions between particles with the same spins contribute to the exchange energy. In analogy with the derivation of the Hartree–Fock equations, equation (7.3), we vary equation (8.3) with respect to the functions $\varphi_j^{(+)}(\mathbf{r})$ and $\varphi_j^{(-)}(\mathbf{r})$, which depend only on position, to obtain the following coupled equations:

$$\begin{aligned}
&\left[-\frac{\hbar^2\nabla^2}{2m} + u(\mathbf{r}) + \int \rho(\mathbf{r}')v(\mathbf{r},\mathbf{r}')\mathrm{d}^3r\right]\varphi_j^{(+)}(\mathbf{r}) \\
&\qquad - \int \rho^{(+)}(\mathbf{r},\mathbf{r}')v(\mathbf{r},\mathbf{r}')\varphi_j^{(+)}(\mathbf{r}')\mathrm{d}^3r' \\
&\quad = \epsilon_j^{(+)}\varphi_j^{(+)}(\mathbf{r}),\ j = 1,\ldots,N_+ \\
&\left[-\frac{\hbar^2\nabla^2}{2m} + u(\mathbf{r}) + \int \rho(\mathbf{r}')v(\mathbf{r},\mathbf{r}')\mathrm{d}^3r'\right]\varphi_j^{(-)}(\mathbf{r}) \\
&\qquad - \int \rho^{(-)}(\mathbf{r},\mathbf{r}')v(\mathbf{r},\mathbf{r}')\varphi_j^{(-)}(\mathbf{r}')\mathrm{d}^3r' \\
&\quad = \epsilon_j^{(-)}\varphi_j^{(-)}(\mathbf{r}),\ j = 1,\ldots,N_-. \qquad (8.4)
\end{aligned}$$

For atomic systems, these equation are explicitly

$$\begin{aligned}
&\left[-\frac{\hbar^2\nabla^2}{2m} - \frac{Ze^2}{|\mathbf{r}|} + e^2\int \frac{\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}\mathrm{d}^3r'\right]\varphi_j^{(\pm)}(\mathbf{r}) \\
&\qquad -e^2\int \frac{\rho^{(\pm)}(\mathbf{r},\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}\varphi_j^{(\pm)}(\mathbf{r}')\mathrm{d}^3r' = \epsilon^{(\pm)}\varphi_j^{(\pm)}(\mathbf{r}). \qquad (8.5)
\end{aligned}$$

The exchange term can be written formally as an electrostatic potential

$$-e^2\int \frac{\rho^{(\pm)}(\mathbf{r},\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}\varphi_j^{(\pm)}(\mathbf{r}')\mathrm{d}^3r' = -e^2\int \frac{\rho_{\mathbf{r},j}^{(\pm)}(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}\mathrm{d}^3r'\varphi_j^{(\pm)}(\mathbf{r})$$

which is the result of a fictitious 'exchange charge density'

$$\rho_{\mathbf{r},j}^{(\pm)}(\mathbf{r}') = \frac{\varphi_j^{(\pm)}(\mathbf{r}')\rho^{(\pm)}(\mathbf{r},\mathbf{r}')}{\varphi_j^{(\pm)}(\mathbf{r})}.$$

The form of this exchange charge density depends on the position **r** of each electron on which it acts, as well as on the state j and spin of each electron. The total charge of this exchange charge density is precisely one elementary charge (assuming that $\varphi_j^{(\pm)}$ is an occupied state):

$$\int \rho_{\mathbf{r},j}^{(\pm)}(\mathbf{r}')\mathrm{d}^3r' = \sum_{i=1}^{N_\pm}\underbrace{\int \varphi_j^{(\pm)}(\mathbf{r}')\varphi_i^{(\pm)}(\mathbf{r}')^*\mathrm{d}^3r'}_{=\delta_{ji}}\varphi_i^{(\pm)}(\mathbf{r})/\varphi_j^{(\pm)}(\mathbf{r}) = 1.$$

Therefore, each electron is in some sense surrounded by an 'exchange hole', which is an oppositely charged cloud with total charge $+e$. This exchange hole originates from the exchange with the polarization of the medium, *i.e.*, the repulsion betweeen electrons with the same spin.

At this point, we should recall equation (8.2), in which we assumed that the single-particle orbitals are eigenfunctions of the spin projection operator $\hat{s}_z$. If we further assume that angular momentum is a good quantum number,

$$\varphi_\nu(x) = R_{n_\nu}(r) Y_{\ell_\nu, m_\nu}(\theta, \varphi) \chi_{\sigma_\nu}(s)$$

we obtain the so-called 'restricted Hartree–Fock' (RHF) procedure. The solutions in this approximation usually have better symmetry properties. In our example, we have

$$\hat{\ell}_z \varphi_\nu(x) = \hbar m_\nu \varphi_\nu(x)$$

and thus

$$\hat{L}_z \Phi^{\mathrm{RHF}}(x_1, \ldots, x_N) = \hbar \left(\sum_\nu m_\nu \right) \Phi^{\mathrm{RHF}}(x_1, \ldots, x_N).$$

A particular variation is the so-called analytic Hartree–Fock or Hartree–Fock–Roothaan procedure. One starts with parametrized single-particle orbitals $\varphi_\nu(x; \alpha_1^{(\nu)}, \ldots, \alpha_M^{(\nu)})$ with known analytic forms. The optimal parameters are determined by setting the derivative of the energy expectation value with respect to the parameters equal to zero.

We should now emphasize that the ground state energy calculated with the restricted Hartree–Fock procedure increases as the restrictions on the single-particle orbitals becomes stronger. We encounter a fundamental problem: if the best possible ground state energy is sought, the Hartree–Fock orbitals should be *free* to vary; however, the resulting wavefunctions have poor symmetry properties. If the symmetry is improved by restricting the variation of the orbitals, the ground state energy increases. This fact is occasionally referred to as the 'symmetry dilemma' of the Hartree–Fock procedure. Projection methods offer a way out by selecting the solution which has minimal energy *and* correct symmetry properties from solutions of the free-variation Hartree–Fock procedure [2].

Chapter 9

Hartree–Fock for translationally invariant systems

We will show in this chapter that the self-consistent problem of the Hartree–Fock approximation can be solved trivially for translationally invariant systems. These are systems of infinite extent, where the external potential is constant and the particle–particle interaction only depends on the relative distance between the particles. The plane waves discussed in Chapter 5 are solutions of the Hartree–Fock equations (or more precisely, of the UHF equations) for such systems. We will prove this by showing that the matrix elements of the UHF operators (*cf.* equation (8.4))

$$\begin{aligned}\langle\beta|\hat{h}^{(+)}_{\mathrm{UHF}}|\alpha\rangle &= \int \mathrm{d}^3r\,\varphi^{(+)}_{\beta}(\mathbf{r})^*\left\{-\frac{\hbar^2\nabla^2}{2m}+u\right\}\varphi^{(+)}_{\alpha}(\mathbf{r})\\ &\quad+\int \mathrm{d}^3r\,\varphi^{(+)}_{\beta}(\mathbf{r})^*\int\rho(\mathbf{r}')v(\mathbf{r}-\mathbf{r}')\mathrm{d}^3r'\,\varphi^{(+)}_{\alpha}(\mathbf{r})\\ &\quad-\int \mathrm{d}^3r\,\varphi^{(+)}_{\beta}(\mathbf{r})^*\int\rho^{(+)}(\mathbf{r},\mathbf{r}')v(\mathbf{r}-\mathbf{r}')\varphi^{(+)}_{\alpha}(\mathbf{r}')\mathrm{d}^3r'\end{aligned}$$

and the corresponding matrix elements $\langle\beta\mid\hat{h}^{(-)}_{\mathrm{UHF}}\mid\alpha\rangle$ for particles with negative spin, are diagonal in the plane wave representation

$$\varphi^{(\pm)}_{\nu}(\mathbf{r})=\frac{1}{\sqrt{\Omega}}\mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}}.$$

We first show that the single-particle term is diagonal, and we will then show that the direct and the exchange terms are diagonal. With **k** replacing the index α, and $\mathbf{k}'$ the index β, we have

$$\begin{aligned}\int_\Omega \mathrm{d}^3r\, \frac{1}{\sqrt{\Omega}}\mathrm{e}^{-i\mathbf{k}'\cdot\mathbf{r}} \left[-\frac{\hbar^2\nabla^2}{2m}+u\right]\frac{1}{\sqrt{\Omega}}\mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}} \\ = \left[\frac{\hbar^2k^2}{2m}+u\right]\frac{1}{\Omega}\int_\Omega \mathrm{d}^3r\,\mathrm{e}^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}} \\ = \left[\frac{\hbar^2k^2}{2m}+u\right]\delta_{\mathbf{k},\mathbf{k}'},\end{aligned}$$

since $u(\mathbf{r})$ = constant. To calculate the direct term, we first evaluate the density

$$\begin{aligned}\rho(\mathbf{r}) &= \sum_{\nu=1}^{N_+}\varphi_\nu^{(+)}(\mathbf{r})^*\varphi_\nu^{(+)}(\mathbf{r})+\sum_{\mu=1}^{N_-}\varphi_\mu^{(-)}(\mathbf{r})^*\varphi_\mu^{(-)}(\mathbf{r}) \\ &= \sum_{\nu=1}^{N_+}\frac{1}{\Omega}+\sum_{\mu=1}^{N_-}\frac{1}{\Omega}=\frac{N_++N_-}{\Omega}=\frac{N}{\Omega}.\end{aligned}$$

We then insert this result in the direct term, which yields

$$\int \mathrm{d}^3r\,\frac{1}{\sqrt{\Omega}}\mathrm{e}^{-i\mathbf{k}'\cdot\mathbf{r}}\int\frac{N}{\Omega}\,v(\mathbf{r}-\mathbf{r}')\mathrm{d}^3r'\frac{1}{\sqrt{\Omega}}\mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}}$$

and expand the interaction potential in a Fourier series:

$$v(\mathbf{r}-\mathbf{r}')=\frac{1}{\Omega}\sum_{\mathbf{q}}v_{\mathbf{q}}\,\mathrm{e}^{i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')}.$$

The direct term then becomes

$$\begin{aligned}&\sum_{\mathbf{q}}v_{\mathbf{q}}\frac{N}{\Omega^3}\int \mathrm{d}^3r\int \mathrm{d}^3r'\,\mathrm{e}^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}}\,\mathrm{e}^{i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')} \\ &= \sum_{\mathbf{q}}v_{\mathbf{q}}\frac{N}{\Omega^3}\int \mathrm{d}^3r'\,\mathrm{e}^{-i\mathbf{q}\cdot\mathbf{r}'}\int \mathrm{d}^3r\,\mathrm{e}^{i(\mathbf{q}+\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}} \\ &= \sum_{\mathbf{q}}v_{\mathbf{q}}\frac{N}{\Omega}\delta_{\mathbf{q},0}\,\delta_{(\mathbf{q}+\mathbf{k}),\mathbf{k}'}=\frac{N}{\Omega}\,v_{\mathbf{q}=0}\,\delta_{\mathbf{k},\mathbf{k}'}.\end{aligned}$$

Here we made use of the assumed translational invariance of the interaction potential, which allows for a simple Fourier series in $(\mathbf{r}-\mathbf{r}')$.

We now consider the exchange term. Let $\sum_{\tilde{\mathbf{k}}}^{+}$ denote the sum over all momenta $\tilde{\mathbf{k}}$ which are occupied by particles with positive spins, and $\sum_{\tilde{\mathbf{k}}}^{-}$ the corresponding sum over particles with negative spin. With this notation, the density matrix becomes

$$\rho^{(+)}(\mathbf{r},\mathbf{r}') = \sum_{\nu=1}^{N_+} \varphi_\nu^{(+)}(\mathbf{r}')^* \varphi_\nu^{(+)}(\mathbf{r}) = \frac{1}{\Omega}\sum_{\tilde{\mathbf{k}}}^{+} \mathrm{e}^{i\tilde{\mathbf{k}}\cdot(\mathbf{r}-\mathbf{r}')}.$$

Again, we expand the interaction potential in a Fourier series and obtain

$$\begin{aligned}
&\int \mathrm{d}^3r \int \mathrm{d}^3r' \, \frac{1}{\sqrt{\Omega}}\,\mathrm{e}^{-i\mathbf{k}'\cdot\mathbf{r}}\,\frac{1}{\Omega}\sum_{\tilde{\mathbf{k}}}^{+}\mathrm{e}^{i\tilde{\mathbf{k}}\cdot(\mathbf{r}-\mathbf{r}')}\,\frac{1}{\Omega}\sum_{\mathbf{q}} v_{\mathbf{q}}\,\mathrm{e}^{i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')}\,\frac{1}{\sqrt{\Omega}}\,\mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}'} \\
=\;& \sum_{\tilde{\mathbf{k}}}^{+}\sum_{\mathbf{q}} \frac{1}{\Omega^3}\underbrace{\int \mathrm{d}^3r'\,\mathrm{e}^{i(\mathbf{k}-\tilde{\mathbf{k}}-\mathbf{q})\cdot\mathbf{r}'}}_{=\Omega\delta_{\mathbf{q},(\mathbf{k}-\tilde{\mathbf{k}})}}\underbrace{\int \mathrm{d}^3r\,\mathrm{e}^{i(\mathbf{q}-\mathbf{k}'+\tilde{\mathbf{k}})\cdot\mathbf{r}}}_{=\Omega\delta_{\mathbf{q},(\mathbf{k}'-\tilde{\mathbf{k}})}} \\
=\;& \frac{1}{\Omega}\sum_{\tilde{\mathbf{k}}}^{+}\delta_{(\mathbf{k}-\tilde{\mathbf{k}}),(\mathbf{k}'-\tilde{\mathbf{k}})}\,v_{(\mathbf{k}-\tilde{\mathbf{k}})} = \frac{1}{\Omega}\sum_{\tilde{\mathbf{k}}}^{+} v_{(\mathbf{k}-\tilde{\mathbf{k}})}\,\delta_{\mathbf{k},\mathbf{k}'}
\end{aligned}$$

and the proof is complete.

The diagonal elements of the Hartree–Fock operators, which are the single-particle energies†, are given by

$$\epsilon_{\mathbf{k}}^{(\pm)} = \frac{\hbar^2k^2}{2m} + u + \frac{N}{\Omega}v_{\mathbf{q}=0} - \frac{1}{\Omega}\sum_{\tilde{\mathbf{k}}}^{(\pm)} v_{(\mathbf{k}-\tilde{\mathbf{k}})}.$$

For the total energy

$$E_{\mathrm{HF}} = \sum_{i=1}^{N}\langle i \mid \hat{t}+\hat{u} \mid i\rangle + \frac{1}{2}\sum_{\substack{i,j=1\\ i\neq j}}^{N}\left(\langle ij \mid \hat{v} \mid ij\rangle - \langle ij \mid \hat{v} \mid ji\rangle\right)$$

we obtain analogously

$$\begin{aligned}
E_{\mathrm{HF}} \;=\;& \sum_{\mathbf{k}}^{+}\left[\frac{\hbar^2k^2}{2m}\right] + \sum_{\mathbf{k}}^{-}\left[\frac{\hbar^2k^2}{2m}\right] + Nu + \frac{1}{2}N\frac{N}{\Omega}v_{\mathbf{q}=0} \\
& -\frac{1}{2\Omega}\sum_{\mathbf{k}}^{+}\sum_{\tilde{\mathbf{k}}}^{+} v_{(\mathbf{k}-\tilde{\mathbf{k}})} - \frac{1}{2\Omega}\sum_{\mathbf{k}}^{-}\sum_{\tilde{\mathbf{k}}}^{-} v_{(\mathbf{k}-\tilde{\mathbf{k}})}.
\end{aligned}$$

---

† The function ϵ_k is called the *dispersion relation.* This terminology is borrowed from optics, where one in general talks about dispersion relations whenever one is concerned with quantities that depend on wavelength.

The calculations show that the plane waves *always* satisfy the Hartree–Fock equations, completely independently of which momentum states are occupied and how many of the occupied states have negative and positive spins. This is very important. Since the Hartree–Fock equations only guarantee that the energy functional is stationary, the question arises for which occupations and, in particular, for which spin distributions the Hartree–Fock energy is *minimal.* A possible distribution can be obtained from the following prescription: put all N_+ particles with positive spins in the momentum space sphere $|\mathbf{k}| = 0, \ldots, k_+$, and correspondingly all N_- particles with negative spins in the momentum sphere $|\mathbf{k}| = 0, \ldots, k_-$ (see figure 9.1). If

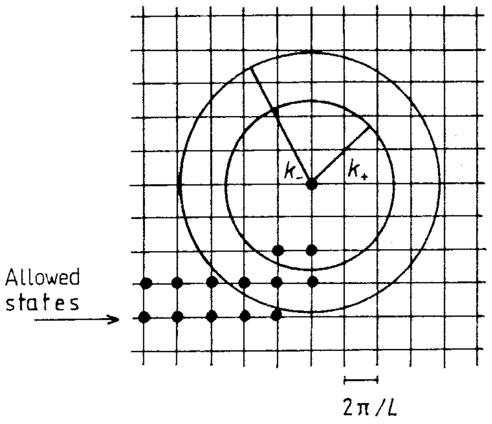


Figure 9.1 *All positive-spin state with $k < k_+$, and all negative-spin states with $k < k_-$ are occupied in the Hartree–Fock ground state.*

the Fourier transform of the particle–particle interaction depends only on $|\mathbf{q}|$ and is monotonically decreasing, this prescription is certain to produce the lowest possible Hartree–Fock energy for the given numbers N_+ and N_-, since by occupying the states in this way we will simultaneously obtain:

(1) the smallest possible kinetic energy, which is positive definite in E_{HF};

(2) the largest possible magnitude of the exchange energy, which is negative definite in E_{HF}. The magnitude of the exchange energy is made as large as possible since a sphere is certainly the geometrical object for which the sum of the distances between interior points are the smallest. In this way, the sum $\sum_{\mathbf{k},\tilde{\mathbf{k}}} v_{|\mathbf{k}-\tilde{\mathbf{k}}|}$ is maximized for monotonically decreasing functions v_q.

For this occupation of the states we have

$$\epsilon_{\mathbf{k}}^{\pm} = \frac{\hbar^2 k^2}{2m} + u + \frac{N}{\Omega} v_{\mathbf{q}=0} - \frac{1}{\Omega} \sum_{\widetilde{\mathbf{k}}=0}^{k_\pm} v_{(\mathbf{k}-\widetilde{\mathbf{k}})}$$

and

$$\begin{aligned} E_{\mathrm{HF}} \quad = \quad & \sum_{k=0}^{k_+} \frac{\hbar^2 k^2}{2m} + \sum_{k=0}^{k_-} \frac{\hbar^2 k^2}{2m} + N u + \frac{1}{2} N \frac{N}{\Omega} v_{\mathbf{q}=0} \\ & - \frac{1}{2\Omega} \sum_{k=0}^{k_+} \sum_{\widetilde{\mathbf{k}}=0}^{k_+} v_{(\mathbf{k}-\widetilde{\mathbf{k}})} - \frac{1}{2\Omega} \sum_{k=0}^{k_-} \sum_{\widetilde{\mathbf{k}}=0}^{k_-} v_{(\mathbf{k}-\widetilde{\mathbf{k}})} . \end{aligned}$$

For the explicit evaluation of these energies, we substitute the sums by integrals according to the prescription

$$\sum_{k=0}^{K} f(\mathbf{k}) \longrightarrow \frac{\Omega}{(2\pi)^3} \int^{K} \mathrm{d}^3 k \, f(\mathbf{k}) .$$

This approximation becomes exact in the thermodynamic limit, *i.e.*, for an infinitely large system. The approximation corresponds to the transition from Fourier series to Fourier integrals. The volume occupied in momentum space by each allowed state is precisely a box with sides $(2\pi/L)$ (see figure 9.1). Thus, each volume element d^3k in momentum space contains

$$\frac{\mathrm{d}^3 k}{\left[(2\pi)/L\right]^3} = \frac{\Omega}{(2\pi)^3} \mathrm{d}^3 k$$

states. This is the origin of the normalization factor of the momentum integral above.

The number of particles with positive and negative spins, respectively, are then obtained as

$$N_+ \quad = \quad \frac{\Omega}{(2\pi)^3} \int^{k_+} \mathrm{d}^3 k = \frac{\Omega}{(2\pi)^3} \cdot 4\pi \frac{k_+^3}{3} = \frac{\Omega}{2} \frac{k_+^3}{3\pi^2} \qquad (9.1)$$

$$\text{and } N_- \quad = \quad \frac{\Omega}{2} \frac{k_-^3}{3\pi^2} . \qquad (9.2)$$

The density of the system is

$$\frac{N}{\Omega} = \frac{N_+}{\Omega} + \frac{N_-}{\Omega} = \frac{1}{2} \frac{k_+^3}{3\pi^2} + \frac{1}{2} \frac{k_-^3}{3\pi^2} .$$

For unpolarized systems, *i.e.*, systems for which $N_+ = N_- = N/2$, which implies that $k_+ = k_- \equiv k_F$, we obtain the fundamental relation

$$\frac{N}{\Omega} = \frac{k_F^3}{3\pi^2}. \tag{9.3}$$

The momentum k_F of the occupied state with the highest energy is called the *Fermi momentum.*

The single-particle energies are obtained as

$$\epsilon_{\mathbf{k}}^{(\pm)} = \frac{\hbar^2 k^2}{2m} + u + \frac{N}{\Omega} v_{\mathbf{q}=0} - \int^{k_\pm} \frac{d^3\tilde{k}}{(2\pi)^3} v_{(\mathbf{k}-\tilde{\mathbf{k}})} \tag{9.4}$$

and the total Hartree–Fock energy becomes

$$\begin{aligned} E_{\mathrm{HF}} = {} & \Omega \int^{k_+} \frac{d^3k}{(2\pi)^3} \frac{\hbar^2 k^2}{2m} + \Omega \int^{k_-} \frac{d^3k}{(2\pi)^3} \frac{\hbar^2 k^2}{2m} + Nu + \frac{1}{2} N \frac{N}{\Omega} v_{\mathbf{q}=0} \\ & - \frac{\Omega}{2} \int^{k_+} \int^{k_+} \frac{d^3k}{(2\pi)^3} \frac{d^3\tilde{k}}{(2\pi)^3} v_{(\mathbf{k}-\tilde{\mathbf{k}})} - \frac{\Omega}{2} \int^{k_-} \int^{k_-} \frac{d^3k}{(2\pi)^3} \frac{d^3\tilde{k}}{(2\pi)^3} v_{(\mathbf{k}-\tilde{\mathbf{k}})}. \end{aligned}$$

We will now explicitly go to the thermodynamic limit, *i.e.*, we will let the volume Ω and the particle number N go to infinity in such a way that the densities (N_+/Ω) and (N_-/Ω) remain constant. The momenta

$$k_\pm = \left[6\pi^2 \frac{N_\pm}{\Omega} \right]^{1/3}$$

will then remain constant, and it is clear that all energy contributions to E_{HF} diverge in this limit. This is not surprising in view of the fact that the energy is an extensive quantity. Consequently, we will instead consider the Hartree–Fock energy per particle (or per unit volume). The kinetic energy contributions can be evaluated by elementary integration, which yields the following total contribution to the Hartree–Fock energy per particle:

$$\begin{aligned} \frac{E_{\mathrm{HF}}}{N} = {} & \frac{\hbar^2}{10m \cdot 2\pi^2} \frac{1}{(N/\Omega)} \left(k_+^5 + k_-^5 \right) + u + \frac{1}{2} \left[\frac{N}{\Omega} \right] v_{\mathbf{q}=0} \\ & - \frac{1}{2(N/\Omega)} \int^{k_+} \int^{k_+} \frac{d^3k}{(2\pi)^3} \frac{d^3\tilde{k}}{(2\pi)^3} v_{(\mathbf{k}-\tilde{\mathbf{k}})} \\ & - \frac{1}{2(N/\Omega)} \int^{k_-} \int^{k_-} \frac{d^3k}{(2\pi)^3} \frac{d^3\tilde{k}}{(2\pi)^3} v_{(\mathbf{k}-\tilde{\mathbf{k}})}. \end{aligned} \tag{9.5}$$

Chapter 10

The homogeneous electron gas in the Hartree–Fock approximation

We will in this chapter discuss the interacting homogeneous electron gas, also known as the free electron gas or the jellium model, as an example of a translationally invariant system. This particular system can be thought of as a model for many metals, if we assume that the charge density of the positive ions of the metal is uniformly smeared out over the volume of the system so that the electrons can move practically freely through the material. This drastic assumption can only be expected to hold in some sense when the electrons which are bound to the ionic cores form closed shells. The valence electrons are then only weakly bound and are therefore only weakly localized in the crystal lattice. Hence, the electron gas can be expected to give some reasonable results for the alkali metals, where the valence electrons indeed are bound very weakly. In fact, we can describe the cohesion of alkali metals rather well with the electron gas model in the Hartree–Fock approximation. (While the cohesive forces of an ionic crystal, such as NaCl, are the immediate result of the electrostatic attraction between the ions, the cohesion of an alkali metal cannot be understood so easily; it originates directly from the delocalization of the electrons, *i.e.*, from the fact that binding the valence electrons to 'many' ion cores yields a state of lower energy than the state consisting of separate atoms.)

The complete Hamiltonian for the electron gas is

$$\hat{H} = \hat{H}_{\mathrm{i}} + \hat{H}_{\mathrm{e}} + \hat{V}_{\mathrm{e-i}}.$$

Here $\hat{H}_{\mathrm{i}}$ is the electrostatic energy of the background ions:

$$\hat{H}_{\mathrm{i}} = \frac{e^2}{2}\int_{\Omega}\mathrm{d}^3R\int_{\Omega}\mathrm{d}^3R'\frac{\rho_i(\mathbf{R})\rho_i(\mathbf{R}')}{|\mathbf{R}-\mathbf{R}'|} = \frac{e^2}{2}\int_{\Omega}\mathrm{d}^3R\int_{\Omega}\mathrm{d}^3R'\frac{(N/\Omega)^2}{|\mathbf{R}-\mathbf{R}'|}$$

which is a simple constant. $\hat{H}_\mathrm{e}$ contains the kinetic energy of the electrons as well as their mutual Coulomb repulsion:

$$\hat{H}_\mathrm{e} = \sum_{i=1}^{N} \frac{\hat{p}_i^2}{2m} + \frac{1}{2} \sum_{\substack{i,j=1 \\ i\neq j}}^{N} \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|}$$

and $\hat{V}_\mathrm{e-i}$ is the interaction of the electrons with the background ions. Hence, $\hat{V}_\mathrm{e-i}$ corresponds to the external potential $\hat{U}$ in the previous notation:

$$\hat{U} \equiv \hat{V}_\mathrm{e-i} = -\sum_{i=1}^{N} \int_\Omega \mathrm{d}^3R \left[\frac{N}{\Omega}\right] \frac{e^2}{|\mathbf{r}_i - \mathbf{R}|}.$$

We take the system to be a cube of volume Ω. With the imposition of periodic boundary conditions we can expand the Coulomb potential in a Fourier series:

$$\frac{e^2}{|\mathbf{r} - \mathbf{r}'|} = \frac{1}{\Omega} \sum_{\mathbf{q}} v_\mathbf{q} e^{i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}')} \qquad (10.1)$$

with

$$v_\mathbf{q} = \int_\Omega \mathrm{d}^3R\, \mathrm{e}^{-i\mathbf{q}\cdot\mathbf{R}} \frac{e^2}{|\mathbf{R}|} = \begin{cases} \frac{4\pi e^2}{q^2} & \text{for } q \neq 0 \\ \int_\Omega \mathrm{d}^3R \frac{e^2}{|\mathbf{R}|} & \text{for } q = 0. \end{cases}$$

Using equation (10.1), we can write $\hat{U}$ as

$$\begin{aligned} \hat{U} = \hat{V}_\mathrm{e-i} &= -\sum_{i=1}^{N} \int_\Omega \mathrm{d}^3R \left[\frac{N}{\Omega}\right] \frac{1}{\Omega} \left[\sum_{q\neq 0} \frac{4\pi e^2}{q^2} \mathrm{e}^{i\mathbf{q}\cdot(\mathbf{r}_i-\mathbf{R})} + \int_\Omega \mathrm{d}^3X \frac{e^2}{|\mathbf{X}|}\right] \\ &= -\left[\frac{N}{\Omega}\right] \frac{1}{\Omega} \sum_{i=1}^{N} \left[\underbrace{\sum_{q\neq 0} \frac{4\pi e^2}{q^2} \underbrace{\int_\Omega \mathrm{d}^3R\, \mathrm{e}^{i\mathbf{q}\cdot(\mathbf{r}_i-\mathbf{R})}}_{=\Omega\delta_{\mathbf{q},0}}}_{=0} + \underbrace{\int_\Omega \mathrm{d}^3R}_{=\Omega} \int_\Omega \mathrm{d}^3X \frac{e^2}{|\mathbf{X}|} \right] \\ &= -N \left[\frac{N}{\Omega}\right] \int_\Omega \mathrm{d}^3X \frac{e^2}{|\mathbf{X}|}. \end{aligned} \qquad (10.2)$$

The fact that we here obtain a constant potential is a result of the artificially imposed periodicity of the problem; we have to a certain extent solved the Poisson equation with periodic boundary conditions.

If we use equation (9.4) for the Hartree–Fock single-particle energies, the external potential

$$u = U/N = -(N/\Omega)\int_\Omega \mathrm{d}^3X\,\frac{e^2}{|\mathbf{X}|}$$

exactly cancels the direct term $(N/\Omega)v_{q=0}$. As a result, the single-particle energies become

$$\epsilon_{\mathbf{k}}^{(\pm)} = \frac{\hbar^2k^2}{2m} - \int^{k_\pm}\frac{\mathrm{d}^3k'}{(2\pi)^3}\,\frac{4\pi e^2}{|\mathbf{k}-\mathbf{k}'|^2}.$$

The constant energy contribution H_i from the ionic background must be included in the calculation of the total energy. Because of the imposed periodicity, we obtain after the substitution $\mathbf{X}\equiv\mathbf{R}-\mathbf{R}'$ the result

$$\begin{aligned} H_\mathrm{i} &= \frac{1}{2}\left[\frac{N}{\Omega}\right]^2\int_\Omega \mathrm{d}^3R\int_\Omega \mathrm{d}^3R'\,\frac{e^2}{|\mathbf{R}-\mathbf{R}'|}\\ &= \frac{1}{2}\left[\frac{N}{\Omega}\right]^2\underbrace{\int_\Omega \mathrm{d}^3R}_{=\Omega}\int_\Omega \mathrm{d}^3X\,\frac{e^2}{|\mathbf{X}|}\\ &= \frac{1}{2}N\left[\frac{N}{\Omega}\right]\int \mathrm{d}^3X\,\frac{e^2}{|\mathbf{X}|}. \end{aligned} \tag{10.3}$$

If we now use equation (9.5) for the Hartree–Fock energy per particle, the constant term u and $\frac{1}{2}\left(\frac{N}{\Omega}\right)v_{\mathrm{q}=0}$ exactly cancel the contribution from the positive background, so that we obtain in total:

$$\begin{aligned} E_\mathrm{HF}^{\mathrm{e-gas}}/N &= H_\mathrm{i}/N + E_\mathrm{HF}/N\\ &= \frac{\hbar^2}{10m2\pi^2}\frac{1}{(N/\Omega)}\left(k_+^5+k_-^5\right)\\ &\quad -\frac{1}{2(N/\Omega)}\int_0^{k_+}\int_0^{k_+}\frac{\mathrm{d}^3k}{(2\pi)^3}\frac{\mathrm{d}^3k'}{(2\pi)^3}\frac{4\pi e^2}{|\mathbf{k}-\mathbf{k}'|^2}\\ &\quad -\frac{1}{2(N/\Omega)}\int_0^{k_-}\int_0^{k_-}\frac{\mathrm{d}^3k}{(2\pi)^3}\frac{\mathrm{d}^3k'}{(2\pi)^3}\frac{4\pi e^2}{|\mathbf{k}-\mathbf{k}'|^2}. \end{aligned}$$

We briefly indicate how to calculate the exchange integrals. We take the z-axis in the integration over $\mathbf{k}'$ to be parallel to $\mathbf{k}$. Thus

$$|\mathbf{k}-\mathbf{k}'|^2 = (\mathbf{k}-\mathbf{k}')\cdot(\mathbf{k}-\mathbf{k}') = k^2 + k'^2 - 2kk'\cos\theta$$

where θ is the angle between $\mathbf{k}'$ and $\mathbf{k}$. With this inserted in the exchange integrals, we obtain

$$\begin{aligned}
&\frac{4\pi e^2}{(2\pi)^3}\int_0^{k_\pm} \mathrm{d}^3k' \frac{1}{|\mathbf{k}-\mathbf{k}'|^2} \\
&= \frac{4\pi e^2}{(2\pi)^3}\int_0^{k_\pm} k'^2\mathrm{d}k' \int_0^{\pi}\int_0^{2\pi} \frac{\sin\theta \mathrm{d}\theta \mathrm{d}\phi}{k^2+k'^2-2kk'\cos\theta}.
\end{aligned}$$

With the variable substitution $x \equiv \cos\theta$, this expression becomes

$$\begin{aligned}
&2\pi\frac{4\pi e^2}{(2\pi)^3}\int_0^{k_\pm} k'^2\mathrm{d}k' \int_{-1}^{1} \frac{\mathrm{d}x}{k^2+k'^2-2kk'x} \\
&= \frac{e^2}{\pi}\int_0^{k_\pm} \mathrm{d}k' \frac{k'}{k}\ln\left|\frac{k+k'}{k-k'}\right|.
\end{aligned}$$

This integral can be evaluated by elementary methods. With the result for the exchange integral we finally obtain for the single-particle energy:

$$\epsilon_k^{\pm} = \frac{\hbar^2k^2}{2m} - \frac{e^2}{\pi}\left[k_\pm + \frac{1}{2k}\left(k_\pm^2 - k^2\right)\ln\left|\frac{k_\pm+k}{k_\pm-k}\right|\right].$$

In order to calculate the exchange-contribution to the total energy per particle, we must perform one additional one-dimensional integration over k. This integral is also an elementary integral. The final result is

$$\begin{aligned}
E_{\mathrm{HF}}^{\mathrm{e-gas}}/N &= \frac{\hbar^2}{10m2\pi^2}\frac{1}{(N/\Omega)}\left(k_+^5 + k_-^5\right) \\
&\quad -\frac{e^2}{(2\pi)^3}\frac{1}{(N/\Omega)}\left(k_+^4 + k_-^4\right). \qquad (10.4)
\end{aligned}$$

We obtain a frequently used representation of the Hartree–Fock energy per particle by expressing the Fermi momenta k_+ and k_- in terms of the density

$$n \equiv \frac{N}{\Omega}$$

and the magnetization, or spin-polarization

$$\xi \equiv \frac{N_+ - N_-}{N}.$$

An unpolarized system then corresponds to the special case $\xi = 0$, whereas for $\xi = \pm 1$ we have a totally polarized ('ferromagnetic') system. From $N_- = N - N_+$, so that $\xi = \frac{2N_+ - N}{N}$, it follows that

$$\begin{aligned}
N_+ &= (1+\xi)N/2 \\
N_- &= (1-\xi)N/2
\end{aligned}$$

so that from equations (9.1) and (9.2) we obtain

$$k_{\pm} = \left[6\pi^2 N_{\pm}/\Omega\right]^{1/3} = \left[3\pi^2 \left(\frac{N}{\Omega}\right)(1 \pm \xi)\right]^{1/3} = \left(3\pi^2 n\right)^{1/3} (1 \pm \xi)^{1/3}.$$

If we insert this expression in equation (10.4), we obtain

$$\begin{aligned} E_{\mathrm{HF}}^{\mathrm{e-gas}}/N &= \frac{\hbar^2}{m}\frac{3}{10}\left(3\pi^2 n\right)^{2/3}\frac{1}{2}\left[(1+\xi)^{5/3} + (1-\xi)^{5/3}\right] \\ &\quad -e^2\frac{3}{4\pi}\left(3\pi^2 n\right)^{1/3}\frac{1}{2}\left[(1+\xi)^{4/3} + (1-\xi)^{4/3}\right]. \end{aligned} \tag{10.5}$$

We obtain another representation of this result if, instead of expressing the energy per particle as a function of density, we express it as a function of the so-called *Wigner–Seitz radius* r_s. This quantity is defined as the radius of the sphere that contains the volume per particle of the system:

$$\frac{\Omega}{N} = \frac{1}{n} = \frac{4\pi}{3} r_s^3. \tag{10.6}$$

If we use this definition in equation (10.5) and furthermore express all lengths in units of the Bohr radius $a_0 = \hbar^2/(me^2)$, we obtain

$$\begin{aligned} E_{\mathrm{HF}}^{\mathrm{e-gas}}/N &= \frac{e^2}{2a_0}\left\{\frac{2.21}{r_s^2}\frac{1}{2}\left[(1+\xi)^{5/3} + (1-\xi)^{5/3}\right]\right. \\ &\quad \left. -\frac{0.916}{r_s}\frac{1}{2}\left[(1+\xi)^{4/3} + (1-\xi)^{5/3}\right]\right\}. \end{aligned} \tag{10.7}$$

From this general formula we can, among other things, conclude that the Hartree–Fock energy for the unpolarized electron gas is

$$E_{\mathrm{HF}}^{\mathrm{e-gas}}(\xi = 0)/N = \frac{e^2}{2a_0}\left[\frac{2.21}{r_s^2} - \frac{0.916}{r_s}\right] \tag{10.8}$$

and that for the completely polarized electron gas we have

$$E_{\mathrm{HF}}^{\mathrm{e-gas}}(\xi = 1)/N < E_{\mathrm{HF}}^{\mathrm{e-gas}}(\xi = 0)/N$$

when r_s is larger than $5.45a_0$. Hence, we should in this case expect a phase transition to a ferromagnetic state. Unfortunately, there are no metals with densities this low, so we cannot expect to observe such a phase transition. Nevertheless, the electron gas model yields the correct result that the alkali metals, for which the model was originally constructed, are not ferromagnetic. Ferromagnetism in other, more complex materials, is a very complicated phenomenon.

If we plot the energy per particle (for an unpolarized system) against r_s, we obtain the picture shown in figure 10.1.

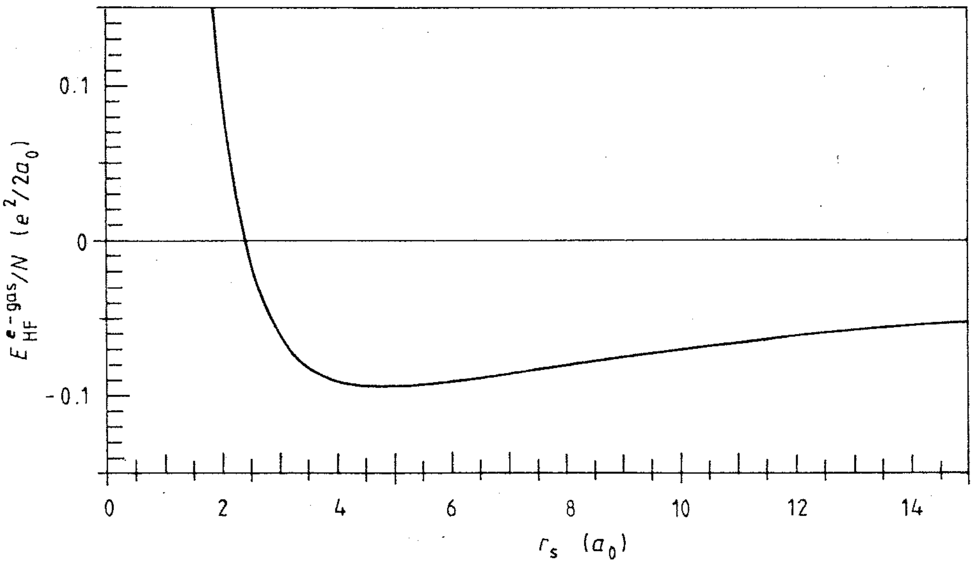


Figure 10.1 *Ground state energy of the homogeneous electron gas in the Hartree–Fock approximation plotted against r_s.*

Since on the one hand the Hartree–Fock energy is less than zero, and on the other hand is an upper bound for the exact ground state energy, we have proved that the system is bound. Thus, we have found a model for the cohesion of alkali metals. The theoretically calculated values

$$(E_{\mathrm{HF}}^{\mathrm{e-gas}}/N)^{\mathrm{min}} = -1.29\,\mathrm{eV}, \quad r_s^{\mathrm{min}} = 4.83a_0$$

agrees surprisingly well with experiments, which, for example for sodium give

$$(E_{\mathrm{HF}}^{\mathrm{e-gas}}/N)_{\mathrm{Na}}^{\mathrm{exp}} = -1.13\,\mathrm{eV}, \quad r_s^{\mathrm{exp}} = 3.96a_0.$$

In Chapter 7 we showed that the Hartree–Fock energy corresponds to first order perturbation theory

$$E_{\mathrm{HF}} = E^{(0)} + E^{(1)} = \langle \Phi \mid \hat{H}_0 \mid \Phi \rangle + \langle \Phi \mid \hat{H}' \mid \Phi \rangle \tag{10.9}$$

when the difference between the exact Hamiltonian and the Hartree–Fock operator is treated as the perturbation:

$$\hat{H}_0 = \hat{H}_{\mathrm{HF}}, \quad \text{and} \quad \hat{H}' = \hat{H} - \hat{H}_{\mathrm{HF}} = \hat{V} - \sum_i \hat{f}_i.$$

In a translationally invariant system in the present sense, equation (10.9) also holds for the partition

$$\hat{H}_0 = \sum_i \frac{\hat{p}_i^2}{2m}, \quad \text{and} \quad \hat{H}' = \hat{V},$$

in which the entire particle–particle interaction is regarded as a perturbation. Even if this assertion is quite obvious in view of the discussion above, we will now explicitly go through the calculation for the electron gas. To do that, we use the representation equation (5.6) of the Hamiltonian in second quantization with Fourier components of the Coulomb potential given by equation (10.1):

$$\begin{aligned}\hat{H} &= \hat{H}_{\mathrm{i}} + \hat{V}_{\mathrm{e-i}} + \hat{H}_{\mathrm{e}} \\ &= \hat{H}_{\mathrm{i}} + \hat{V}_{\mathrm{e-i}} + \sum_{\mathbf{k},\sigma} \frac{\hbar^2 k^2}{2m} \hat{c}^{\dagger}_{\mathbf{k}\sigma}\hat{c}_{\mathbf{k}\sigma} + \frac{1}{2\Omega}\left(N^2 - N\right) v_{\mathbf{q}=0} \\ &\quad + \frac{1}{2\Omega} \sum_{\mathbf{q}\neq 0} \sum_{\mathbf{k}\sigma} \sum_{\mathbf{k}'\sigma'} \frac{4\pi e^2}{q^2} \hat{c}^{\dagger}_{(\mathbf{k}+\mathbf{q}),\sigma} \hat{c}^{\dagger}_{(\mathbf{k}'-\mathbf{q}),\sigma'} \hat{c}_{\mathbf{k}',\sigma'} \hat{c}_{\mathbf{k},\sigma}.\end{aligned}$$

The contribution from the Fourier component $v_{\mathbf{q}=0}$ will be calculated separately by using the fermion anti-commutation relations, equation (2.4). The constant terms $\hat{H}_{\mathrm{i}}$, $\hat{V}_{\mathrm{e-i}}$ and $N^2/(2\Omega)v_{\mathbf{q}=0}$ cancel mutually (*cf.* equations (10.1), (10.2) and (10.3)). The remaining constant expression

$$-\frac{N}{2\Omega} v_{\mathbf{q}=0} = -\frac{N}{2\Omega} \int_{\Omega} \mathrm{d}^3 R \frac{e^2}{|\mathbf{R}|}$$

can be neglected in the thermodynamic limit. To show this, we transform the integral to an integral over the unit cube through the change of scale given by $R^{\mathrm{new}} = R^{\mathrm{old}}/L$. The result is

$$-\frac{N}{2\Omega} v_{\mathbf{q}=0} = -\frac{N}{2\Omega} L^2 \int_{-1}^{1} \mathrm{d}^3 R \frac{e^2}{|\mathbf{R}|} = -\frac{cN}{2\Omega^{1/3}}$$

where c is a constant which does not depend on volume. The corresponding energy contribution *per particle* will thus vanish as $\Omega^{-1/3}$ in the thermodynamic limit.

In all, we are then left with

$$\hat{H} = \sum_{\mathbf{k},\sigma} \frac{\hbar^2 k^2}{2m} \hat{c}^{\dagger}_{\mathbf{k},\sigma}\hat{c}_{\mathbf{k},\sigma} + \frac{1}{2\Omega} \sum_{\substack{\mathbf{k},\sigma \\ \mathbf{k}',\sigma'}} \sum_{\mathbf{q}\neq 0} \frac{4\pi e^2}{q^2} \hat{c}^{\dagger}_{(\mathbf{k}+\mathbf{q}),\sigma} \hat{c}^{\dagger}_{(\mathbf{k}'-\mathbf{q}),\sigma'} \hat{c}_{\mathbf{k}',\sigma} \hat{c}_{\mathbf{k},\sigma}. \tag{10.10}$$

We will now use this representation of the Hamiltonian to prove the statement that we made above: the Hartree–Fock energy of the electron gas corresponds precisely to the zeroth and first order terms in perturbation theory, if the entire interaction is regarded as a perturbation. Since the zeroth order terms immediately give us the kinetic energy of the electron gas, we only need to show that the first-order matrix elements

$$E^{(1)} = \frac{1}{2\Omega} \sum_{\substack{\mathbf{k},\sigma \\ \mathbf{k}',\sigma'}} \sum_{\mathbf{q}\neq 0} \frac{4\pi e^2}{q^2} \langle \Phi \mid \hat{c}^{\dagger}_{(\mathbf{k}+\mathbf{q}),\sigma} \hat{c}^{\dagger}_{(\mathbf{k}'-\mathbf{q}),\sigma'} \hat{c}_{\mathbf{k}',\sigma} \hat{c}_{\mathbf{k},\sigma} \mid \Phi \rangle$$

of the ground state Slater determinant $\mid \Phi\rangle$ precisely yield the exchange term, which we calculated above, of the Hartree–Fock energy. The occurring matrix elements can only be non-zero when the created states are the same as the annihilated ones, *i.e.*, when either

$$(\mathbf{k}+\mathbf{q},\sigma) = (\mathbf{k}',\sigma') \quad \text{and} \quad (\mathbf{k}'-\mathbf{q},\sigma') = (\mathbf{k},\sigma)$$

or when

$$(\mathbf{k}+\mathbf{q},\sigma) = (\mathbf{k},\sigma) \quad \text{and} \quad (\mathbf{k}'-\mathbf{q},\sigma') = (\mathbf{k}',\sigma').$$

The second possibility is ruled out, since it is equivalent to $\mathbf{q} = 0$ and was already excluded from the sum. The matrix element is then only non-zero when $\mathbf{q} = \mathbf{k}' - \mathbf{k}$ and $\sigma = \sigma'$. We can then write

$$\begin{aligned} &\langle \Phi \mid \hat{c}^\dagger_{(\mathbf{k}+\mathbf{q}),\sigma} \hat{c}^\dagger_{(\mathbf{k}'-\mathbf{q}),\sigma'} \hat{c}_{\mathbf{k}',\sigma'} \hat{c}_{\mathbf{k},\sigma} \mid \Phi\rangle \\ = \;& \delta_{\mathbf{q},(\mathbf{k}'-\mathbf{k})} \delta_{\sigma,\sigma'} \langle \Phi \mid \hat{c}^\dagger_{\mathbf{k}',\sigma} \hat{c}^\dagger_{\mathbf{k},\sigma} \hat{c}_{\mathbf{k}'\sigma} \hat{c}_{\mathbf{k},\sigma} \mid \Phi\rangle. \end{aligned}$$

Because $\mathbf{q} \neq 0$ and $\mathbf{k}' = \mathbf{k} + \mathbf{q}$, we always have that $\mathbf{k}' \neq \mathbf{k}$, and we can anti-commute the two operators in the middle to obtain

$$-\delta_{\mathbf{q},(\mathbf{k}'-\mathbf{k})} \delta_{\sigma,\sigma'} \langle \Phi \mid \hat{c}^\dagger_{\mathbf{k}',\sigma} \hat{c}_{\mathbf{k}',\sigma} \hat{c}^\dagger_{\mathbf{k},\sigma} \hat{c}_{\mathbf{k},\sigma} \mid \Phi\rangle = -\delta_{\mathbf{q},(\mathbf{k}'-\mathbf{k})} \delta_{\sigma,\sigma'} n_{\mathbf{k}'\sigma} n_{\mathbf{k}\sigma}.$$

Thus, we have the first order energy contribution

$$E^{(1)} = -\frac{1}{2\Omega} \sum_{\sigma} \sum_{\mathbf{k},\mathbf{k}'} \frac{4\pi e^2}{|\mathbf{k}-\mathbf{k}'|^2} n_{\mathbf{k},\sigma} n_{\mathbf{k}'\sigma}.$$

If we now choose the ground state occupation we discussed previously, namely

$$n_{\widetilde{\mathbf{k}}\sigma} = \begin{cases} \theta(k_+ - \widetilde{k}) & \text{for } \sigma = \text{`}+\text{'} \\ \theta(k_- - \widetilde{k}) & \text{for } \sigma = \text{`}-\text{'} \end{cases}$$

we immediately obtain the previous exchange term

$$E^{(1)} = -\frac{1}{2\Omega} \sum_{\mathbf{k}=0}^{k_+} \sum_{\mathbf{k}'=0}^{k_+} \frac{4\pi e^2}{|\mathbf{k}-\mathbf{k}'|^2} - \frac{1}{2\Omega} \sum_{\mathbf{k}=0}^{k_-} \sum_{\mathbf{k}'=0}^{k_-} \frac{4\pi e^2}{|\mathbf{k}-\mathbf{k}'|^2}$$

which was what we wanted to prove.

At this point the question arises as to whether we can obtain parts of the correlation energy in the same way by including higher order terms in the perturbation expansion. The question can indeed in principle be answered with a yes, but the calculation is anything but simple. It turns out that every order in perturbation theory beyond the present one diverges. Only the summation of the entire perturbation series, or at least infinite sub-series, which is possible for the limiting case of $r_s \to 0$ by diagrammatical methods, leaves a finite, sensible result. It is possible to overcome these problems, but only at a great effort until we have had a detailed discussion of Feynman diagrams. We will first discuss another possible way of considering at least a part of the correlation energy. This possibility comes from the observation that the main reason for the divergence of the higher order perturbation terms originates in the long-range tail of the Coulomb potential. Hence, one thing that seems natural to do is to divide the total Coulomb interaction into a short-range and a long-range part. We can then calculate the correlation energy of the short-range part by, for example, perturbation theory, since this part should not give rise to divergent expressions. However, a non-perturbative approach (or infinite order summation) is required to calculate the long-range correlation energy. The division into a long-range and a short-range part can be done in the following way:

$$\hat{H} = \sum_i \frac{\hat{p}_i^2}{2m} + \frac{1}{2}\sum_{i\neq j}\sum_{\mathbf{k}\neq 0} \frac{4\pi e^2}{\Omega k^2} \mathrm{e}^{i\mathbf{k}\cdot(\mathbf{r}_i-\mathbf{r}_j)} = \sum_i \frac{\hat{p}_i^2}{2m} + \hat{V}_{\mathrm{sr}} + \hat{V}_{\mathrm{lr}}$$

where

$$\hat{V}_{\mathrm{sr}} = \frac{1}{2}\sum_{i\neq j}\sum_{k>k_c} \frac{4\pi e^2}{\Omega k^2} \mathrm{e}^{i\mathbf{k}\cdot(\mathbf{r}_i-\mathbf{r}_j)} \tag{10.11}$$

and

$$\hat{V}_{\mathrm{lr}} = \frac{1}{2}\sum_{i\neq j}\sum_{\substack{k\leq k_c\\ k\neq 0}} \frac{4\pi e^2}{\Omega k^2} \mathrm{e}^{i\mathbf{k}\cdot(\mathbf{r}_i-\mathbf{r}_j)}. \tag{10.12}$$

Here the limiting momentum k_c is a suitably chosen constant. We will return later to how to determine this constant. The Fourier transform of $\hat{V}_{\mathrm{sr}}$

$$\sum_{k>k_c} \frac{4\pi/\Omega}{k^2} \mathrm{e}^{i\mathbf{k}\cdot(\mathbf{r}_i-\mathbf{r}_j)} = \frac{F(k_c|\mathbf{r}_i - \mathbf{r}_j|)}{|\mathbf{r}_i - \mathbf{r}_j|}$$

where

$$F(y) = 1 - \frac{2}{\pi}\int_0^y \frac{\sin(x)}{x}\mathrm{d}x = 1 - \frac{2}{\pi}\mathrm{Si}(y)$$

shows that $\hat{V}_{sr}$ indeed is a short-range potential: it follows from the properties of the sine-integral, $\mathrm{Si}(x)$, that for large y this function tends to zero in an oscillatory fashion and that the function value $F(0)$ is unity. Thus, we obtain a reasonable screened Coulomb potential in this case.

The long-range part, which is just the difference between the exact Coulomb potential and the the short-range part $\hat{V}_{\mathrm{sr}}$, *i.e.*

$$\hat{V}_{\mathrm{lr}} = \frac{(2/\pi)\mathrm{Si}(k_c|\mathbf{r}_i - \mathbf{r}_j|)}{|\mathbf{r}_i - \mathbf{r}_j|}$$

is finite for $\mathbf{r}_i - \mathbf{r}_j = 0$, where it assumes the value $(2/\pi)k_c$.

We conclude this chapter by stating the result for the short-range correlation energy from second-order perturbation theory. We have to calculate

$$E_{\text{corr}}^{(\text{sr})} = -\sum_n \frac{\left|\langle \Phi_n \mid \hat{V}_{\text{sr}} \mid \Phi_0\rangle\right|^2}{E_n - E_0}.$$

what about divergences?

Here Φ_0 is the Slater determinant of plane waves in the ground state occupation and E_0 is the corresponding kinetic energy (the expectation value of $\hat{H}_0$). The summation runs in principle over the complete system of all configurations Φ_n, which can be constructed from plane waves. However, the matrix element

$$\begin{aligned}&\langle \Phi_n \mid \hat{V}_{\text{sr}} \mid \Phi_0\rangle \\ &= \frac{1}{2\Omega}\sum_{\substack{\mathbf{p}\sigma\\ \mathbf{p}'\sigma'}}\sum_{k>k_c}\frac{4\pi e^2}{k^2}\langle \Phi_n \mid \hat{c}^\dagger_{(\mathbf{p}+\mathbf{k})\sigma}\hat{c}^\dagger_{(\mathbf{p}'-\mathbf{k})\sigma'}\hat{c}_{\mathbf{p}'\sigma'}\hat{c}_{\mathbf{p}\sigma} \mid \Phi_0\rangle\end{aligned}$$

vanishes whenever Φ_n differs from Φ_0 in more than the configuration of two orbitals. This reduces drastically the number of terms in the sum. The remaining terms can be integrated approximately (see Raimes [3]). The dominant contributions in (k_c/k_F) are

$$E_{\text{corr}}^{\text{sr}}/N = \left[\frac{2}{\pi}(1-\ln 2)\ln(k_c/k_F)^2\right]\frac{e^2}{2a_0} + C. \tag{10.13}$$

We give a heuristic estimate due to Raimes [3] for the constant C

$$C = -0.0095\frac{e^2}{2a_0}.$$

So long as the value of k_c is not determined, this result is not very useful. The final determination of k_c will be carried out in the next chapter, where we will discuss the long-range correlation in terms of plasma oscillations.

Chapter 11

Long-range correlations in the electron-gas: plasmons

A gas of charged particles, which move against the background of oppositely charged particles, is called a neutral plasma. It is known from classical physics, for example from gas discharge tubes, that such systems can exhibit collective density oscillations, so-called plasma oscillations. The fundamental frequency of such oscillations can easily be derived from classical considerations: let us assume that we displace a part of the total charge a distance $\mathbf{x}$. If n is the particle density of these charges, a polarization

$$\mathbf{P} = ne\mathbf{x}$$

will arise. This polarization will in its turn give rise to an electric field

$$\mathbf{E} = -4\pi\mathbf{P}.$$

This field acts as a restoring force $e\mathbf{E}$ on the displaced charges. Their motion can then be described by Newton's equation

$$m\ddot{\mathbf{x}} = -4\pi ne^2\mathbf{x}.$$

This is the equation of a harmonic oscillator with the frequency

$$\omega_p = \sqrt{\frac{4\pi e^2 n}{m}} \tag{11.1}$$

which is generally called the *plasma frequency*.

One would then expect that the electron gas in metals can also display such plasma oscillations, and there is indeed clear experimental evidence for this: if the metal is bombarded with electrons of a fixed energy, the energy loss spectrum, *i.e.*, the fraction $N(\Delta E)/N$ of the electrons which have lost an energy ΔE, will show clear maxima at integer multiples of $\hbar\omega_p$. These electrons have excited one or several quanta of plasma oscillation, which are called *plasmons.*

If we use the definition equation (10.6) of the atomic radius r_s, we can write the plasma frequency in terms of this quantity:

$$\hbar\omega_p = \frac{\sqrt{3}}{r_s^{3/2}}\frac{e^2}{a_0}.$$

For metallic densities, we obtain values of $\hbar\omega_p$ between 3 and 30 eV. Compared to thermal excitations of electrons at room temperature, which are approximately of an energy of 0.02 eV, this is a very large value.

Since such plasma oscillations can occur in the electron gas, it is natural to attempt to transform the Hamiltonian to a form which contains an explicit harmonic-oscillator part of the form

$$\frac{1}{2}\left(\hat{P}_{\mathbf{k}}^{\dagger}\hat{P}_{\mathbf{k}} + \omega_p^2\hat{Q}_{\mathbf{k}}^{\dagger}\hat{Q}_{\mathbf{k}}\right)$$

with suitable collective coordinates $Q_{\mathbf{k}}$ and corresponding momenta $P_{\mathbf{k}}$. Such a procedure was first suggested by Bohm and Pines [5]. The transformation of the Hamiltonian consists of several steps: first we find appropriate collective coordinates

$$\hat{\tilde{Q}}_{\mathbf{k}} = \tilde{Q}_{\mathbf{k}}(\hat{\mathbf{r}}_1, \ldots, \hat{\mathbf{r}}_N)$$

which are written as functions of the electron coordinates. We do not gain much so long as we merely express a part of the Hamiltonian in these collective coordinates. Rather, the crucial point is to introduce *independent* variables $Q_{\mathbf{k}}$, and impose the constraint that

$$\hat{Q}_{\mathbf{k}} \quad \text{corresponds to} \quad \hat{\tilde{Q}}_{\mathbf{k}} = \tilde{Q}_{\mathbf{k}}(\hat{\mathbf{r}}_i).$$

We will see under what conditions we can replace the operators $\hat{\tilde{Q}}_{\mathbf{k}}$ with the operators $\hat{Q}_{\mathbf{k}}$. In principle, we are looking for a solution of the Schrödinger equation

$$\hat{H}(\hat{\mathbf{r}}_i, \hat{\mathbf{p}}_i)\Psi(\mathbf{r}_i) = E\Psi(\mathbf{r}_i)$$

such that $\Psi(\mathbf{r}_i)$ is independent of $Q_{\mathbf{k}}$, *i.e.*,

$$\frac{\partial}{\partial Q_{\mathbf{k}}}\Psi = 0.$$

Expressed in terms of the canonical momentum $\hat{P}_{\mathbf{k}} = -i\hbar\frac{\partial}{\partial Q_{\mathbf{k}}}$, this condition becomes

$$\hat{P}_{\mathbf{k}}\psi = 0. \tag{11.2}$$

Under this condition, we can transform the Schrödinger equation by adding zero to it:

$$\left(\hat{H}(\hat{\mathbf{r}}_i,\hat{\mathbf{p}}_i)+\widetilde{H}(\hat{P}_{\mathbf{k}})\right)\Psi(\mathbf{r}_i)=E\Psi(\mathbf{r}_i).$$

We will finally bring this transformed Schrödinger equation to the desired form by acting on it with a unitary transformation $\hat{U}$ so that the resulting equation

$$\underbrace{\left[\hat{U}^\dagger\left(\hat{H}+\hat{\tilde{H}}\right)\hat{U}\right]}_{\equiv\mathcal{H}(\hat{Q}_{\mathbf{k}},\hat{P}_{\mathbf{k}},\mathbf{r}_i,\mathbf{p}_i)}\left[\hat{U}^\dagger\Psi\right]=E\ \underbrace{\left[\hat{U}^\dagger\Psi\right]}_{\equiv\Psi(Q_{\mathbf{k}},\mathbf{r}_i)} \tag{11.3}$$

contains a harmonic-oscillator part. The transformed wavefunction depends explicitly on the collective coordinates. We are, however, interested in a solution such that it satisfies the transformed condition equation (11.2):

$$\begin{aligned} 0 &= \left(\hat{U}^\dagger\hat{P}_{\mathbf{k}}\hat{U}\right)\hat{U}^\dagger\left(\Psi(\mathbf{r}_i)\right) \\ &= \left(\hat{U}^\dagger\hat{P}_{\mathbf{k}}\hat{U}\right)\Psi(\mathbf{r}_i,Q_{\mathbf{k}}). \end{aligned}$$

We will solve the problem that we have obtained in this way by using perturbation theory. We will take the oscillator part and the remaining kinetic energy of the electrons as the unperturbed Hamiltonian H_0. Thus, the zeroth order wavefunction will be constructed from the product of a Slater determinant of plane waves and oscillator wavefunctions in the collective coordinates. In what now follows, we will discuss the individual steps of the transformation in detail.

To define the collective coordinates, we first consider the Fourier expansion of the density:

$$\rho(\mathbf{r})=\frac{1}{\Omega}\sum_{\mathbf{k}}\rho_{\mathbf{k}}\mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}}$$

where

$$\rho_{\mathbf{k}}=\int\rho(\mathbf{r})\mathrm{e}^{-i\mathbf{k}\cdot\mathbf{r}}\mathrm{d}^3r.$$

If we interpret the density as matrix elements of the density operator $\hat{\rho}(\mathbf{r})$ introduced earlier (*cf.* Chapter 6)

$$\rho(\mathbf{r})=\langle\Psi\mid\hat{\rho}(\mathbf{r})\mid\Psi\rangle$$

and introduce the operators $\hat{\rho}_{\mathbf{k}}$ by

$$\rho_{\mathbf{k}}\equiv\langle\Psi\mid\hat{\rho}_{\mathbf{k}}\mid\Psi\rangle$$

we can also interpret the Fourier expansion as an operator equation:

$$\hat{\rho}(\mathbf{r})=\frac{1}{\Omega}\sum_{\mathbf{k}}\mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}}\hat{\rho}_{\mathbf{k}}.$$

Explicitly, the Fourier components are

$$\begin{aligned}\hat{\rho}_{\mathbf{k}} &= \int \hat{\rho}(\mathbf{r})\mathrm{e}^{-i\mathbf{k}\cdot\mathbf{r}}\mathrm{d}^3r \\ &= \int \left[\sum_{j=1}^{N} \delta(\mathbf{r}-\hat{\mathbf{r}}_j)\right] \mathrm{e}^{-i\mathbf{k}\cdot\mathbf{r}}\mathrm{d}^3r \\ &= \sum_{j=1}^{N} \mathrm{e}^{-i\mathbf{k}\cdot\hat{\mathbf{r}}_j}.\end{aligned}$$

These momentum components correspond to small density packages which execute oscillations according to the aforementioned classical considerations. It is then natural to choose these as collective coordinates. For convenience we will however include a constant and define

$$\tilde{Q}_{\mathbf{k}}(\hat{\mathbf{r}}_i) \equiv iM_k\hat{\rho}_{\mathbf{k}}$$

where

$$M_k \equiv \sqrt{\frac{4\pi e^2}{k^2\Omega}}.$$

We have

$$(\hat{\rho}_{\mathbf{k}})^\dagger = \sum_{j=1}^{N} \mathrm{e}^{i\mathbf{k}\cdot\hat{\mathbf{r}}_j^\dagger} = \sum_{j=1}^{N} \mathrm{e}^{-i(-\mathbf{k})\cdot\hat{\mathbf{r}}_j} = \hat{\rho}_{-\mathbf{k}}$$

which implies that

$$\hat{\tilde{Q}}_{\mathbf{k}}^\dagger = -\hat{\tilde{Q}}_{-\mathbf{k}}$$

in agreement with the property of $\hat{\tilde{Q}}_{\mathbf{k}}$ that it changes the momentum of a plane wave $\varphi_\nu(\mathbf{r}_\nu) = \exp(i\mathbf{k}'\cdot\mathbf{r}_\nu)/\sqrt{\Omega}$ by $\mathbf{k}$:

$$\begin{aligned}\hat{\tilde{Q}}_{\mathbf{k}}\varphi_\nu(\mathbf{r}_\nu) &= \frac{iM_k\mathrm{e}^{-i\mathbf{k}\cdot\mathbf{r}_\nu}\mathrm{e}^{i\mathbf{k}'\cdot\mathbf{r}_\nu}}{\sqrt{\Omega}} \\ &= \frac{iM_k\mathrm{e}^{i(\mathbf{k}'-\mathbf{k})\cdot\mathbf{r}_\nu}}{\sqrt{\Omega}}.\end{aligned}$$

Hence, the operators $\tilde{Q}_{\mathbf{k}}$ are *not* self-adjoint.

We can then formally rewrite the entire Coulomb interaction as

$$
\begin{aligned}
\hat{H} &= \sum_{i=1}^{N} \frac{\hat{p}_i^2}{2m} + \frac{1}{2} \sum_{\substack{i,j=1 \\ i\neq j}} \sum_{k\neq 0} \frac{4\pi e^2}{k^2\Omega} \mathrm{e}^{i\mathbf{k}\cdot(\hat{\mathbf{r}}_i - \hat{\mathbf{r}}_j)} \\
&= \sum_{i=1}^{N} \frac{\hat{p}_i^2}{2m} + \frac{1}{2} \sum_{i,j=1}^{N} \sum_{k\neq 0} \frac{4\pi e^2}{k^2\Omega} \mathrm{e}^{i\mathbf{k}\cdot(\hat{\mathbf{r}}_i - \hat{\mathbf{r}}_j)} - \frac{N}{2} \sum_{k\neq 0} \frac{4\pi e^2}{k^2\Omega} \\
&= \sum_{i=1}^{N} \frac{\hat{p}_i^2}{2m} + \frac{1}{2} \sum_{k\neq 0} \hat{\tilde{Q}}_{\mathbf{k}}^{\dagger} \hat{\tilde{Q}}_{\mathbf{k}} - \frac{N}{2} \sum_{k\neq 0} \frac{4\pi e^2}{k^2\Omega}.
\end{aligned}
$$

Since the plasma oscillations represent the motions of many electrons, the oscillations are mostly due to the long-range part of the Coulomb interactions. Therefore, it seems reasonable to perform the transformation to collective coordinates only for this part of the interaction, and to leave the short-range part as a function of the electron coordinates. With the partition of the Coulomb potential interaction into a long-range part and a short-range part that we derived in the previous chapter (equations (10.11) and (10.12)), we obtain

$$
\hat{H} = \sum_{i=1}^{N} \frac{\hat{p}_i^2}{2m} + \frac{1}{2} \sum_{0\neq k<k_c} \left(\hat{\tilde{Q}}_{\mathbf{k}}^{\dagger} \hat{\tilde{Q}}_{\mathbf{k}} - N M_k^2 \right) + \hat{V}_{\mathrm{sr}}.
$$

Up to this point we have merely rewritten the Hamiltonian. In the next step we will introduce $\hat{Q}_{\mathbf{k}}$ as independent coordinates. (In the end, these will of course replace the $\hat{\tilde{Q}}_{\mathbf{k}}$.) We demand that $\hat{Q}_{\mathbf{k}}$ satisfy

$$
\hat{Q}_{\mathbf{k}}^{\dagger} = -\hat{Q}_{(-\mathbf{k})}.
$$

For the canonically conjugated operators, $\hat{P}_{\mathbf{k}}$, it follows from

$$
\left[\hat{Q}_{\mathbf{k}}, \hat{P}_{\mathbf{k}'}\right] = i\hbar\delta_{\mathbf{k},\mathbf{k}'}
$$

that

$$
\left[\hat{Q}_{\mathbf{k}}^{\dagger}, \hat{P}_{\mathbf{k}'}^{\dagger}\right] = -\left[\hat{Q}_{\mathbf{k}}, \hat{P}_{\mathbf{k}'}\right]^{\dagger} = -\left(i\hbar\delta_{\mathbf{k},\mathbf{k}'}\right)^{*} = i\hbar\delta_{\mathbf{k},\mathbf{k}'}.
$$

These commutation relations are consistent only if

$$
\hat{P}_{\mathbf{k}}^{\dagger} = -\hat{P}_{(-\mathbf{k})}
$$

since then

$$
\begin{aligned}
\left[\hat{Q}_{\mathbf{k}'}, \hat{P}_{\mathbf{k}}^{\dagger}\right] &= \left[-\hat{Q}_{(-\mathbf{k}')}^{\dagger}, \hat{P}_{\mathbf{k}}^{\dagger}\right] = -i\hbar\delta_{\mathbf{k},(-\mathbf{k}')} \\
&= -i\hbar\delta_{\mathbf{k}',(-\mathbf{k})} = \left[\hat{Q}_{\mathbf{k}'}, \left(\hat{P}_{(-\mathbf{k})}\right)\right].
\end{aligned}
$$

We should also note that the collective operators $\hat{Q}_{\mathbf{k}}$ of course must commute with one another just as the $\hat{\tilde{Q}}_{\mathbf{k}}$.

For the additional term, we choose the operator

$$\hat{\tilde{H}} \equiv \frac{1}{2} \sum_{k<k_c} \left(\hat{P}^{\dagger}_{\mathbf{k}} - 2\hat{\tilde{Q}}^{\dagger}_{\mathbf{k}} \right) \hat{P}_{\mathbf{k}} = \sum_{k<k_c} \left(\frac{1}{2} \hat{P}^{\dagger}_{\mathbf{k}} \hat{P}_{\mathbf{k}} + iM \hat{\rho}^{\dagger}_{\mathbf{k}} \hat{P}_{\mathbf{k}} \right)$$

which, in a field-theoretical language, describes a free field $\hat{P}_{\mathbf{k}}$ and the interaction of this field with the electron field $\hat{\rho}_{\mathbf{k}}$. The operator $\hat{\tilde{H}}$ is self-adjoint, which one readily confirms from the remarks above and by renaming the summation indices $\mathbf{k} \to -\mathbf{k}$ ($\hat{\tilde{Q}}_{\mathbf{k}}$ and $\hat{P}_{\mathbf{k}}$ commute, since they act on different sets of coordinates). Apparently $\hat{\tilde{H}}$ gives no contribution when acting on the solution function that we are looking for (see equation (11.2). For the transformation $\hat{U}$ we take

$$\begin{aligned} \hat{U} &= \exp\left[+i\hbar \sum_{k<k_c} \hat{Q}^{\dagger}_{\mathbf{k}} \hat{\tilde{Q}}_{\mathbf{k}} \right] \\ &= \exp\left[-\frac{1}{\hbar} \sum_{k<k_c} \hat{Q}^{\dagger}_{\mathbf{k}} M_{\mathbf{k}} \hat{\rho}_{\mathbf{k}} \right] . \end{aligned}$$

The operator $\hat{U}$ defined in this way is unitary, since

$$\begin{aligned} \hat{U}^{\dagger} &= \exp\left[-\frac{i}{\hbar} \sum_{k<k_c} \hat{\tilde{Q}}^{\dagger}_{\mathbf{k}} \hat{Q}_{\mathbf{k}} \right] \\ &= \exp\left[-\frac{1}{\hbar} \sum_{k<k_c} \left(-\hat{Q}^{\dagger}_{(-\mathbf{k})} \right) \left(-\hat{\tilde{Q}}_{(-\mathbf{k})} \right) \right] = \hat{U}^{-1}. \end{aligned}$$

By using the identity

$$\exp(-S)\hat{A}\exp(+\hat{S}) = \hat{A} + \left[\hat{A}, \hat{S} \right]$$

provided

$$\left[\left[\hat{A}, \hat{S} \right], \hat{S} \right] = 0$$

we can quickly derive the following relations:

$$\begin{aligned} \hat{U}^{\dagger} \hat{Q}_{\mathbf{k}} \hat{U} &= \hat{Q}_{\mathbf{k}} \\ \hat{U}^{\dagger} \hat{\tilde{Q}}_{\mathbf{k}} \hat{U} &= \hat{\tilde{Q}}_{\mathbf{k}} \\ \hat{U}^{\dagger} \hat{\mathbf{r}}_i \hat{U} &= \hat{\mathbf{r}}_i \end{aligned}$$

$$\begin{aligned}
\hat{U}^\dagger \hat{P}^\dagger_{\mathbf{k}} \hat{U} &= \hat{P}^\dagger_{\mathbf{k}} + \left[\hat{P}^\dagger_{\mathbf{k}}, \frac{i}{\hbar} \sum_{\tilde{k}<k_c} \hat{Q}_{\tilde{\mathbf{k}}} \hat{\tilde{Q}}_{\tilde{\mathbf{k}}} \right] \\
&= \hat{P}^\dagger_{\mathbf{k}} + \frac{i}{\hbar}(-i\hbar) \sum_{\tilde{k}<k_c} \delta_{\mathbf{k},\tilde{\mathbf{k}}} \hat{\tilde{Q}}_{\tilde{\mathbf{k}}} \\
&= \hat{P}^\dagger_{\mathbf{k}} + \hat{\tilde{Q}}_{\mathbf{k}} \\
\hat{U}^\dagger \hat{\mathbf{p}}_i \hat{U} &= \hat{\mathbf{p}}_i + \left[\hat{\mathbf{p}}_i, \frac{i}{\hbar} \sum_{k<k_c} \hat{Q}^\dagger_{\mathbf{k}} i M_k \sum_j \mathrm{e}^{-i\mathbf{k}\cdot\hat{\mathbf{r}}_j} \right] \\
&= \hat{\mathbf{p}}_i + \sum_{k<k_c} \frac{i}{\hbar} \hat{Q}^\dagger_{\mathbf{k}} i M_k \sum_j \hbar \delta_{i,j} (-\mathbf{k}) \mathrm{e}^{-i\mathbf{k}\cdot\hat{\mathbf{r}}_j} \\
&= \hat{\mathbf{p}}_i + \sum_{k<k_c} \mathbf{k} M_k \hat{Q}^\dagger_{\mathbf{k}} \mathrm{e}^{-i\mathbf{k}\cdot\hat{\mathbf{r}}_i} \\
&= \hat{\mathbf{p}}_i + \sum_{k<k_c} \mathbf{k} M_k \hat{Q}_{\mathbf{k}} \mathrm{e}^{+i\mathbf{k}\cdot\hat{\mathbf{r}}_i}.
\end{aligned}$$

We write these relations once again in an abbreviated form:

$$\hat{Q}^{(\mathrm{new})}_{\mathbf{k}} = \hat{Q}^{(\mathrm{old})}_{\mathbf{k}} \qquad \hat{\mathbf{r}}^{(\mathrm{new})}_i = \hat{\mathbf{r}}^{(\mathrm{old})}_i \qquad \hat{P}^{(\mathrm{new})}_{\mathbf{k}} = \hat{P}^{(\mathrm{old})}_{\mathbf{k}} + \hat{\tilde{Q}}^{(\mathrm{old/new})}_{\mathbf{k}}$$

and

$$\hat{\mathbf{p}}^{(\mathrm{new})}_i = \hat{\mathbf{p}}^{(\mathrm{old})}_i + \left[\sum_{k<k_c} \hat{Q}_{\mathbf{k}} \mathbf{k} M_k \mathrm{e}^{i\mathbf{k}\cdot\hat{\mathbf{r}}_i} \right]^{(\mathrm{old/new})}.$$

With the help of these relations we can immediately calculate the transformed Hamiltonian (*cf.* equation (11.3)):

$$\hat{\mathcal{H}} = \left[\sum_{i=1}^{N} \frac{\hat{p}_i^2}{2m} + \hat{V}_{\mathrm{sr}} \right] + \hat{H}_{\mathrm{pl}} + \hat{H}^{(I)}_{\mathrm{e-pl}} + \hat{H}(II)_{\mathrm{e-pl}}, \tag{11.4}$$

where

$$\begin{aligned}
\hat{H}_{\mathrm{pl}} &= \frac{1}{2} \sum_{\substack{k<k_c \\ k\neq 0}} \left[\hat{P}^\dagger_{\mathbf{k}} \hat{P}_{\mathbf{k}} + \omega_p^2 \hat{Q}^\dagger_{\mathbf{k}} \hat{Q}_{\mathbf{k}} - N \frac{4\pi e^2}{k^2 \Omega} \right] \\
\hat{H}^{(I)}_{\mathrm{e-pl}} &= \sum_{i=1}^{N} \sum_{0<k<k_c} \frac{M_k}{2m} \mathbf{k} \cdot (2\hat{\mathbf{p}}_i - \hbar\mathbf{k}) \, \hat{Q}_{\mathbf{k}} \mathrm{e}^{i\mathbf{k}\cdot\hat{\mathbf{r}}_i} \\
\hat{H}^{(II)}_{\mathrm{e-pl}} &= \sum_{i=1}^{N} \sum_{\substack{0<k,k'<k_c \\ -\mathbf{k}\neq\mathbf{k}'}} \frac{M_k M_{k'}}{2m} \mathbf{k} \cdot \mathbf{k}' \hat{Q}_{\mathbf{k}'} \hat{Q}_{\mathbf{k}} \mathrm{e}^{i(\mathbf{k}+\mathbf{k}')\cdot\hat{\mathbf{r}}_i}.
\end{aligned}$$

Thus, we obtain one part which only depends on the electron coordinates $\hat{\mathbf{p}}_i$ and $\hat{\mathbf{r}}_i$ and which describes an electron gas with short-range interactions. Furthermore, we have an harmonic-oscillator part in the collective coordinates, which reproduces the plasma oscillations, and, finally, we have two terms which contain both particle and collective coordinates and which consequently describe an electron–plasmon interaction.

To understand the individual contributions better, we go over to second quantization. To do this, we first define the usual oscillator creation and annihilation operators (the non-hermiticity of the operators $\hat{P}_{\mathbf{k}}$ and $\hat{Q}_{\mathbf{k}}$ can easily be taken into account and does not lead to any complications):

$$\begin{aligned} \hat{b}^{\dagger}_{\mathbf{k}} &\equiv \frac{1}{\sqrt{2\hbar\omega_p}}\left(\omega_p\hat{Q}^{\dagger}_{\mathbf{k}} - i\hat{P}_{\mathbf{k}}\right) \\ \hat{b}_{\mathbf{k}} &\equiv \frac{1}{\sqrt{2\hbar\omega_p}}\left(\omega_p\hat{Q}_{\mathbf{k}} + i\hat{P}^{\dagger}_{\mathbf{k}}\right). \end{aligned}$$

For these operators, we have

$$\hat{b}^{\dagger}_{\mathbf{k}}\hat{b}_{\mathbf{k}} = \frac{1}{2\hbar\omega_p}\left(\omega_p^2\hat{Q}^{\dagger}_{\mathbf{k}}\hat{Q}_{\mathbf{k}} + \hat{P}_{\mathbf{k}}\hat{P}^{\dagger}_{\mathbf{k}} + i\omega_p\hat{Q}^{\dagger}_{\mathbf{k}}\hat{P}^{\dagger}_{\mathbf{k}} - i\omega_p\hat{P}_{\mathbf{k}}\hat{Q}_{\mathbf{k}}\right)$$

and furthermore, with $\left[\hat{Q}_{\mathbf{k}}, \hat{P}_{\mathbf{k}}\right] = i\hbar$, we have

$$\hat{b}^{\dagger}_{\mathbf{k}}\hat{b}_{\mathbf{k}} = \frac{1}{2\hbar\omega_p}\left(\omega_p^2\hat{Q}^{\dagger}_{\mathbf{k}}\hat{Q}_{\mathbf{k}} + \hat{P}^{\dagger}_{\mathbf{k}}\hat{P}_{\mathbf{k}} + i\omega_p\left(\hat{Q}^{\dagger}_{\mathbf{k}}\hat{P}^{\dagger}_{\mathbf{k}} - \hat{Q}_{\mathbf{k}}\hat{P}_{\mathbf{k}}\right) - \hbar\omega_p\right).$$

Analogously, we obtain the relation

$$\hat{b}_{\mathbf{k}}\hat{b}^{\dagger}_{\mathbf{k}} = \frac{1}{2\hbar\omega_p}\left[\omega_p^2\hat{Q}^{\dagger}_{\mathbf{k}}\hat{Q}_{\mathbf{k}} + \hat{P}^{\dagger}_{\mathbf{k}}\hat{P}_{\mathbf{k}} + i\omega_p\left(\hat{Q}^{\dagger}_{\mathbf{k}}\hat{P}^{\dagger}_{\mathbf{k}} - \hat{Q}_{\mathbf{k}}\hat{P}_{\mathbf{k}}\right) + \hbar\omega_p\right].$$

From these relations the commutation relation

$$\left[\hat{b}_{\mathbf{k}}, \hat{b}^{\dagger}_{\mathbf{k}}\right] = 1$$

follows. Thus, the plasmons are bosons, which is what we would expect of oscillator quanta.

Furthermore, we have

$$\begin{aligned} &\sum_{0<k<k_c} \hbar\omega_p\left(\hat{b}^{\dagger}_{\mathbf{k}}\hat{b}_{\mathbf{k}} + \frac{1}{2}\right) \\ &\quad = \sum_{0<k<k_c} \frac{1}{2}\left[\omega_p^2\hat{Q}^{\dagger}_{\mathbf{k}}\hat{Q}_{\mathbf{k}} + \hat{P}^{\dagger}_{\mathbf{k}}\hat{P}_{\mathbf{k}} + i\omega_p\left(\hat{Q}^{\dagger}_{\mathbf{k}}\hat{P}^{\dagger}_{\mathbf{k}} - \hat{Q}_{\mathbf{k}}\hat{P}_{\mathbf{k}}\right)\right]. \end{aligned}$$

In this last expression, we see that the part

$$\frac{1}{2}i\omega_p \sum_{0<k<k_c} \left(\hat{Q}^\dagger_{\mathbf{k}}\hat{P}^\dagger_{\mathbf{k}} - \hat{Q}_{\mathbf{k}}\hat{P}_{\mathbf{k}}\right)$$

vanishes if we insert the relations $\hat{Q}^\dagger_{\mathbf{k}} = -\hat{Q}_{-\mathbf{k}}$ and $\hat{P}^\dagger_{\mathbf{k}} = -\hat{P}_{-\mathbf{k}}$ and take into account that for each vector $\mathbf{k}$ in the sphere with radius k_c, the vector $-\mathbf{k}$ is also contained in the sphere:

$$\sum_{0<k<k_c} \hat{Q}^\dagger_{\mathbf{k}}\hat{P}^\dagger_{\mathbf{k}} = \sum_{0<k<k_c} \left(\hat{Q}_{-\mathbf{k}}\right)\left(\hat{P}_{-\mathbf{k}}\right) = \sum_{0<k<k_c} \hat{Q}_{\mathbf{k}}\hat{P}_{\mathbf{k}}.$$

We can then write the part of the Hamiltonian that only contains the plasmons in the following form:

$$\hat{H}_{\mathrm{pl}} = \sum_{\substack{k<k_c\\ k\neq 0}} \left[\hbar\omega_p\left(\hat{b}^\dagger_{\mathbf{k}}\hat{b}_{\mathbf{k}} + \frac{1}{2}\right) - \frac{N}{\Omega}\frac{2\pi e^2}{k^2}\right]. \tag{11.5}$$

We can now write the operator $\hat{H}^{(I)}_{\mathrm{e-pl}}$ in second quantization with respect to the electron coordinates. By using

$$\langle \mathbf{p}'\sigma' \mid e^{i\mathbf{k}\cdot\mathbf{r}} \mid \mathbf{p}\sigma\rangle = \delta_{\sigma,\sigma'}\delta_{\mathbf{p}',(\mathbf{k}+\mathbf{p})}$$

we obtain

$$\begin{aligned}\hat{H}^{(I)}_{\mathrm{e-pl}} &= \sum_i \sum_{\substack{0<k<k_c\\ k\neq 0}} \frac{M_k}{2m}\left(2\mathbf{k}\cdot\hat{\mathbf{p}}_i - \hbar k^2\right)\hat{Q}_{\mathbf{k}}e^{i\mathbf{k}\cdot\mathbf{r}_i}\\ &= \sum_{\mathbf{p},\sigma} \sum_{\substack{0<k<k_c\\ k\neq 0}} \frac{M_k}{2m}\left(2\mathbf{k}\cdot\mathbf{p} - \hbar k^2\right)\hat{Q}_{\mathbf{k}}\hat{c}^\dagger_{(\mathbf{k}+\mathbf{p}),\sigma}\hat{c}_{\mathbf{p},\sigma}.\end{aligned}$$

We invert the definition of the plasmon creation and annihilation operators,

$$\hat{Q}_{\mathbf{k}} = \sqrt{\frac{\hbar}{2\omega_p}}\left(\hat{b}_{\mathbf{k}} - \hat{b}^\dagger_{-\mathbf{k}}\right)$$

and with this result we obtain

$$\begin{aligned}\hat{H}^{(I)}_{\mathrm{e-pl}} &= \sum_{\mathbf{p},\sigma}\sum_{0<k<k_c} \frac{M_k}{2m}\sqrt{\frac{\hbar}{2\omega_p}}\left(2\mathbf{k}\cdot\mathbf{p} - \hbar k^2\right)\\ &\quad\times\left(\hat{b}_{\mathbf{k}}\hat{c}^\dagger_{\mathbf{k}+\mathbf{p},\sigma}\hat{c}_{\mathbf{p},\sigma} - \hat{b}^\dagger_{-\mathbf{k}}\hat{c}^\dagger_{\mathbf{k}+\mathbf{p},\sigma}\hat{c}_{\mathbf{p},\sigma}\right).\end{aligned} \tag{11.6}$$

This operator describes processes in which the momentum of an electron increases an amount **k** by absorbing (annihilating) a plasmon with momentum **k** (the first term), or by emitting (creating) a plasmon with momentum −**k** (the second term).

The second electron–plasmon interaction operator $\hat{H}^{(II)}_{\text{e-pl}}$ is usually omitted for the reason that it contains the sum over the phase factors

$$\sum_{i=1}^{N} e^{i(\mathbf{k}'+\mathbf{k})\cdot\mathbf{r}_i}$$

which vanishes for a random distribution of the electron coordinates $\mathbf{r}_i$. This approximation is known as the *random phase approximation* (RPA). If we write this operator in second quantization, we obtain

$$\begin{aligned}\hat{H}^{(II)}_{\text{e-pl}} \;=\; & \sum_{\substack{0<k,k'<k_c\\ -\mathbf{k}\neq\mathbf{k}'}} \sum_{\mathbf{p},\sigma} \frac{\hbar\omega_p}{4N}\left(\frac{\mathbf{k}}{k}\right)\left(\frac{\mathbf{k}'}{k'}\right) \\ & \times \left[\hat{b}_{\mathbf{k}}\hat{b}_{\mathbf{k}'} + \hat{b}^{\dagger}_{-\mathbf{k}}\hat{b}^{\dagger}_{-\mathbf{k}'} - \hat{b}^{\dagger}_{-\mathbf{k}}\hat{b}_{\mathbf{k}'} - \hat{b}_{\mathbf{k}}\hat{b}^{\dagger}_{-\mathbf{k}'}\right]\hat{c}^{\dagger}_{(\mathbf{k}+\mathbf{k}'+\mathbf{p})\sigma}\hat{c}_{\mathbf{p},\sigma}. \qquad (11.7)\end{aligned}$$

Thus, when we neglect this part, we neglect all processes where the momentum of an electron increases by an amount $(\mathbf{k}+\mathbf{k}')$ either by absorbing two plasmons (with momenta $\mathbf{k},\mathbf{k}'$) or by emitting two plasmons (with momenta $-\mathbf{k},-\mathbf{k}'$), or by absorbing and emitting one plasmons of each momentum $\pm\mathbf{k}$ and $\pm\mathbf{k}'$.

In summary, we have cast the original Hamiltonian into a form that contains two different kinds of particles, electrons and plasmons, and where the electrons interact both with the plasmons as well as with one another. However, the interactions between the electrons are now only short-ranged. The question whether the transformation is useful can ultimately be answered in more detail beyond the simple arguments given so far, if we can show that the interaction term is small. This is indeed the case. The tedious calculations will not be carried through in detail here. It suffices to say that this can be proved by another unitary transformation, after which the remainder is truly negligible. This transformation changes the up till now large terms so that the electrons acquires an effective k-dependent mass and that the plasmons acquire a k-dependent eigenfrequency, so that they both show dispersion:

$$m \longrightarrow m^*(k) \quad \text{and} \quad \omega_p \longrightarrow \omega(k).$$

In the following considerations, we will totally ignore these small effects and calculate the ground state energy in first-order perturbation theory.

We choose the interaction-free term as H_0:

$$\hat{H}_0 = \sum_{i=1}^{N} \frac{\hat{p}_i^2}{2m} + \hat{H}_{\mathrm{pl}}.$$

The wavefunction is then to zeroth order given by

$$\Psi_0(Q_{\mathbf{k}}, x_i) = \varphi_i(Q_{\mathbf{k}})\Phi(x_i)$$

where the collective part is a product of oscillator ground state functions

$$\varphi(Q_{\mathbf{k}}) = C \prod_{0<k<k_c} \mathrm{e}^{-(1/2)(\omega_p/\hbar)Q_{\mathbf{k}}^* Q_{\mathbf{k}}}$$

(C is a normalization constant), while the electron part is the usual Slater determinant of plane waves;

$$\Phi(x_i) = \frac{1}{\sqrt{N!}} \det_{k<k_F,\sigma} \left[\mathrm{e}^{i\mathbf{k}_j\cdot\mathbf{r}_i}\chi_{\sigma_j}(s_i)\right].$$

The zeroth-order energy is

$$E^{(0)} = \langle \Psi_0 \mid \sum_i \frac{\hat{p}_i^2}{2m} + \hat{H}_{\mathrm{pl}} \mid \Psi_0 \rangle = \langle \Phi \mid \sum_i \frac{\hat{p}_i^2}{2m} \mid \Phi \rangle + \langle \varphi \mid \hat{H}_{\mathrm{pl}} \mid \varphi \rangle.$$

The kinetic energy has already been calculated in the previous section (*cf.* equation (10.8)), with the result

$$\langle \Phi \mid \sum_i \frac{\hat{p}_i^2}{2m} \mid \Phi \rangle = N \frac{2.21}{r_s^2} \left[\frac{e^2}{2a_0}\right].$$

For the plasmon contribution, we use the fact that since we are calculating the ground state energy, we only need the energy of the zero-point motions:

$$\begin{aligned}
\langle \varphi \mid \hat{H}_{\mathrm{pl}} \mid \varphi \rangle &= \sum_{\substack{k<k_c \\ k\neq 0}} \left[\frac{\hbar\omega_p}{2} - \frac{N}{\Omega}\frac{2\pi e^2}{k^2}\right] \\
&= \frac{\Omega}{(2\pi)^3} \int_0^{k_c} 4\pi k^2 \mathrm{d}k \left[\frac{\hbar\omega_p}{2} - \frac{N}{\Omega}\frac{2\pi e^2}{k^2}\right] \\
&= \frac{\Omega\hbar\omega_p k_c^3}{12\pi^2} - \frac{Ne^2 k_c}{\pi}.
\end{aligned}$$

With $k_F^3 = 3\pi\frac{N}{\Omega}$ and the definition $\beta \equiv k_c/k_F$, this expression takes the form

$$\langle \varphi \mid \hat{H}_{\mathrm{pl}} \mid \varphi \rangle = \frac{1}{4}N\hbar\omega_p\beta^3 - \frac{1}{\pi}Ne^2 k_F\beta.$$

We regard the short-range part of the electron–electron interaction as a perturbation and obtain the first-order correction to the ground state energy. The operator $\hat{H}^{(I)}_{\text{e-pl}}$, which we can readily express in second quantization, changes the plasmon number; thus, any matrix element between states of equal plasmon number will vanish. In particular, this holds for the expectation value involving $|\,\Psi_0\rangle$, so that this part of the Hamiltonian does not contribute to $E^{(1)}$.

$$\begin{aligned} E^{(1)} &= \langle\Psi_0 \mid \hat{V}_{\text{sr}} \mid \Psi_0\rangle = \langle\Phi \mid \hat{V}_{\text{sr}} \mid \Phi\rangle \\ &= -\frac{4\pi e^2}{\Omega} \sum_{\substack{k,k'<k_F \\ |\mathbf{k}-\mathbf{k}'|>k_F}} \frac{1}{|\mathbf{k}-\mathbf{k}'|^2} \\ &= -\frac{4\pi e^2}{\Omega}\left[\frac{\Omega}{(2\pi)^3}\right]^2 \int^{k_F} \mathrm{d}^3k \int^{k_F}_{|\mathbf{k}-\mathbf{k}'|>k_F} \mathrm{d}^3k' \frac{1}{|\mathbf{k}-\mathbf{k}'|^2}. \end{aligned}$$

This integral can be evaluated by elementary integrations (see, for example, Raimes [4]. The result is

$$E^{(1)} = \frac{3Ne^2k_F}{4\pi}\left(1+\frac{\beta^2}{2}-\frac{\beta^4}{48}\right) + \frac{1}{\pi}Ne^2k_F\beta.$$

With $\hbar\omega_p = \sqrt{3}/r_s^{3/2}[e^2/a_o]$, we then obtain in all

$$E^{(0)} + E^{(1)} = N\left[\frac{2.21}{r_s^2} + \frac{0.8866\beta^3}{r_s^{3/2}} - \frac{0.916}{r_s}\left(1+\frac{\beta^2}{2}-\frac{\beta^4}{48}\right)\right]\frac{e^2}{2a_o}. \quad (11.8)$$

Thus, we have calculated the energy as a function of the so far unknown quantity β, or, equivalently, k_c. The following considerations will show that we may determine β by minimizing the energy $E^{(0)} + E^{(1)}$ with respect to β. We have

$$\begin{aligned} E^{(0)} + E^{(1)} &= \langle\varphi\Phi \mid \hat{T}_{\text{e}} + \hat{H}_{\text{pl}} + \hat{V}_{\text{sr}} + \hat{H}^{(I)}_{\text{e-pl}} \mid \varphi\Phi\rangle \\ &\cong \langle\varphi\Phi \mid \hat{T}_{\text{e}} + \hat{H}_{\text{pl}} + \hat{V}_{\text{sr}} + \hat{H}^{(I)}_{\text{e-pl}} + \hat{H}^{(II)}_{\text{e-pl}} \mid \varphi\Phi\rangle \\ &= \langle\varphi\Phi \mid \hat{U}^\dagger\hat{U}\left(\hat{T}_{\text{e}} + \hat{H}_{\text{pl}} + \hat{H}^{(I)}_{\text{e-pl}} + \hat{H}^{(II)}_{\text{e-pl}} + \hat{V}_{\text{sr}}\right)\hat{U}^\dagger\hat{U} \mid \varphi\Phi\rangle \\ &= \langle\hat{U}\varphi\Phi \mid \hat{H} + \hat{\hat{H}} \mid \hat{U}\varphi\Phi\rangle \\ &\cong \langle\hat{U}\varphi\Phi \mid \hat{H} \mid \hat{U}\varphi\Phi\rangle. \end{aligned}$$

After integrating over the plasmon coordinates, the expectation value of the original Hamiltonian in the electron part of the wavefunction remains. This part is not the exact ground state, but only an approximation of it. In particular, this wavefunction in this approximation depends on k_c:

$$E^{(0)} + E^{(1)} \cong \langle \Psi(k_c) \mid \hat{H} \mid \Psi(k_c) \rangle.$$

By Ritz' theorem, we will obtain an upper bound for the ground state energy when we minimize with respect to k_c. The very small contribution proportional to β^4 in equation (11.8) will then be negligible (a more careful consideration will show that this term is of the same order as contributions already neglected in the present approximation), and we obtain

$$k_c = 0.677 r_s^{-1/2} = 0.353 r_s^{+1/2} k_F$$

which gives

$$\beta = 0.353 r_s^{1/2}.$$

As an example to illustrate the order of magnitude, we consider sodium, for which $r_s \approx 4a_o$. This yields $\beta = 0.71$ and $k_c^{-1} = 2.95\ a_o$, so that the remaining short-range forces are indeed limited to only a few neighboring electrons.

With β fixed in this way, the energy, equation (11.8), is then finally determined. In this calculation, the constraint equation (11.2) was however disregarded. One can easily convince oneself that the transformed constraint

$$\begin{aligned} 0 &= \left(\hat{U}^\dagger \hat{P}_{\mathbf{k}}^{(\mathrm{old})} \hat{U}\right) \hat{U}^\dagger \Psi^{(\mathrm{old})}\left(x_j\right) \\ &= \left(\hat{P}_{\mathbf{k}}^{(\mathrm{old})} + \hat{\tilde{Q}}_{\mathbf{k}}\right) \Psi^{(\mathrm{new})}\left(Q_{\mathbf{k}}, x_j\right) \end{aligned} \tag{11.9}$$

is not satisfied by the above wavefunction $\Psi_0\left(Q_{\mathbf{k}}, x_j\right) = \varphi(Q_{\mathbf{k}} \Phi(x_j)$. However, it can be shown [6], that a small change in the wavefunction so that it satisfies equation (11.9), has a negligible effect on the *ground state energy*. However, a corresponding statement does not necessarily hold for other observables of the system.

It should be emphasized that the energy, equation (11.8), obtained by this projection contains part of the long-ranged correlation energy due to the transformation to collective coordinates that was carried through. To isolate this contribution, we subtract the Hartree–Fock energy, equation (10.8). Using the value determined above for β, we obtain per particle

$$\begin{aligned} E_{\mathrm{corr}}^{(\mathrm{lr})}/N &= \left(E^{(0)} + E^{(1)} - E_{\mathrm{HF}}^{\mathrm{e-gas}}\right)/N \\ &= \left(-\frac{0.458}{r_s}\beta^2 + \frac{0.866}{r_s^{3/2}}\beta^3 + \frac{0.019}{r_s}\beta^4\right)\frac{e^2}{2a_o} \\ &= -0.0190\frac{e^2}{2a_o} + \mathrm{O}(r_s). \end{aligned}$$

We can now finally give a definite value for the short-ranged correlation energy, equation (10.13), that was calculated in the end of the previous chapter. We obtain per particle:

$$E^{(\mathrm{sr})}_{\mathrm{corr}}/N = (0.0622\ln(r_s) - 0.139)\,\frac{e^2}{2a_\mathrm{o}} + \mathrm{O}(r_s).$$

If we add the long-range and short-range contributions, we obtain in total for the correlation energy per particle:

$$E_{\mathrm{corr}}/N = (0.0622\ln(r_s) - 0.158)\,\frac{e^2}{2a_\mathrm{o}}. \tag{11.10}$$

We will later derive this approximation for the correlation energy of the free electron gas by using the perturbation theory of Gell-Mann and Brueckner (Chapter 22).

Chapter 12

Phonons

We have in the last two chapters approximated the ion lattice in a metal by a constant charge distribution. This is obviously a very rough approximation which only leads to semi-reasonable quantitative results for a few simple metals. A better approximation is obtained by using the Hamiltonian

$$\hat{H} = \hat{H}_{\mathrm{i}} + \hat{H}_{\mathrm{e}} + \hat{V}_{\mathrm{e-i}}$$

where

$$\begin{aligned}
\hat{H}_{\mathrm{e}} &= \sum_{i=1}^{N} \frac{\hat{p}_i^2}{2m} + \frac{e^2}{2} \sum_{\substack{i,j=1 \\ i \neq j}}^{N} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|} \equiv \hat{T}_{\mathrm{e}} + \hat{V} \\
\hat{H}_{\mathrm{i}} &= \sum_{j=1}^{J} \frac{\hat{p}_j^2}{2M_j} + \frac{1}{2} \sum_{\substack{j,k=1 \\ j \neq k}}^{J} w\left(\mathbf{R}_j - \mathbf{R}_k\right) \equiv \hat{T}_{\mathrm{i}} + \hat{W} \\
\hat{V}_{\mathrm{e-i}} &= \sum_{n=1}^{N} \sum_{j=1}^{J} v_{\mathrm{e-i}}\left(\mathbf{r}_n - \mathbf{R}_j\right) .
\end{aligned}$$

This is also an approximation, since we are treating the ions as particles without inner structure with a fixed interaction potential $\hat{W}$. We abbreviate the set of electron coordinates by

$$\underline{\mathbf{r}} = (\mathbf{r}_1, \ldots, \mathbf{r}_N)$$

and the set of ion coordinates by

$$\underline{\mathbf{R}} = (\mathbf{R}_1, \ldots, \mathbf{R}_J)$$

so that we can write the Hamiltonian as

$$\hat{H} = \hat{H}(\underline{\mathbf{r}}, \underline{\mathbf{R}}) = \hat{H}_{\mathrm{i}}(\underline{\mathbf{R}}) + \hat{H}_{\mathrm{e}}(\underline{\mathbf{r}}) + \hat{V}_{\mathrm{e-i}}(\underline{\mathbf{r}}, \underline{\mathbf{R}}).$$

We will search for solutions of the full Schrödinger equation

$$\hat{H}\Psi_n(\underline{\mathbf{r}},\underline{\mathbf{R}}) = E_n\Psi_n(\underline{\mathbf{r}},\underline{\mathbf{R}})$$

where the ionic motion is coupled to the electronic motions. A partial decoupling can be obtained by the so-called *Born-Oppenheimer approximation.* This approximation is based on the large mass difference between the electrons and the ions. Because of this mass difference, the ions move much more slowly in their oscillations about their equilibrium positions than the electrons. Consequently, the electrons are approximately in a stationary state for each instantaneous configuration of the ions. Conversely, for each instantaneous configuration, the electron cloud will slightly modify the ion–ion interactions by screening them.

Thus, we first of all solve the electronic Schrödinger equation

$$\left[\hat{H}_{\mathrm{e}}(\underline{\mathbf{r}}) + \hat{V}_{\mathrm{e-i}}(\underline{\mathbf{r}},\underline{\mathbf{R}})\right] \psi_m(\underline{\mathbf{r}},\underline{\mathbf{R}}) = \epsilon_m(\underline{\mathbf{R}})\psi_m(\underline{\mathbf{r}},\underline{\mathbf{R}}) \tag{12.1}$$

for each fixed set of ion coordinates $\underline{\mathbf{R}}$. For each fixed $\underline{\mathbf{R}}$, $\{\psi_m(\underline{\mathbf{r}},\underline{\mathbf{R}})\}$ is a complete system in the electron many-particle Hilbert space. For fixed $\underline{\mathbf{R}}$, we can then expand the exact many-body wavefunction:

$$\Psi_n(\underline{\mathbf{r}},\underline{\mathbf{R}}) = \sum_{m=1}^{\infty} \chi_{nm}(\underline{\mathbf{R}})\psi_m(\underline{\mathbf{r}},\underline{\mathbf{R}}).$$

We obtain a set of expansion coefficients χ_{nm} for each $\underline{\mathbf{R}}$. We insert this completely general representation of $\Psi_n(\mathbf{r},\underline{\mathbf{R}})$ in the full Schrödinger equation to obtain

$$\sum_m \psi_m(\underline{\mathbf{r}},\underline{\mathbf{R}}) \left[\hat{T}_{\mathrm{i}} + \hat{W}(\underline{\mathbf{R}})\right] \chi_{nm}(\underline{\mathbf{R}}) + \sum_m \chi_{nm}(\underline{\mathbf{R}}) \left[\hat{T}_{\mathrm{i}}(\underline{\mathbf{R}})\psi_m(\underline{\mathbf{r}},\underline{\mathbf{R}})\right]$$
$$+\sum_m \chi_{nm}(\underline{\mathbf{R}}) \underbrace{\left[\hat{T}_{\mathrm{e}} + \hat{V} + \hat{V}_{\mathrm{e-i}}\right] \psi_m(\underline{\mathbf{r}},\underline{\mathbf{R}})}_{=\epsilon_m(\underline{\mathbf{R}})\psi_m(\underline{\mathbf{r}},\underline{\mathbf{R}})} = E_n \sum_m \chi_{nm}(\underline{\mathbf{R}})\psi_m(\underline{\mathbf{r}},\underline{\mathbf{R}}).$$

If we multiply this equation by $\psi_k(\underline{\mathbf{r}},\underline{\mathbf{R}})$, integrate over the electron coordinates $\mathrm{d}^{3N}r$, and use the orthogonality of ψ_m, we arrive at

$$\left[\hat{T}_{\mathrm{i}} + \hat{W}(\underline{\mathbf{R}}) + \epsilon_k(\underline{\mathbf{R}})\right] \chi_{nk}(\underline{\mathbf{R}}) + \sum_m \chi_{nm}(\underline{\mathbf{R}})\langle\psi_k \mid \hat{T}_{\mathrm{i}}(\underline{\mathbf{R}}) \mid \psi_m\rangle$$
$$= E_n\chi_{nk}(\underline{\mathbf{R}}).$$

Here, the matrix elements $\langle\psi_k \mid \hat{T}_{\mathrm{i}}(\underline{\mathbf{R}}) \mid \psi_m\rangle$ are functions of $\underline{\mathbf{R}}$, since we integrated only over the electron coordinates. We result is a system of infinitely many coupled equation. The Born–Oppenheimer approximation consists of neglecting the *off-diagonal* matrix elements $\langle \psi_k \mid \hat{T}_{\rm i}(\underline{\mathbf{R}}) \mid \psi_m \rangle$. In this way, we obtain the approximate equation

$$\left[\hat{T}_{\rm i} + \hat{W}(\underline{\mathbf{R}}) + \epsilon_k(\underline{\mathbf{R}}) + \langle \psi_k \mid \hat{T}_{\rm i}(\underline{\mathbf{R}}) \mid \psi_k \rangle\right] \chi_{nk}(\underline{\mathbf{R}}) = E_n \chi_{nk}(\underline{\mathbf{R}}) \qquad (12.2)$$

where the electron eigenvalues ϵ_k and the matrix elements $\langle \psi_k \mid \hat{T}_{\rm i} \mid \psi_k \rangle$ act as potential terms for the ionic motions. We can solve the Schrödinger equation (12.2) for the ionic motion and the electron Schrödinger equation (12.1) separately. If the conditions for the validity of the Born–Oppenheimer approximation, which were described in the beginning of this chapter, are satisfied, we can assume that the neglected matrix elements are small. This assumption can be shown to be correct at the end of the calculations.

The electronic Schrödinger equation must in principle be solved for each set of fixed ion coordinates $\underline{\mathbf{R}}$. This is of course not possible, but it is not even necessary for solids. We know from experience that in practice, only the equilibrium position of the crystal lattice is important. Therefore, it is natural to expand all the occurring potentials about the equilibrium positions. Before we do this, however, we make a brief digression to discuss the equilibrium positions themselves, *i.e.*, the crystal lattice.

An ideal crystal lattice is a periodic arrangement of points, which are invariant under so-called primitive translations

$$\mathbf{R}_m^{(0)} = m_1\mathbf{a}_1 + m_2\mathbf{a}_2 + m_3\mathbf{a}_3, \; m_i \in \mathcal{Z}$$

where $\mathcal{Z}$ is the set of integers. The choice of the linearly independent vectors $\mathbf{a}_i$ is not unique, which is clear from figure 12.1. The set of these points is also known as a *Bravais lattice*. The individual Bravais lattices are classified

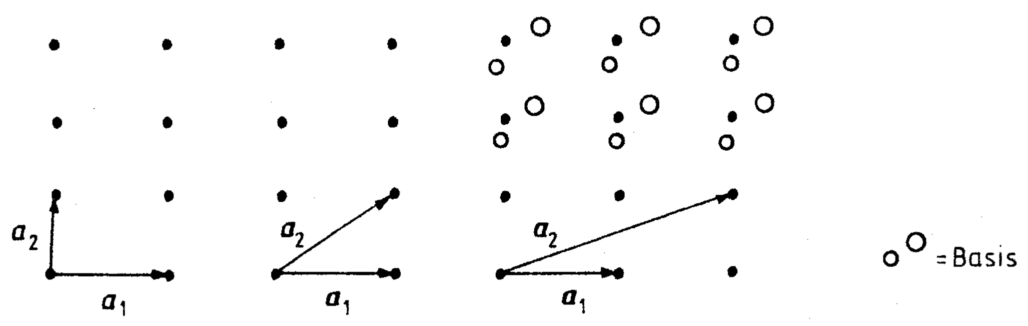


Figure 12.1 *For this diatomic crystal, the basis contains two atoms. A few choices for primitive translation vectors are shown.*

according to additional point symmetry operations, such as rotations or reflections. Because of the simultaneous constraint of translational symmetry, the number of geometrically different point lattices is severely reduced; for example, there are five in two dimensions, and in three dimensions there are 14 different Bravais lattices.

If each point in the Bravais lattice is assigned a *basis*, which can consist of one or several atoms or ions, we obtain the real crystal. It should be emphasized that the point symmetries of the Bravais lattice are not necessarily point symmetries of the crystal, since the basis can break these symmetries, if it consists of several atoms. For example, the right-angle Bravais lattice pictured in figure 12.1 is symmetric under reflection in horizontal and vertical lines cutting the unit cells in half, whereas the crystal with the indicated basis is not.

The parallelepipedes spanned by the vectors $\mathbf{a}_i$ form the unit cells of the lattice. The unit cells completely fill the entire space. However, most frequently one uses other unit cells, the so-called *Wigner–Seitz cells.* These are constructed by drawing all lines which are perpendicular bisectors of the lines from a particular lattice point to all its nearest neighbors, as shown in figure 12.2. The unit cells constructed in this way have the advantage that they are invariant under the point symmetry of the lattice. These symmetries are clearly seen, as in the hexagonal Bravais lattice illustrated above.

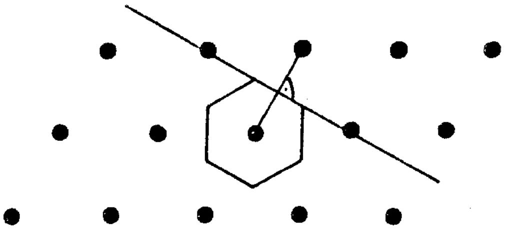


Figure 12.2 *Construction of the Wigner–Seitz cell for a hexagonal lattice.*

We now define new basis vectors by

$$\mathbf{b}_1 \equiv \frac{\mathbf{a}_2 \times \mathbf{a}_3}{(\mathbf{a}_1 \cdot \mathbf{a}_2 \times \mathbf{a}_3)} \quad \mathbf{b}_2 \equiv \frac{\mathbf{a}_3 \times \mathbf{a}_1}{(\mathbf{a}_1 \cdot \mathbf{a}_2 \times \mathbf{a}_3)} \quad \mathbf{b}_3 \equiv \frac{\mathbf{a}_1 \times \mathbf{a}_2}{(\mathbf{a}_1 \cdot \mathbf{a}_2 \times \mathbf{a}_3)}.$$

The components of any vector in one or the other basis are called contra and covariant components, respectively, in vector calculus.

Given any vectors $\mathbf{x} = x_1\mathbf{a}_1 + x_2\mathbf{a}_2 + x_3\mathbf{a}_3$ and $\mathbf{y} = y_1\mathbf{b}_1 + y_2\mathbf{b}_2 + y_3\mathbf{b}_3$, it follows that the scalar product of them is

$$\mathbf{x} \cdot \mathbf{y} = x_1 y_1 + x_2 y_2 + x_3 y_3.$$

The union of the points

$$\mathbf{G}_n \equiv n_1(2\pi\mathbf{b}_1) + n_2(2\pi\mathbf{b}_2) + n_3(2\pi\mathbf{b}_3) \quad \text{with } n_i \in \mathcal{Z}$$

is called the *reciprocal lattice* (of the original lattice). The origin of the name comes from the fact that the basis vectors $\mathbf{b}_i$ have the dimension of a reciprocal length. As is easily verified, the lattices $\mathbf{R}_m^{(0)}$ and $\mathbf{G}_n$ are *mutually* reciprocal, so that the reciprocal lattice of $\mathbf{G}_n$ is the original (real-space) lattice $\mathbf{R}_m^{(0)}$.

The Wigner–Seitz cell of the reciprocal lattice $\mathbf{G}_n$ is called the *Brillouin zone.* The scalar product of a lattice vector and a reciprocal lattice vector follows from the general scalar product above:

$$\mathbf{R}_m^{(0)} \cdot \mathbf{G}_n = 2\pi\left(m_1 n_1 + m_2 n_2 + m_3 n_3\right) \equiv 2\pi N \quad \text{with } N \in \mathcal{Z}. \qquad (12.3)$$

We will frequently use this relation.

Let us now consider a macroscopic volume Ω with sides $L_1\mathbf{a}_1$, $L_2\mathbf{a}_2$ and $L_3\mathbf{a}_3$, so that the volume contains $L_1 \cdot L_2 \cdot L_3$ unit cells. For the sake of simplicity, we will in the remainder of this section consider only monatomic crystals, in which the unit cell only contains a single atom or ion. The number of ions, J, is then equal to the number of unit cells:

$$J = L_1 \cdot L_2 \cdot L_3.$$

To describe the extensive properties of the crystal, we will apply periodic boundary conditions in all three directions $\mathbf{a}_i$ so that we imagine the system continued periodically in these directions. (We recognize this procedure from the discussion of translationally invariant systems.) Each group of translations along $\mathbf{a}_i$ $(i = 1, 2, 3)$ then becomes a cyclic group of order L_i. Because each such group then is an abelian group, it has only one-dimensional irreducible representations, *i.e.*, the representations are numbers in the complex plane. From the fact that each group is cyclic, it follows that these numbers are the L_i roots of unity, *i.e.*, complex numbers whose L_ith power is unity. These numbers lie on the unit circle in the complex plane. The irreducible representations of each group can then be written $\exp(iq_i\mathbf{b}_i \cdot \mathbf{a}_i)$, where $q_i = 2\pi n_i/L_i$ with $n_i \in \mathcal{Z}$. The irreducible representations of the element $\mathbf{R}_m^{(0)}$ of the full translation group of the crystal, which is a product of the cyclic groups, are then

$$\Gamma_{\mathbf{q}}\left(\mathbf{R}_m^{(0)}\right) = e^{i\mathbf{q}\cdot\mathbf{R}_m^{(0)}} \quad \text{with} \quad \begin{cases} \mathbf{q} = q_1\mathbf{b}_1 + q_2\mathbf{b}_2 + q_3\mathbf{b}_3 \\ q_i = 2\pi n_i/L_i \end{cases} \quad \text{with } n_i \in \mathcal{Z}.$$

Since this representation matrix is one-dimensional, it is identical to its group characters. From the orthogonality of characters we readily obtain the following two results:

$$\begin{aligned}
\sum_{n_i=1}^{L_i} e^{i\mathbf{q}\cdot\mathbf{R}_m^{(0)}} &= \begin{cases} J & \text{for } \mathbf{R}_m^{(0)} = 0 \\ 0 & \text{otherwise} \end{cases} \\
\sum_{m_i=1}^{L_i} e^{i\mathbf{q}\cdot\mathbf{R}_m^{(0)}} &= \begin{cases} J & \text{for } \mathbf{q} \text{ a reciprocal lattice vector } \mathbf{G} \\ 0 & \text{otherwise.} \end{cases}
\end{aligned}$$

In the first of these two equations, the summation over $n_i = 1, \ldots, L_i$ includes all q-vectors which lie in the unit cells spanned by the vectors $\mathbf{b}_i$. Instead, we can of course sum over the Brillouin zone (BZ). If we also use

$$\mathbf{R}_m^{(0)} = m_1\mathbf{a}_1 + m_2\mathbf{a}_2 + m_3\mathbf{a}_3 = 0$$

only if $\mathbf{m} = (m_1, m_2, m_3) = (0, 0, 0)$, we can use the shorter notation

$$\begin{aligned}
\sum_{\mathbf{q}\in \mathrm{BZ}} e^{i\mathbf{q}\cdot\mathbf{R}_m^{(0)}} &= J\delta_{\mathbf{m},0} &\quad (12.4) \\
\sum_{\mathbf{R}_m^{(0)}\in\Omega} e^{i\mathbf{q}\cdot\mathbf{R}_m^{(0)}} &= J\Delta_{\mathbf{q},0}. &\quad (12.5)
\end{aligned}$$

In equation (12.5), we have used Δ to denote a Kronecker-delta modulus reciprocal lattice vector $\mathbf{G}$.

That concludes the short digression on crystal lattices.

We will now further analyze the Schrödinger equation, equation (12.2), for the ionic motion. To do so, we begin by collecting all potential energy terms into one total potential, $\widetilde{W}(\mathbf{R}_1, \ldots, \mathbf{R}_J)$, and for ease of notation we will not explicitly indicate the dependence of $\widetilde{W}$ on the electronic state ψ_k. The Schrödinger equation then becomes

$$\left[\hat{T}_{\mathrm{I}} + \widetilde{W}(\underline{\mathbf{R}})\right] \chi_\ell(\underline{\mathbf{R}}) = E_\ell \chi_\ell(\underline{\mathbf{R}}).$$

Because the ions in a solid body essentially stay at the lattice sites, we can expand $\widetilde{W}$ about these equilibrium positions. With $\mathbf{R}_j \equiv \mathbf{R}_j^{(0)} + \mathbf{u}_j$, we obtain

$$\begin{aligned}
\widetilde{W}(\mathbf{R}_1, \ldots, \mathbf{R}_J) &= \widetilde{W}(\mathbf{R}_1^{(0)}, \ldots, \mathbf{R}_J^{(0)}) \\
&\quad + \sum_{m=1}^{J} \mathbf{u}_m \cdots \nabla_{R_m} \widetilde{W}\Big|_{\underline{\mathbf{R}}^{(0)}}
\end{aligned}$$

$$+\frac{1}{2!}\sum_{m,n=1}^{J}\sum_{\mu,\nu=1}^{3} u_m^\mu u_n^\nu A_{mn}^{\mu\nu}$$
$$+\frac{1}{3!}\sum_{m,n,\ell=1}^{J}\sum_{\mu,\nu,\lambda=1}^{3} u_m^\mu u_n^\nu u_\ell^\lambda B_{mn\ell}^{\mu\nu\lambda}+\cdots.$$

The coefficients are derived from the ion–ion potential, for example

$$A_{mn}^{\mu\nu}=\left.\frac{\partial^2\widetilde{W}}{\partial R_m^\mu \partial R_n^\nu}\right|_{\underline{\mathbf{R}}^{(0)}}.$$

The linear term in this expansion vanishes, since each coefficient is precisely the sum of all forces acting on each ion, and this force must be zero from the definition of the equilibrium position. Thus, we can approximately write the Hamiltonian for the ionic motion as

$$\hat{T}_\mathrm{i}+\widetilde{W}(\underline{\mathbf{R}})=\widetilde{W}(\underline{\mathbf{R}}^{(0)})+\hat{H}_\mathrm{ph}+\hat{H}_\mathrm{ph-ph}$$

where

$$\hat{H}_\mathrm{ph}=\sum_{j=1}^{J}\frac{\hat{p}_j^2}{2M}+\frac{1}{2}\sum_{m,n=1}^{J}\sum_{\mu,\nu=1}^{3} u_m^\mu u_n^\nu A_{mn}^{\mu\nu} \tag{12.6}$$

and

$$\hat{H}_\mathrm{ph-ph}=\frac{1}{3!}\sum_{m,n,\ell=1}^{3}\sum_{\mu,\nu,\lambda=1}^{3} u_m^\mu u_n^\nu u_\ell^\lambda B_{mn\ell}^{\mu\nu\lambda}. \tag{12.7}$$

The first term, $\widetilde{W}(\underline{\mathbf{R}}^{(0)})$, is constant and is not interesting for the discussion on ionic motion.

We will now examine $\hat{H}_\mathrm{ph}$ a little more closely. To do so, we will, just as we did for the plasmons, make a transformation to collective oscillator coordinates, so-called *normal coordinates*:

$$\hat{U}_\mathbf{q}^\mu \equiv \frac{1}{\sqrt{J}}\sum_{\mathbf{R}_m^{(0)}\in\Omega} \hat{u}_m^\mu e^{-i\mathbf{q}\cdot\mathbf{R}_m^{(0)}} \qquad \mu=1,2,3.$$

Here the sum extends over all lattice points in the system volume Ω. This definition holds for arbitrary vectors $\mathbf{q}$. From equation (12.3), however, we see that for any reciprocal lattice vector $\mathbf{G}$

$$\hat{\mathbf{U}}_{\mathbf{q}+\mathbf{G}}=\hat{\mathbf{U}}_\mathbf{q}$$

so it is customary to discuss the normal coordinates only for vectors $\mathbf{q}$ in the first Brillouin zone. Furthermore, it is convenient to restrict the discussion to the discrete set of vectors $\mathbf{q}$

$$\mathbf{q}=q_1\mathbf{b}_1+q_2\mathbf{b}_2+q_3\mathbf{b}_3 \quad \text{with } q_i=2\pi\frac{n_i}{L_i},\ n_i\in\mathcal{Z}.$$

This set of vectors is quasi-continuous. We can with the help of the theorem (12.4) derive the inverse relation

$$\frac{1}{\sqrt{J}}\sum_{\mathbf{q}\in\mathrm{BZ}} \hat{U}^{\mu}_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{R}^{(0)}_m} = \sum_{\mathbf{R}^{(0)}_n\in\Omega} \hat{u}^{\mu}_m \underbrace{\frac{1}{J}\sum_{\mathbf{q}\in\mathrm{BZ}} e^{i\mathbf{q}\cdot(\mathbf{R}^{(0)}_m-\mathbf{R}^{(0)}_n)}}_{=\delta_{m,n}} = \hat{u}^{\mu}_m .$$

We introduce the operators

$$\hat{P}^{\mu}_{\mathbf{q}} \equiv -i\hbar\frac{\partial}{\partial U^{\mu}_{\mathbf{q}}}$$

which are conjugate to the normal coordinates $\hat{U}^{\mu}_{\mathbf{q}}$. The momentum operator $\hat{p}_j$ can then be expressed in terms of $\hat{P}^{\mu}_{\mathbf{q}}$

$$\begin{aligned}
\hat{p}^{\mu}_m &= -i\hbar\frac{\partial}{\partial R^{\mu}_m} = -i\hbar\frac{\partial}{\partial u^{\mu}_m} = -i\hbar\sum_{\mathbf{q}\in\mathrm{BZ}}\sum_{\nu=1}^{3}\frac{\partial U^{\nu}_{\mathbf{q}}}{\partial u^{\mu}_m}\frac{\partial}{\partial U^{\nu}_{\mathbf{q}}} \\
&= -i\hbar\sum_{\mathbf{q}\in\mathrm{BZ}}\sum_{\nu=1}^{3}\frac{\delta_{\mu\nu}}{\sqrt{J}}e^{-i\mathbf{q}\cdot\mathbf{R}^{(0)}_m}\frac{\partial}{\partial U^{\nu}_{\mathbf{q}}} \\
&= \frac{1}{\sqrt{J}}\sum_{\mathbf{q}\in\mathrm{BZ}} e^{-i\mathbf{q}\cdot\mathbf{R}^{(0)}_m}\hat{P}^{\mu}_{\mathbf{q}} .
\end{aligned}$$

The inverse relation can be obtained from equation (12.5) as

$$\begin{aligned}
\frac{1}{\sqrt{J}}\sum_{\mathbf{R}^{(0)}_m\in\Omega} e^{i\mathbf{q}\cdot\mathbf{R}^{(0)}_m}\hat{p}^{\mu}_m &= \sum_{\mathbf{q}'\in\mathrm{BZ}}\hat{P}^{\mu}_{\mathbf{q}'}\underbrace{\frac{1}{J}\sum_{\mathbf{R}^{(0)}_m\in\Omega} e^{+i(\mathbf{q}-\mathbf{q}')\cdot\mathbf{R}^{(0)}_m}}_{=\Delta_{\mathbf{q},\mathbf{q}'}} \\
&= \hat{P}^{\mu}_{\mathbf{q}} .
\end{aligned}$$

For the coordinates defined in this way, we apparently have

$$\hat{\mathbf{U}}^{\dagger}_{\mathbf{q}} = \hat{\mathbf{U}}_{-\mathbf{q}} \quad \text{and} \quad \hat{\mathbf{P}}^{\dagger}_{\mathbf{q}} = \hat{\mathbf{P}}_{-\mathbf{q}} .$$

Next, we express the kinetic energy, equation (12.6), in the new coordinates:

$$\begin{aligned}
\frac{1}{2M}\sum_{\mathbf{m}}\hat{\mathbf{p}}_{\mathbf{m}}\cdot\hat{\mathbf{p}}_{\mathbf{m}} &= \frac{1}{2M}\sum_{\mathbf{q},\mathbf{q}'\in\mathrm{BZ}}\underbrace{\frac{1}{J}\sum_{\mathbf{m}} e^{-i(\mathbf{q}+\mathbf{q}')\cdot\mathbf{R}^{(0)}_m}}_{=\Delta_{\mathbf{q}',-\mathbf{q}}}\hat{\mathbf{P}}_{\mathbf{q}'}\cdot\hat{\mathbf{P}}_{\mathbf{q}} \\
&= \frac{1}{2M}\sum_{\mathbf{q}\in\mathrm{BZ}}\hat{\mathbf{P}}_{-\mathbf{q}}\cdot\hat{\mathbf{P}}_{\mathbf{q}} = \frac{1}{2M}\sum_{\mathbf{q}\in\mathrm{BZ}}\hat{\mathbf{P}}^{\dagger}_{\mathbf{q}}\cdot\hat{\mathbf{P}}_{\mathbf{q}} .
\end{aligned}$$

Instead of summing over all $\mathbf{R}_m^{(0)} = m_1\mathbf{a}_1 + m_2\mathbf{a}_2 + m_3\mathbf{a}_3$ in Ω, we have here summed over all integer vectors $\mathbf{m} = (m_1, m_2, m_3)$.

An analogous calculation for the potential energy yields

$$\begin{aligned}\frac{1}{2}\sum_{\mathbf{m},\mathbf{n}}\sum_{\mu,\nu}\hat{u}_m^\mu\hat{u}_n^\nu A_{mn}^{\mu\nu} &= \frac{1}{2}\sum_{\mathbf{m},\mathbf{n}}\sum_{\mu,\nu}\frac{1}{J}\sum_{\mathbf{q}',\mathbf{q}\in \mathrm{BZ}}\hat{U}_{\mathbf{q}'}^\mu\hat{U}_{\mathbf{q}}^\nu e^{i\mathbf{q}'\cdot\mathbf{R}_m^{(0)}}e^{i\mathbf{q}\cdot\mathbf{R}_n^{(0)}}A_{mn}^{\mu\nu}\\ &= \frac{1}{2}\sum_{\mathbf{q}\mathbf{q}'\in\mathrm{BZ}}\sum_{\mu,\nu}\hat{U}_{\mathbf{q}'}^\mu\hat{U}_{\mathbf{q}}^\nu\frac{1}{J}\sum_{\mathbf{m}}e^{i(\mathbf{q}+\mathbf{q}')\cdot\mathbf{R}_m^{(0)}}\sum_{\mathbf{n}}e^{i\mathbf{q}\cdot(\mathbf{R}_n^{(0)}-\mathbf{R}_m^{(0)})}A_{mn}^{\mu\nu}.\end{aligned}$$

We can simplify this expression by writing

$$\mathbf{R}_n^{(0)} - \mathbf{R}_m^{(0)} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3 - m_1\mathbf{a}_1 - m_2\mathbf{a}_2 - m_3\mathbf{a}_3 = \mathbf{R}_{n-m}^{(0)}$$

for the difference between lattice vectors. To further simplify the expression for the potential energy, we examine in which way the matrix

$$A_{ab}^{\alpha\beta} = \left.\frac{\partial^2\widetilde{W}(\mathbf{R}_1^{(0)}\ldots\mathbf{R}_a^{(0)}\ldots\mathbf{R}_b^{(0)}\ldots\mathbf{R}_J^{(0)})}{\partial R_a^\alpha\partial R_b^\beta}\right|_{\substack{\mathbf{R}_a=\mathbf{R}_a^{(0)}\\ \mathbf{R}_b=\mathbf{R}_b^{(0)}}}$$

displays the translational invariance of the problem. For a constant vector $\mathbf{C}$ and $\mathbf{X}_m \equiv \mathbf{R}_m - \mathbf{C}$ we have $\partial/\partial R_m^\mu = \partial/\partial X_m^\mu$, and because of the translational invariance of the ion–ion potential

$$\widetilde{W}(\mathbf{R}_1,\ldots,\mathbf{R}_J) = \widetilde{W}(\mathbf{X}_1,\ldots,\mathbf{X}_J)$$

we also have

$$A_{ab}^{\alpha\beta} = \left.\frac{\partial^2\widetilde{W}(\mathbf{X}_1^{(0)}\ldots\mathbf{X}_a\ldots\mathbf{X}_b\ldots\mathbf{X}_J^{(0)})}{\partial X_a^\alpha\partial X_b^\beta}\right|_{\substack{\mathbf{X}_a=\mathbf{X}_a^{(0)}\\ \mathbf{X}_b=\mathbf{X}_b^{(0)}}}.$$

In particular, if we choose $\mathbf{C} = \mathbf{R}_a^{(0)}$, we obtain

$$A_{ab}^{\alpha\beta} = \left.\frac{\partial\widetilde{W}}{\partial X_a^\alpha\partial X_b^\beta}\right|_{\substack{\mathbf{X}_a=0\\ \mathbf{X}_b=\mathbf{R}_b^{(0)}-\mathbf{R}_a^{(0)}=\mathbf{R}_{b-a}^{(0)}}} = A_{0,b-a}^{\alpha,\beta}. \qquad (12.8)$$

We can then sum the expression

$$\sum_{\mathbf{n}} e^{\mathbf{q}\cdot(\mathbf{R}_n^{(0)}-\mathbf{R}_m^{(0)})}A_{mn}^{\mu\nu}$$

over the difference $\mathbf{k} \equiv \mathbf{n}-\mathbf{m}$ for each fixed m by using the periodic boundary conditions:

$$\sum_{\mathbf{n}} e^{i\mathbf{q}\cdot(\mathbf{R}_n^{(0)}-\mathbf{R}_m^{(0)})}A_{mn}^{\mu\nu} = \sum_{\mathbf{k}} e^{i\mathbf{q}\cdot\mathbf{R}_{\mathbf{k}}^{(0)}}A_{0,k}^{\mu\nu} \equiv \Lambda_{\mathbf{q}}^{\mu\nu}. \qquad (12.9)$$

With equations (12.8) and (12.9), the potential energy can be written

$$\frac{1}{2}\sum_{\mathbf{q}\mathbf{q}'\in \mathrm{BZ}}\sum_{\mu,\nu}\hat{U}^{\mu}_{\mathbf{q}'}\hat{U}^{\nu}_{\mathbf{q}}\underbrace{\frac{1}{J}\sum_{\mathbf{m}}\mathrm{e}^{i(\mathbf{q}+\mathbf{q}')\cdot\mathbf{R}^{(0)}_{m}}}_{=\Delta_{\mathbf{q},\mathbf{q}'}}\Lambda^{\mu\nu}_{\mathbf{q}}$$

$$= \frac{1}{2}\sum_{\mathbf{q}\in \mathrm{BZ}}\sum_{\mu,\nu}\hat{U}^{\mu}_{-\mathbf{q}}\hat{U}^{\nu}_{\mathbf{q}}\Lambda^{\mu\nu}_{\mathbf{q}}.$$

If we use a matrix notation, this expression can be written

$$\frac{1}{2}\sum_{\mathbf{q}\in \mathrm{BZ}}\hat{\mathbf{U}}^{\dagger}_{\mathbf{q}}\Lambda_{\mathbf{q}}\hat{\mathbf{U}}_{\mathbf{q}}.$$

We now proceed to show that the 3×3-matrix $\Lambda_{\mathbf{q}}$ is symmetric for each $\mathbf{q}$. First of all, we have

$$A^{\alpha\beta}_{a,b} = A^{\alpha\beta}_{-a,-b} \tag{12.10}$$

since

$$\frac{\partial^2\widetilde{W}}{\partial R^{\alpha}_{a}\partial R^{\beta}_{b}} = \frac{\partial^2\widetilde{W}}{\partial(-R^{\alpha}_{a})\partial(-R^{\beta}_{b})} = \frac{\partial^2\widetilde{W}}{\partial R^{\alpha}_{-a}\partial R^{\beta}_{-b}}.$$

Furthermore, we can interchange the order in which the two derivatives are taken, so that

$$A^{\alpha\beta}_{a,b} = A^{\beta\alpha}_{b,a}. \tag{12.11}$$

If we combine equations (12.11), (12.8) and (12.10), we obtain

$$A^{\mu\nu}_{0,k} = A^{\nu\mu}_{k,0} = A^{\nu\mu}_{0,-k} = A^{\nu\mu}_{0,k}$$

so that we finally arrive at

$$\Lambda^{\mu\nu}_{\mathbf{q}} = \sum_{\mathbf{k}}\mathrm{e}^{i\mathbf{q}\cdot\mathbf{R}^{(0)}_{k}}A^{\mu\nu}_{0,k} = \sum_{\mathbf{k}}\mathrm{e}^{i\mathbf{q}\cdot\mathbf{R}^{(0)}_{k}}A^{\nu\mu}_{0,k} = \Lambda^{\nu\mu}_{\mathbf{q}}.$$

The matrix $\Lambda_{\mathbf{q}}$ is symmetric, so we can diagonalize it with an orthogonal transformation $Y_{\mathbf{q}}$:

$$Y_{\mathbf{q}}\Lambda_{\mathbf{q}}Y^{\dagger}_{\mathbf{q}} = \begin{bmatrix} \lambda^{1}_{\mathbf{q}} & 0 & 0 \\ 0 & \lambda^{2}_{\mathbf{q}} & 0 \\ 0 & 0 & \lambda^{3}_{\mathbf{q}} \end{bmatrix}.$$

We now define new coordinates through

$$\begin{bmatrix} \hat{Q}^{1}_{\mathbf{q}} \\ \hat{Q}^{2}_{\mathbf{q}} \\ \hat{Q}^{3}_{\mathbf{q}} \end{bmatrix} \equiv \begin{bmatrix} \quad Y^{\mu\nu}_{\mathbf{q}} \quad \end{bmatrix} \begin{bmatrix} \hat{U}^{1}_{\mathbf{q}} \\ \hat{U}^{2}_{\mathbf{q}} \\ \hat{U}^{3}_{\mathbf{q}} \end{bmatrix}.$$

In terms of these, the potential energy takes the form

$$\begin{aligned}\frac{1}{2}\sum_{\mathbf{q}} \hat{\mathbf{U}}_{\mathbf{q}}^{\dagger} \Lambda_{\mathbf{q}} \hat{\mathbf{U}}_{\mathbf{q}} &= \frac{1}{2}\sum_{\mathbf{q}} \hat{\mathbf{U}}_{\mathbf{q}}^{\dagger} Y_{\mathbf{q}}^{\dagger} Y_{\mathbf{q}} \Lambda_{\mathbf{q}} Y_{\mathbf{q}}^{\dagger} Y_{\mathbf{q}} \hat{\mathbf{U}}_{\mathbf{q}} \\ &= \frac{1}{2}\sum_{\mathbf{q}} \sum_{\mu=1}^{3} \hat{Q}_{\mathbf{q}}^{\mu\dagger} \lambda_{\mathbf{q}}^{\mu} \hat{Q}_{\mathbf{q}}^{\mu}.\end{aligned}$$

It is easy to confirm that the kinetic energy remains invariant under the coordinate transformation $Y_{\mathbf{q}}$. For

$$\hat{P}_{\mathbf{q}}^{\nu(\mathrm{new})} = -i\hbar \frac{\partial}{\partial Q_{\mathbf{q}}^{\nu}}$$

we have

$$\begin{aligned}\hat{P}_{\mathbf{q}}^{\nu(\mathrm{old})} &= -i\hbar \frac{\partial}{\partial U_{\mathbf{q}}^{\nu}} = -i\hbar \sum_{\mu=1}^{3} \frac{\partial Q_{\mathbf{q}}^{\mu}}{\partial U_{\mathbf{q}}^{\nu}} \frac{\partial}{\partial Q_{\mathbf{q}}^{\mu}} \\ &= -i\hbar \sum_{\mu=1}^{3} Y_{\mathbf{q}}^{\mu\nu} \frac{\partial}{\partial Q_{\mathbf{q}}^{\mu}} = \sum_{\mu=1}^{3} Y_{\mathbf{q}}^{\mu\nu} \hat{P}_{\mathbf{q}}^{\mu(\mathrm{new})}\end{aligned}$$

so that in matrix notation we can write

$$\hat{\mathbf{P}}_{\mathbf{q}}^{(\mathrm{old})} = Y_{\mathbf{q}}^{\dagger} \hat{\mathbf{P}}_{\mathbf{q}}^{(\mathrm{new})}.$$

Since the scalar product is invariant under the orthogonal transformation $Y_{\mathbf{q}}$, it follows that

$$\frac{1}{2M}\sum_{\mathbf{q}} \hat{\mathbf{P}}_{\mathbf{q}}^{\dagger(\mathrm{old})} \cdot \hat{\mathbf{P}}_{\mathbf{q}}^{(\mathrm{old})} = \frac{1}{2M}\sum_{\mathbf{q}} \hat{\mathbf{P}}_{\mathbf{q}}^{\dagger(\mathrm{new})} \cdot \hat{\mathbf{P}}_{\mathbf{q}}^{(\mathrm{new})}.$$

The Hamiltonian for the lattice motion then finally becomes

$$\hat{H}_{\mathrm{ph}} = \sum_{\mu=1}^{3} \sum_{\mathbf{q}\in\mathrm{BZ}} \left[\frac{1}{2M} \hat{P}_{\mathbf{q}}^{\mu\dagger} \hat{P}_{\mathbf{q}}^{\mu} + \frac{M}{2} \omega_{\mathbf{q},\mu}^{2} \hat{Q}_{\mathbf{q}}^{\mu\dagger} \hat{Q}_{\mathbf{q}}^{\mu}\right] \tag{12.12}$$

where we have defined

$$\omega_{\mathbf{q},\mu} \equiv \sqrt{\frac{\lambda_{\mathbf{q}}^{\mu}}{M}}. \tag{12.13}$$

We have then succeeded in showing that the ionic motion can be approximately transformed to a system of *independent* oscillators with eigenfrequencies $\omega_{\mathbf{q},\mu}$. The quanta of these oscillators are called *phonons.* The only approximation that we have done in this, is to omit the higher order terms in the Taylor expansion about the equilibrium positions. We will, however, briefly discuss these terms later.

The eigenvalues satisfy $\omega_{\mathbf{q},\mu} = \omega_{-\mathbf{q},\mu}$. This follows from combining the definition (12.9) with equation (12.10):

$$\begin{aligned}\Lambda_{\mathbf{q}}^{\mu\nu} = \sum_{\mathbf{k}} \mathrm{e}^{i\mathbf{q}\cdot\mathbf{R}_{\mathbf{k}}^{(0)}} A_{0,k}^{\mu\nu} &= \sum_{\mathbf{k}} \mathrm{e}^{i\mathbf{q}\cdot\mathbf{R}_{\mathbf{k}}^{(0)}} A_{0,-k}^{\mu\nu} \\ &= \sum_{\mathbf{k}} \mathrm{e}^{-i\mathbf{q}\cdot\mathbf{R}_{-\mathbf{k}}^{(0)}} A_{0,-k}^{\mu\nu} = \Lambda_{\mathbf{q}}^{\mu\nu} .\end{aligned}$$

The matrices $\Lambda_{\mathbf{q}}$ and $\Lambda_{-\mathbf{q}}$ are thus identical, hence also (by suitable enumeration) the eigenvalues $\omega_{\pm\mathbf{q},\mu}$. It also follows directly from the definition equation (12.9) of the matrix $\Lambda_{\mathbf{q}}$ that $\omega_{\mathbf{q},\mu} = \omega_{\mathbf{q}+\mathbf{G},\mu}$. Consequently,we only need to calculate the dispersion relation $\omega(\mathbf{q})$ in the first Brillouin zone. The exact calculation of such a dispersion relation is quite tedious, since the matrix $\Lambda_{\mathbf{q}}$, from which we obtain the eigenvalues $\omega_{\mathbf{q},\mu}$ by diagonalization, consists of the Fourier transform of the second derivative of the interaction potential of *all* ions. In most cases, it suffices to take into account only nearest neighbors or next nearest neighbors. Typically, one then obtains the picture shown in figure 12.3.

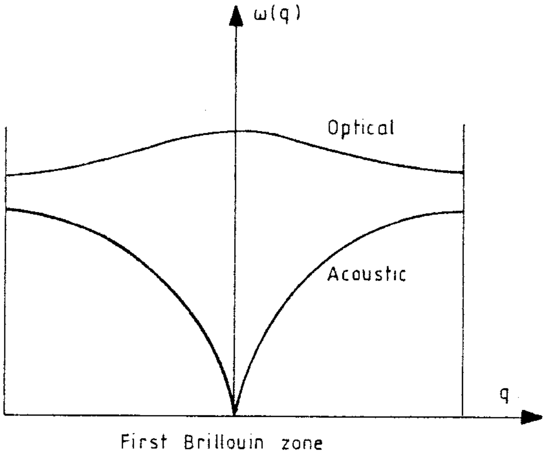


Figure 12.3 *The optical and acoustic phonon branches are depicted schematically.*

If the basis consists of only *one* ion, one obtains a dispersion curve which is linear in q for small q: $\omega(q \to 0) = cq$. Small q means large wavelengths, so these modes are the usual sound waves in condensed matter. This means that

$$s = \left.\frac{\mathrm{d}\omega}{\mathrm{d}q}\right|_{q=0}$$

is the sound velocity of the medium. Phonons with a dispersion curve of this kind are called acoustic phonons.

If the crystal contains several different atoms, optical phonon branches will appear in the dispersion curve. The quanta are called optical phonons because they can be excited by photons in the visible region.

We have up to this point not said anything about the polarization, *i.e.*, the direction of oscillation of the three different modes $\omega_{\mathbf{q},\mu}$, $\mu = 1, 2, 3$. However, we have already calculated these implicitly. The three vector components $Q^1_{\mathbf{q}}, Q^2_{\mathbf{q}}, Q^3_{\mathbf{q}}$ of the oscillations with frequencies $\omega_{\mathbf{q},1}, \omega_{\mathbf{q},2}, \omega_{\mathbf{q},3}$, are precisely the projections of the original displacement vectors $\mathbf{U}_{\mathbf{q}}$ of the particles on the row vectors of the orthogonal matrix $Y_{\mathbf{q}}$:

$$\mathbf{U} = Y^{\dagger}\mathbf{Q} = \begin{pmatrix} Y_{11}Q^1 + Y_{21}Q^2 + Y_{31}Q^3 \\ Y_{12}Q^1 + \dots \\ Y_{13}Q^1 + \dots \end{pmatrix} = Q^1\xi_1 + Q^2\xi_3 + Q^3\xi_3.$$

Thus, the column vectors of the matrix $Y^{\dagger}$, which are the row vectors of the matrix Y, give the polarization directions ξ_μ of the three modes $\omega_{\mathbf{q},\mu}$. The polarization directions depend, of course, on $\mathbf{q}$, just as the frequencies do. Depending on the direction of oscillation $\xi_{\mathbf{q},\mu}$ relative to the direction of propagation $\mathbf{q}$, one distinguishes between transverse and longitudinal phonons:

$$\xi_{\mathbf{q},\mu} \cdot \mathbf{q} = \begin{cases} 0 & \text{for purely transverse phonons} \\ |\xi_{\mathbf{q},\mu}| \cdot |\mathbf{q}| & \text{for purely logitudinal phonons.} \end{cases}$$

We cast $\hat{H}_{\text{ph}}$ in second quantization by introducing creation and annihilation operators (analogously to how we did with the plasmons):

$$\begin{aligned} \hat{b}_{\mathbf{q},\mu} &\equiv (2\hbar M\omega_{\mathbf{q},\mu})^{-1/2}\left(M\omega_{\mathbf{q},\mu}\hat{Q}^{\mu}_{\mathbf{q}} + i\hat{P}^{\mu\dagger}_{\mathbf{q}}\right) \\ \hat{b}^{\dagger}_{\mathbf{q},\mu} &\equiv (2\hbar M\omega_{\mathbf{q},\mu})^{-1/2}\left(M\omega_{\mathbf{q},\mu}\hat{Q}^{\mu\dagger}_{\mathbf{q}} - i\hat{P}^{\mu}_{\mathbf{q}}\right). \end{aligned}$$

It can be shown that these operators satisfy the boson commutation relations, and that $\hat{H}_{\text{ph}}$ can be written in the form

$$\hat{H}_{\text{ph}} = \sum_{\mathbf{q}\in\text{BZ}} \sum_{\mu=1}^{3} \hbar\omega_{\mathbf{q},\mu}\left(\hat{b}^{\dagger}_{\mathbf{q},\mu}\hat{b}_{\mathbf{q},\mu} + \frac{1}{2}\right). \tag{12.14}$$

This is the Hamiltonian of a system of non-interacting bosons. The anharmonic terms, *i.e.*, the higher terms in the Taylor expansion about the equilibrium positions, which we have neglected up to this point, can also be interpreted in terms of creation and annihilation operators. In order to write these terms explicitly, we use the inverse transformation

$$\hat{Q}^{\mu}_{\mathbf{q},\mu} = \left[\frac{\hbar}{2M\omega_{\mathbf{q},\mu}}\right]^{1/2}\left(\hat{b}_{\mathbf{q},\mu} + \hat{b}^{\dagger}_{-\mathbf{q},\mu}\right).$$

This yields

$$\begin{aligned}\hat{u}^{\mu}_{m} &= \frac{1}{\sqrt{J}}\sum_{\mathbf{q}\in\mathrm{BZ}} \mathrm{e}^{i\mathbf{q}\cdot\mathbf{R}^{(0)}_{m}}\hat{U}^{\mu}_{\mathbf{q}} \\ &= \frac{1}{\sqrt{J}}\sum_{\mathbf{q}\in\mathrm{BZ}} \mathrm{e}^{i\mathbf{q}\cdot\mathbf{R}^{(0)}_{m}}\sum_{\alpha=1}^{3}\hat{Q}^{\alpha}_{\mathbf{q}}\xi^{\mu}_{\mathbf{q},\alpha}\end{aligned}$$

so that

$$\hat{u}^{\mu}_{m} = \sum_{\mathbf{q}\in\mathrm{BZ}}\sum_{\alpha=1}^{3}\left[\frac{\hbar}{2MJ\omega_{\mathbf{q},\mu}}\right]^{1/2}\mathrm{e}^{i\mathbf{q}\cdot\mathbf{R}^{(0)}_{m}}\xi^{\mu}_{\mathbf{q},\alpha}\left(\hat{b}_{\mathbf{q},\alpha}+\hat{b}^{\dagger}_{-\mathbf{q},\alpha}\right). \tag{12.15}$$

Here, $\xi^{\mu}_{\mathbf{q},\alpha}$ denotes the μth component of the polarization vector $\xi_{\mathbf{q},\alpha}$.

If we insert these expressions in the third-order term

$$\hat{H}_{\mathrm{ph-ph}} = \frac{1}{3!}\sum_{m,n,\ell=1}^{J}\sum_{\mu,\nu,\lambda=1}^{3} u^{\mu}_{m}u^{\nu}_{n}u^{\lambda}_{\ell}B^{\mu\nu\lambda}_{mn\ell}$$

and also use

$$\begin{aligned}&\sum_{m,n,\ell=1}^{J}\mathrm{e}^{i\mathbf{q}\cdot\mathbf{R}^{(0)}_{m}}\mathrm{e}^{i\mathbf{q}'\cdot\mathbf{R}^{(0)}_{n}}\mathrm{e}^{i\mathbf{q}''\cdot\mathbf{R}^{(0)}_{\ell}}B^{\mu\nu\lambda}_{mn\ell} \\ &= \sum_{\mathbf{m}}\mathrm{e}^{i(\mathbf{q}+\mathbf{q}'+\mathbf{q}'')\cdot\mathbf{R}^{(0)}_{m}}\sum_{\mathbf{n}}\mathrm{e}^{\mathbf{q}'\cdot(\mathbf{R}^{(0)}_{n}-\mathbf{R}^{(0)}_{m})}\sum_{\ell}\mathrm{e}^{i\mathbf{q}''\cdot(\mathbf{R}^{(0)}_{\ell}-\mathbf{R}^{(0)}_{m})} \\ &\quad\times B^{\mu\,\nu\,\lambda}_{0,(n-m),(\ell-m)} \\ &= \Delta_{(\mathbf{q}+\mathbf{q}'+\mathbf{q}''),0}\sum_{\mathbf{k}}\mathrm{e}^{i\mathbf{q}'\cdot\mathbf{R}^{(0)}_{\mathbf{k}}}\sum_{\mathbf{g}}\mathrm{e}^{i\mathbf{q}''\cdot\mathbf{R}^{(0)}_{\mathbf{g}}}B^{\mu\,\nu\,\lambda}_{0,\mathbf{k},\mathbf{g}}\end{aligned}$$

and finally define

$$\begin{aligned}\Gamma^{\alpha\alpha'\alpha''}_{\mathbf{q},\mathbf{q}',\mathbf{q}''} &\equiv \sum_{\mu,\nu,\lambda}\xi^{\mu}_{\mathbf{q},\alpha}\xi^{\nu}_{\mathbf{q}',\alpha'}\xi^{\lambda}_{\mathbf{q}'',\alpha''}\sum_{\mathbf{k}}\mathrm{e}^{i\mathbf{q}'\cdot\mathbf{R}^{(0)}_{\mathbf{k}}} \\ &\quad\times\sum_{\mathbf{g}}\mathrm{e}^{i\mathbf{q}''\cdot\mathbf{R}^{(0)}_{\mathbf{g}}}B^{\mu\nu\lambda}_{0,\mathbf{k},\mathbf{g}}\end{aligned}$$

we obtain for the phonon–phonon interaction:

$$\begin{aligned}\hat{H}_{\mathrm{ph-ph}} &= \frac{1}{3!}\left[\frac{\hbar}{2MJ}\right]^{3/2}\sum_{\substack{\mathbf{q}\mathbf{q}'\mathbf{q}''\\ \alpha\alpha'\alpha''}}\frac{\Gamma^{\alpha\alpha'\alpha''}_{\mathbf{q}\mathbf{q}'\mathbf{q}''}}{\sqrt{\omega_{\mathbf{q},\alpha}\omega_{\mathbf{q}',\alpha'}\omega_{\mathbf{q}'',\alpha''}}} \\ &\quad\times\Delta_{(\mathbf{q}+\mathbf{q}'+\mathbf{q}''),0}\left(\hat{b}_{\mathbf{q},\alpha}+\hat{b}^{\dagger}_{-\mathbf{q},\alpha}\right)\left(\hat{b}_{\mathbf{q}',\alpha'}+\hat{b}^{\dagger}_{-\mathbf{q}',\alpha'}\right) \\ &\quad\times\left(\hat{b}_{\mathbf{q}'',\alpha''}+\hat{b}^{\dagger}_{-\mathbf{q}'',\alpha''}\right).\end{aligned}$$

When this expression is multiplied out, it yields a sum of three-phonon processes which are subjected to momentum conservation $\mathbf{q}+\mathbf{q}'+\mathbf{q}''=\mathbf{G}$. Such processes obviously play an important role when many phonons are excited, as is the case at high temperatures. They are important for the description of thermal conductivity and thermal expansion of crystal lattices.

After these remarks on the ionic motion, we now continue with the electronic problem. The Taylor expansion of the electron–ion potential leads to first order to

$$\begin{aligned} V_{\mathrm{e-i}}(\mathbf{r},\underline{\mathbf{R}}) &= \sum_{n=1}^{N}\sum_{j=1}^{J} v_{\mathrm{e-i}}(\mathbf{r}_n-\mathbf{R}_j) \\ &= \sum_{n=1}^{N}\sum_{j=1}^{J} v_{\mathrm{e-i}}(\mathbf{r}_n-\mathbf{R}_j^{(0)}-\mathbf{u}_j) \\ &= \sum_{n=1}^{N}\sum_{j=1}^{J}\left\{v_{\mathrm{e-i}}(\mathbf{r}_n\mathbf{R}_j^{(0)})-\mathbf{u}_j\cdot\nabla_{\mathbf{R}_j}\left[v_{\mathrm{e-i}}(\mathbf{r}_n-\mathbf{R}_j)\right]\Big|_{\mathbf{R}_j^{(0)}}+\ldots\right\} \\ &= \sum_n\sum_j v_{\mathrm{e-i}}\left(\mathbf{r}_n-\mathbf{R}_j^{(0)}\right)+\sum_n\sum_j \mathbf{u}_j\cdot\left[\nabla v_{\mathrm{e-i}}(\mathbf{r}_j-\mathbf{R}_j^{(0)})+\ldots\right]. \end{aligned}$$

We then arrive at the following expression for the total Hamiltonian for the electronic problem, equation (12.1):

$$\hat{H}_{\mathrm{e}}+\hat{V}_{\mathrm{e-i}}=\hat{H}_{\mathrm{e}}^{(0)}+\hat{H}_{\mathrm{e-ph}}$$

where

$$\hat{H}_{\mathrm{e}}^{(0)}=\hat{T}_{\mathrm{e}}+\frac{1}{2}\sum_{\substack{i,\ell=1\\ i\neq\ell}}^{N}\frac{e^2}{|\mathbf{r}_i-\mathbf{r}_\ell|}+\sum_{n=1}^{N}\sum_{j=1}^{J}v_{\mathrm{e-i}}(\mathbf{r}_n-\mathbf{R}_j^{(0)})$$

and

$$\hat{H}_{\mathrm{e-ph}}=\sum_{n=1}^{N}\tilde{v}(\mathbf{r}_n).$$

In this expression, we have only kept the first-order term of the higher-order terms in the Taylor expansion:

$$\tilde{v}(\mathbf{r})=\sum_{j=1}^{J}\mathbf{u}_j\cdot\left[(\nabla v_{\mathrm{e-i}})\left(\mathbf{r}-\mathbf{R}_j^{(0)}\right)\right].$$

The solution of the $\hat{H}_{\mathrm{e}}^{(0)}$-problem, *i.e.*, the calculation of the electron states in a fixed potential which is periodic with the lattice, is usually done with the so-called pseudo-potential method. The electron–electron potential is then usually regarded only as a screening of the ion potential. The electron states calculated in this way are called *Bloch states.* They are of the form

$$\psi_{\mathbf{k},\sigma}(x) = \frac{1}{\sqrt{J}} \mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}} \chi_\sigma(s) \varphi_{\mathbf{k}}(\mathbf{r}),$$

where

$$\varphi_{\mathbf{k}}(\mathbf{r} + \mathbf{R}_n^{(0)}) = \varphi_{\mathbf{k}}(\mathbf{r})$$

for all lattice vectors $\mathbf{R}_n^{(0)}$. In what follows, we will assume that these single-particle functions are known. If $\hat{c}^\dagger_{\mathbf{k}\sigma}$ and $\hat{c}_{\mathbf{k}\sigma}$ are the creation and annihilation operators of these one-electron states, we can write the operator $\hat{H}_{\mathrm{e-ph}}$, which eventually will have the form of electron–phonon interaction, in second quantization as

$$\hat{H}_{\mathrm{e-ph}} = \sum_{\mathbf{k},\mathbf{k}'\in \mathrm{BZ}} \sum_\sigma \langle \psi_{\mathbf{k}'\sigma} \mid \tilde{v} \mid \psi_{\mathbf{k}\sigma} \rangle \hat{c}^\dagger_{\mathbf{k}'\sigma} \hat{c}_{\mathbf{k}\sigma}.$$

Since the Bloch functions satisfy

$$\psi_{\mathbf{k}\sigma} = \psi_{(\mathbf{k}+\mathbf{G})\sigma}$$

it suffices to carry out the double sum over the first Brillouin zone.

To proceed, we expand the electron–ion potential in a Fourier series:

$$v_{\mathrm{e-i}}(\mathbf{y}) = \frac{1}{\Omega} \sum_{\mathbf{q}} v_{\mathrm{e-i}}(\mathbf{q}) \mathrm{e}^{i\cdot\mathbf{q}}$$

and

$$\nabla_{\mathbf{y}} v_{\mathrm{e-i}}(\mathbf{y}) = \frac{i}{\Omega} \sum_{\mathbf{q}} \mathbf{q} v_{\mathrm{e-i}}(\mathbf{q}) \mathrm{e}^{i\mathbf{q}\cdot\mathbf{y}}.$$

This yields

$$\begin{aligned} \tilde{v}(\mathbf{r}) &= \frac{i}{\Omega} \sum_{j=1}^{J} \mathbf{u}_j \cdot \sum_{\mathbf{q}} \mathbf{q} v_{\mathrm{e-i}}(\mathbf{q}) \mathrm{e}^{i\mathbf{q}\cdot(\mathbf{r}-\mathbf{R}_j^{(0)})} \\ &= \frac{i}{\Omega} \sum_{\mathbf{q}} \mathrm{e}^{i\mathbf{q}\cdot\mathbf{r}} v_{\mathrm{e-i}}(\mathbf{q}) \mathbf{q} \cdot \left[\sum_j \mathbf{u}_j \mathrm{e}^{-i\mathbf{q}\cdot\mathbf{R}_j^{(0)}} \right]. \end{aligned}$$

By using equation (12.15) we obtain

$$\begin{aligned}
&\sum_{j=1}^{J} \mathbf{u}_j e^{-i\mathbf{q}\cdot\mathbf{R}_j^{(0)}} \\
&\quad = \sum_{\substack{\mathbf{q}'\in\mathrm{BZ}\\ \alpha}} \left[\frac{\hbar}{2MJ\omega_{\mathbf{q}',\alpha}}\right]^{1/2} \underbrace{\sum_j e^{i(\mathbf{q}'-\mathbf{q})\cdot\mathbf{R}_j^{(0)}}}_{=J\Delta_{\mathbf{q},\mathbf{q}'}} \xi_{\mathbf{q}',\alpha}\left(\hat{b}_{\mathbf{q}',\alpha}+\hat{b}^{\dagger}_{-\mathbf{q}',\alpha}\right) \\
&\quad = \sum_{\alpha} \left[\frac{\hbar J}{2M\omega_{\mathbf{q},\alpha}}\right]^{1/2} \xi_{\mathbf{q},\alpha}\left(\hat{b}_{\mathbf{q},\alpha}+\hat{b}^{\dagger}_{-\mathbf{q},\alpha}\right)
\end{aligned}$$

so, in total

$$\widetilde{v}(\mathbf{r}) = \frac{i}{\Omega}\sum_{\mathbf{q},\alpha}\left[\frac{\hbar J}{2M\omega_{\mathbf{q},\alpha}}\right]^{1/2} e^{i\mathbf{q}\cdot\mathbf{r}} v_{\mathrm{e-i}}(\mathbf{q})\mathbf{q}\cdot\xi_{\mathbf{q},\alpha}\left(\hat{b}_{\mathbf{q},\alpha}+\hat{b}^{\dagger}_{-\mathbf{q},\alpha}\right).$$

Here we see that the electron–phonon interaction apparently vanishes for purely transverse phonons, since for these we have $\mathbf{q}\cdot\xi = 0$.

It should further be remarked that the sum over $\mathbf{q}$, which stems from the Fourier transform of the electron–ion potential, extends over all vectors $\mathbf{q}$, and is not restricted only to those in the first Brillouin zone. However, the phonons created only have momenta which are contained in the first Brillouin zone, since

$$\hat{b}^{\dagger}_{\mathbf{q},\alpha} = \hat{b}^{\dagger}_{(\mathbf{q}+\mathbf{G}),\alpha} \quad \text{and} \quad \hat{b}_{\mathbf{q},\alpha} = \hat{b}_{(\mathbf{q}+\mathbf{G}),\alpha}.$$

This follows immediately from the definition of the normal coordinates $\hat{U}^{\alpha}_{\mathbf{q}}$ and $\hat{P}^{\alpha}_{\mathbf{q}}$, from which the creation and annihilation operators were formed by linear combinations.

Since each allowed vector $\mathbf{q}$ can be written unambiguously as the sum of a vector in the first Brillouin zone and a reciprocal lattice vector, we can split up the sum over $\mathbf{q}$ in the following way:

$$\sum_{\mathbf{q}} f(\mathbf{q}) = \sum_{\mathbf{q}\in\mathrm{BZ}}\sum_{\mathbf{G}} f(\mathbf{q}+\mathbf{G}).$$

With

$$\omega_{\mathbf{q},\alpha} = \omega_{(\mathbf{q}+\mathbf{G}),\alpha} \text{ and } \xi_{\mathbf{q},\alpha} = \xi_{(\mathbf{q}+\mathbf{G}),\alpha}$$

we then finally obtain

$$\begin{aligned}
\widetilde{v}(\mathbf{r}) &= \frac{i}{\Omega}\sum_{\mathbf{q}\in\mathrm{BZ}}\sum_{\alpha}\sum_{\mathbf{G}}\left[\frac{\hbar J}{2M\omega_{\mathbf{q},\alpha}}\right]^{1/2} e^{i(\mathbf{q}+\mathbf{G})\cdot\mathbf{r}} v_{\mathrm{e-i}}(\mathbf{q}+\mathbf{G}) \\
&\quad \times(\mathbf{q}+\mathbf{G})\cdot\xi_{\mathbf{q},\alpha}\left(\hat{b}_{\mathbf{q},\alpha}+\hat{b}^{\dagger}_{-\mathbf{q},\alpha}\right).
\end{aligned}$$

The only part in this expression that depends on $\mathbf{r}$ is the exponential. To write $\hat{H}_{\mathrm{e-ph}}$ in second quantization, we need the matrix elements of the exponential and the Bloch functions:

$$\langle \psi_{\mathbf{k}',\sigma} \mid \mathrm{e}^{i(\mathbf{q}+\mathbf{G})\cdot\mathbf{r}} \mid \psi_{\mathbf{k}\sigma}\rangle = \underbrace{\sum_{s} \chi_{\sigma}^{*}(s)\chi_{\sigma}(s)}_{=1} \frac{1}{J} \int \mathrm{d}^3 r\, \mathrm{e}^{i(\mathbf{k}+\mathbf{q}+\mathbf{G}-\mathbf{k}')\cdot\mathbf{r}}$$

$$\times \varphi_{\mathbf{k}'}^{*}(\mathbf{r})\varphi_{\mathbf{k}}(\mathbf{r}).$$

In the calculations of the integrals, we can use the fact that the functions $\varphi_{\mathbf{k}}(\mathbf{r})$ are periodic with the lattice and that the lattice constants are small compared to the scale with which the exponential functions change appreciably. Consequently, it is a very good approximation to substitute the unit cell average value $\overline{\varphi_{\mathbf{k}'}^{*}\varphi_{\mathbf{k}}}$ for the product $\varphi_{\mathbf{k}'}^{*}\varphi_{\mathbf{k}}$ in each unit cell (and thus for the entire volume Ω). The matrix element then becomes

$$\frac{1}{J}\overline{\varphi_{\mathbf{k}'}^{*}\varphi_{\mathbf{k}}} \int_{\Omega} \mathrm{d}^3 r\, \mathrm{e}^{i(\mathbf{k}+\mathbf{q}+\mathbf{G}-\mathbf{k}')\cdot\mathbf{r}} = \frac{\Omega}{J}\overline{\varphi_{\mathbf{k}'}^{*}\varphi_{\mathbf{k}}}\,\delta_{\mathbf{k}',\mathbf{k}+\mathbf{q}+\mathbf{G}}.$$

In particular, for the case $\mathbf{k}' = \mathbf{k}+\mathbf{q}+\mathbf{G}$ we have the exact result

$$\begin{aligned} &\frac{1}{J}\int_{\Omega} \mathrm{d}^3 r\, \mathrm{e}^{i(\mathbf{k}+\mathbf{q}+\mathbf{G}-\mathbf{k}')\cdot\mathbf{r}} \varphi_{\mathbf{k}'}^{*}(\mathbf{r})\varphi_{\mathbf{k}}(\mathbf{r}) \\ &= \frac{1}{J}\int_{\Omega} \mathrm{d}^3 r\, \varphi_{\mathbf{k}+\mathbf{q}+\mathbf{G}}^{*}(\mathbf{r})\varphi_{\mathbf{k}}(\mathbf{r}) = \int_{\text{unit cell}} \mathrm{d}^3 r\, \varphi_{\mathbf{k}+\mathbf{q}+\mathbf{G}}^{*}(\mathbf{r})\varphi_{\mathbf{k}}(\mathbf{r}) \\ &\equiv \langle \varphi_{\mathbf{k}+\mathbf{q}+\mathbf{G}} \mid \varphi_{\mathbf{k}}\rangle, \end{aligned}$$

where the overlap integral is evaluated over one unit cell. Hence, the unit cell average above is for the case $\mathbf{k}' = \mathbf{k}+\mathbf{q}+\mathbf{G}$ exactly equal to the overlap integral:

$$\overline{\varphi_{\mathbf{k}+\mathbf{q}+\mathbf{G}}^{*}\varphi_{\mathbf{k}}} = \frac{\langle \varphi_{\mathbf{k}+\mathbf{q}+\mathbf{G}} \mid \varphi_{\mathbf{k}}\rangle}{\Omega/J}$$

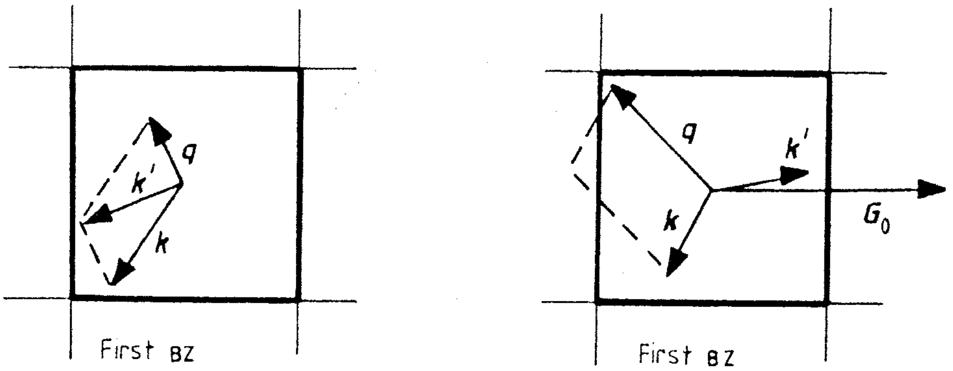
normalized with respect to the unit cell volume.

We then obtain in total

$$\langle \psi_{\mathbf{k}'\sigma} \mid \mathrm{e}^{i(\mathbf{q}+\mathbf{G})\cdot\mathbf{r}} \mid \psi_{\mathbf{k}\sigma}\rangle = \langle \varphi_{\mathbf{k}+\mathbf{q}+\mathbf{G}} \mid \varphi_{\mathbf{k}}\rangle \delta_{\mathbf{k}',\mathbf{k}+\mathbf{q}+\mathbf{G}}.$$

Due to the Kronecker-delta, not only does the sum over $\mathbf{k}'$ reduce to a single term, but the sum over reciprocal lattice vectors $\mathbf{G}$ is also reduced. For $\mathbf{k},\mathbf{q} \in$ BZ there can only be a single reciprocal lattice vector $\mathbf{G}(\mathbf{k},\mathbf{q})$ such that $\mathbf{k}'$ also lies in the first Brillouin zone. This is clearly illustrated in figure 12.4. We have

$$\mathbf{G}(\mathbf{k},\mathbf{q}) = \begin{cases} 0 & \text{if } \mathbf{k}+\mathbf{q} \text{ is in the first BZ} \\ G_0 & \text{otherwise} \end{cases}$$



$k' = k + q$

$k' = k + q + G_0$

Figure 12.4 *If* $\mathbf{k} + \mathbf{q}$ *is not in the first BZ, we can write* $\mathbf{k}' = \mathbf{k} + \mathbf{q} + \mathbf{G}_0$, *where* $\mathbf{k}'$ *is in the first BZ, and* $\mathbf{G}_0$ *is a reciprocal lattice vector.*

The entire electron–phonon interaction is then

$$\begin{aligned}\hat{H}_{\text{e-ph}} &= \frac{i}{\Omega}\sum_{\mathbf{k},\mathbf{q}\in\text{BZ}}\sum_{\sigma}\sum_{\alpha=1}^{3}\left[\frac{\hbar J}{2M\omega_{\mathbf{q},\alpha}}\right]^{1/2}\langle\varphi_{\mathbf{k}+\mathbf{q}+\mathbf{G}}\mid\varphi_{\mathbf{k}}\rangle v_{\text{e-i}}(\mathbf{q}+\mathbf{G}) \\ &\quad\times(\mathbf{q}+\mathbf{G})\cdot\xi_{\mathbf{q},\alpha}\left(\hat{b}_{\mathbf{q},\alpha}+\hat{b}^{\dagger}_{-\mathbf{q},\alpha}\right)\hat{c}^{\dagger}_{(\mathbf{k}+\mathbf{q}+\mathbf{G})\sigma}\hat{c}_{\mathbf{k}\sigma} \qquad (12.16)\end{aligned}$$

The interaction thus consists of processes in which the momentum of an electron changes by $\mathbf{q}+\mathbf{G}$, either by absorption of a phonon of momentum $\mathbf{q}$ or by emission of a phonon of momentum $(-\mathbf{q})$. If also $\mathbf{G} = 0$, the process is called a normal process, and if $\mathbf{G} = \mathbf{G}_0$ (see figure 12.4), the process is called an Umklapp process. (Such a distinction between normal and Umklapp processes can also be made for the case of the phonon–phonon interaction discussed previously.) The electron–phonon interaction equation (12.16) plays a role for example in the description of the electrical conductivity.

Chapter 13

Superconductivity

The most striking consequence of the electron–phonon interaction is superconductivity: below a certain temperature, the transition temperature, the electrical resistivity of many materials disappears. We cannot here go into the phenomenology of superconductivity, and can only address the basic concepts of the theory of Bardeen, Cooper and Schrieffer (BCS)[7] and of Bogoliubov [8] and of Valatin [9]. Our goal is just to show how helpful many-particle theory is to the understanding of superconductivity. Furthermore, we should get a hint of the importance of symmetry-breaking and anomalous expectation values. We will in this chapter only discuss phonon-mediated superconductivity within the weak-coupling BCS theory.

The first clue as to the nature of the phenomenon is offered by the fact that the transition temperature is different for different isotopes of the same material. This means that the motion of the nuclei, *i.e.*, the phonons, plays a role. The system of electrons and phonons will be described as in Chapter 12 by a Hamiltonian of the form

$$\hat{H} = \hat{H}_{\mathrm{e}}^{(0)} + \hat{H}_{\mathrm{e-ph}} + \hat{H}_{\mathrm{ph}}.$$

Here

$$\hat{H}_{\mathrm{e}}^{(0)} = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} \hat{c}^{\dagger}_{\mathbf{k}\sigma} \hat{c}_{\mathbf{k}\sigma}$$

already contains the effect of the rigid, periodic lattice. Hence, we will in this chapter by 'electrons' mean Bloch states. For later use, we introduce the ground state of $\hat{H}_{\mathrm{e}}^{(0)}$: all states with single-particle energies ϵ_k below the Fermi energy ϵ_F, which depends on the number of electrons, are occupied; all others are empty (we will assume that $\epsilon_k = \epsilon_{-k}$):

$$| \Psi_n \rangle = \prod_{\substack{\epsilon_k < \epsilon_F \\ \sigma}} \hat{c}^{\dagger}_{\mathbf{k}\sigma} \mid \mathrm{vac} \rangle = \prod_{\epsilon_k < \epsilon_F} \left(\hat{c}^{\dagger}_{\mathbf{k}\uparrow} \hat{c}^{\dagger}_{-\mathbf{k}\downarrow} \right) \mid \mathrm{vac} \rangle . \qquad (13.1)$$

The operator

$$\hat{H}_{\text{ph}} = \sum_{q \in \text{BZ}} \omega_q \left(\hat{b}_{\mathbf{q}}^{\dagger} \hat{b}_{\mathbf{q}} + \frac{1}{2} \right)$$

describes the phonons, which we assume do not interact with one another. For simplicity, we also restrict ourselves to one polarization. The electron–phonon interaction, $\hat{H}_{\text{e-ph}}$, results in an effective electron–electron interaction by the exchange of phonons. We write $\hat{H}_{\text{e-ph}}$ as

$$\hat{H}_{\text{e-ph}} = \sum_{\mathbf{k},\mathbf{q} \in \text{BZ}} \sum_{\sigma} V_q \left(\hat{b}_{\mathbf{q}} + \hat{b}_{-\mathbf{q}}^{\dagger} \right) \hat{c}_{(\mathbf{k}+\mathbf{q})\sigma}^{\dagger} \hat{c}_{\mathbf{k}\sigma}$$

where we for simplicity have ignored Umklapp processes and have taken the interaction V_q to depend only of the magnitude of $\mathbf{q}$. The operator $\hat{H}_{\text{e-ph}}$ does not commute with the phonon-number operator, $\sum_{\mathbf{q}} \hat{b}_{\mathbf{q}}^{\dagger} \hat{b}_{\mathbf{q}}$, but does commute with the electron number operator, $\sum_{\mathbf{k}\sigma} \hat{c}_{\mathbf{k}\sigma}^{\dagger} \hat{c}_{\mathbf{k}\sigma}$. Hence, a state with a fixed number of phonons cannot be an eigenstate of $\hat{H}$. To get some understanding of how this affects the time-evolution of a single electron under $\hat{H}$, we consider a small time-increment δ from an initial time $t = 0$ and Taylor-expand:

$$f(t_0 + \delta) \cong f(t_0) + \delta \frac{\partial f}{\partial t} |_{t=t_0} .$$

At time $t_0 = 0$, the initial state is

$$| \phi(t = 0) \rangle \quad = \quad \hat{c}_{\mathbf{k}\sigma}^{\dagger} \mid \text{vac} \rangle$$

and at $t = \delta$, the state is

$$\begin{aligned} | \phi(t = \delta) \rangle \quad &\cong \quad \left(1 - i\delta \hat{H} \right) | \phi(t) \rangle |_{t=0} \\ &= \quad \left[(1 - i\delta\epsilon_k)\, \hat{c}_{\mathbf{k}\sigma}^{\dagger} - i\delta \sum_{\mathbf{q}} V_q \hat{b}_{-\mathbf{q}}^{\dagger} \hat{c}_{(\mathbf{k}+\mathbf{q})\sigma}^{\dagger} \right] | \text{vac} \rangle . \end{aligned}$$

This time-evolution shows that the electron will emit a phonon with a certain probability, and V_q gives the corresponding probability amplitude. In the further time evolution, the possibility of reabsorbing phonons enters in addition to the possibility of emitting a second phonon. This simple argument demonstrates that:

(1) the electron is surrounded by a phonon cloud due to the interaction $\hat{H}_{\text{e-ph}}$;

(2) as a consequence, the properties of the electron, in particular its dispersion relation ϵ_k, will be changed.

We can treat the electron–phonon interaction as a perturbation and calculate the electron energies using perturbation theory. In second order we obtain a reduction in the electron energy. We use the standard formula

$$(\Delta E)^{(2)} = \sum_{n_e,n_{\text{ph}}} \frac{\langle \phi_{1,0} \mid \hat{H}_{\text{e-ph}} \mid \phi_{n_e,n_{\text{ph}}} \rangle \langle \phi_{n_e,n_{\text{ph}}} \mid \hat{H}_{\text{e-ph}} \mid \phi_{1,0} \rangle}{W_{1,0} - W_{n_e,n_{\text{ph}}}}.$$

The sum runs over all eigenstates $\mid \phi_{n_e,n_{\text{ph}}} \rangle$ of $\left(\hat{H}_{\text{e}}^{(0)} + \hat{H}_{\text{ph}}\right)$ with n_{e} electrons and n_{ph} phonons, respectively. If we set

$$\mid \phi_{1,0} \rangle = \hat{c}^\dagger_{\mathbf{k}\sigma} \mid \text{vac} \rangle \quad W_{1,0} = \epsilon_k$$

we obtain

$$\hat{H}_{\text{e-ph}} \mid \phi_{1,0} \rangle = \sum_{\mathbf{q},\mathbf{p},\alpha} V_q \left(\hat{b}_{\mathbf{q}} + \hat{b}^\dagger_{-\mathbf{q}}\right) \hat{c}^\dagger_{(\mathbf{p}+\mathbf{q})\alpha} \underbrace{\hat{c}_{\mathbf{p},\alpha} \hat{c}^\dagger_{\mathbf{k}\sigma}}_{=\delta_{\mathbf{p},\mathbf{k}}\delta_{\alpha\sigma} - \hat{c}^\dagger_{\mathbf{k}\sigma}\hat{c}_{\mathbf{p}\alpha}} \mid \text{vac} \rangle$$

and since $\hat{b}_{\mathbf{q}} \mid \text{vac} \rangle = 0 = \hat{c}_{\mathbf{p}\alpha} \mid \text{vac} \rangle$, we furthermore obtain

$$\hat{H}_{\text{e-ph}} = \sum_{\mathbf{q}} V_q \hat{b}^\dagger_{-\mathbf{q}} \hat{c}^\dagger_{(\mathbf{k}+\mathbf{q})\sigma} \mid \text{vac} \rangle.$$

In the sum

$$\sum_{n_e,n_{\text{ph}}} \mid \phi_{n_e,n_{\text{ph}}} \rangle \langle \phi_{n_e,n_{\text{ph}}} \mid$$

only the state

$$\hat{b}^\dagger_{-\mathbf{q}} \hat{c}^\dagger_{(\mathbf{k}+\mathbf{q})\sigma} \mid \text{vac} \rangle$$

with energy

$$W_{1,1} = \epsilon_{k+q} + \omega_{-q} = \epsilon_{k+q} + \omega_q$$

leaves a non-vanishing contribution. The energy shift then becomes

$$\begin{aligned}
(\Delta E)^{(2)} &= \sum_{\mathbf{q}} V_q \frac{1}{\epsilon_k - (\epsilon_{k+q} + \omega_q)} \langle \phi_{1,0} \mid \hat{H}_{\text{e-ph}} \hat{b}^\dagger_{-\mathbf{q}} \hat{c}^\dagger_{(\mathbf{k}+\mathbf{q})\sigma} \mid \text{vac} \rangle \\
&= \sum_{\mathbf{q}} \frac{V_q}{\epsilon_k - (\epsilon_{k+q} + \omega_q)} \\
&\quad \times \sum_{\mathbf{q}',\mathbf{p}'\alpha'} V_{q'} \langle \text{vac} \mid \hat{c}_{\mathbf{q}\sigma} \left(\hat{b}_{\mathbf{q}'} + \hat{b}^\dagger_{-\mathbf{q}'}\right) \hat{c}^\dagger_{(\mathbf{p}'+\mathbf{q}')\alpha'} \hat{c}_{\mathbf{p}'\alpha'} \hat{b}^\dagger_{-\mathbf{q}} \hat{c}^\dagger_{(\mathbf{k}+\mathbf{q})\sigma} \mid \text{vac} \rangle \\
&= \sum_{\mathbf{q}} \frac{V_q}{\epsilon_k - (\epsilon_{k+q} + \omega_q)}
\end{aligned}$$

$$\times \sum_{\mathbf{q}'\mathbf{p}'\alpha'} V_{q'} \langle \text{vac} \mid \underbrace{\hat{b}_{\mathbf{q}'}\hat{b}^\dagger_{-\mathbf{q}}}_{=\delta_{\mathbf{q}',-\mathbf{q}}+\hat{b}^\dagger_{-\mathbf{q}}\hat{b}_{\mathbf{q}'}} \hat{c}_{\mathbf{k}\sigma}\hat{c}^\dagger_{(\mathbf{p}'+\mathbf{q}')\alpha'} \underbrace{\hat{c}_{\mathbf{p}'\alpha'}\hat{c}^\dagger_{(\mathbf{k}+\mathbf{q})\sigma}}_{=\delta_{\alpha'\sigma}\delta_{\mathbf{p}',(\mathbf{k}+\mathbf{q})}-\hat{c}^\dagger_{(\mathbf{k}+\mathbf{q})\sigma}\hat{c}_{\mathbf{p}'\alpha'}} \mid \text{vac}\rangle$$

$$= \sum_{\mathbf{q}} \frac{V_q V_{-q}}{\epsilon_k - (\epsilon_{k+q} + \omega_q)} \underbrace{\langle \text{vac} \mid \hat{c}_{\mathbf{k}\sigma}\hat{c}^\dagger_{\mathbf{k}\sigma} \mid \text{vac}\rangle}_{=1}.$$

Finally, we use $V_{-q} = V_q^*$, which must hold for any potential which is real in coordinate space, and obtain

$$(\Delta E)^{(2)}_{\mathbf{k}} = \sum_{\mathbf{q}} \frac{|V_q|^2}{\epsilon_k - (\epsilon_{k+q} + \omega_q)}.$$

What we obtain is a modified dispersion relation for the electron under consideration. One says that the electron properties are renormalized.

If one calculates second-order energy-shift of a two-electron state $\hat{c}^\dagger_{\mathbf{k}\sigma}\hat{c}^\dagger_{\mathbf{k}'\sigma'} \mid \text{vac}\rangle$, a contribution which consists of the exchange of a phonon with momentum $\mathbf{q}$ appears in addition to the energy-shift above for each electron. The phonon-exchange term is

$$\begin{aligned}(\Delta E)^{(2)}_{\mathbf{k},\mathbf{k}'} \quad = \quad & \sum_q \frac{|V_q|^2}{\epsilon_k - (\epsilon_{k+q} + \omega_q)} + \frac{|V_q|^2}{\epsilon_{k'} - (\epsilon_{k'-q} + \omega_q)} \\ & + \sum_{\mathbf{q}} |V_q|^2 \left[\frac{1}{(\epsilon_k + \epsilon_{k'}) - (\epsilon_{k+q} + \epsilon_{k'} + \omega_q)} \right. \\ & \left. + \frac{1}{(\epsilon_k + \epsilon_{k'}) - (\epsilon_{k'-q} + \epsilon_k + \omega_q)} \right] \\ & \times \langle \text{vac} \mid \hat{c}_{\mathbf{k}'\sigma'}\hat{c}_{\mathbf{k}\sigma}\hat{c}^\dagger{}_{(\mathbf{k}+\mathbf{q})\sigma}\hat{c}^\dagger{}_{(\mathbf{k}'-\mathbf{q})\sigma'} \mid \text{vac}\rangle\end{aligned}$$

The matrix element in the last term vanishes unless $\mathbf{q} = 0$ or $\sigma = \sigma'$ and $\mathbf{k}' = \mathbf{k} + \mathbf{q}$, *i.e.*, unless $\mathbf{k} = \mathbf{k}' - \mathbf{q}$. Note that the phonon-exchange term has the form of a contribution in *first*-order perturbation theory with an effective electron–electron potential

$$\frac{1}{2} \sum_{\mathbf{q}} \sum_{\substack{\mathbf{k}\sigma \\ \mathbf{k}'\sigma'}} V^{\text{eff}}_q(\mathbf{k}, \mathbf{k}') \hat{c}^\dagger_{(\mathbf{k}+\mathbf{q})\sigma} \hat{c}^\dagger_{(\mathbf{k}'-\mathbf{q})\sigma'} \hat{c}_{\mathbf{k}'\sigma'} \hat{c}_{\mathbf{k}\sigma}$$

where

$$V^{\text{eff}}_q(\mathbf{k}, \mathbf{k}') = |V_q|^2 \left[\frac{1}{\epsilon_k - (\epsilon_{k+q} + \omega_q)} + \frac{1}{\epsilon_{k'} - (\epsilon_{k'-q} + \omega_q)} \right]. \qquad (13.2)$$

It is also clear that such a term (among many others) appears if the initial state in addition to $(\mathbf{k}\sigma)$ and $(\mathbf{k}'\sigma')$ contains other electrons and possibly other phonons, and that such a term also appears as an intermediate state in higher order perturbation theory. In these cases, processes for which

$$\epsilon_{k+q} - \epsilon_k \approx \epsilon_{k'} - \epsilon_{k'-q} \tag{13.3}$$

are particularly important (in the example above, equation (13.3) holds exactly in second order perturbation theory for the non-vanishing contributions). Equation (13.2) becomes with the approximation equation (13.3)

$$V_q^{\text{eff}} \cong |V_q|^2 \frac{2\omega_q}{(\epsilon_{k+q} - \epsilon_k)^2 - \omega_q^2}. \tag{13.4}$$

For the two electrons to affect one another through this indirect scattering process, the final states $(\mathbf{k}+\mathbf{q}, \sigma)$ and $(\mathbf{k}'-\mathbf{q}, \sigma')$ must be unoccupied. Right at the Fermi energy ϵ_F, occupied and unoccupied states lie closely together and can therefore easily be mixed, and the effective interaction equation (13.4) becomes relatively large and attractive:

$$\epsilon_k,\, \epsilon_{k'},\, \epsilon_{k+q},\, \epsilon_{k'-q} \cong \epsilon_F \;\Rightarrow\; V_q^{\text{eff}} \cong -\frac{|V_q|^2}{\omega_q}.$$

The picture of the superconducting mechanism is hinted at in this attractive interaction. An electron deforms the crystal lattice in its surrounding, which implies that the electron emits phonons; the deformation and polarization acts as an attraction on other electrons.

The elementary calculations above can be more elegantly formulated with the methods that we will discuss in later chapters. Here, we only wanted to demonstrate that the electron–phonon coupling can lead to an effective electron–electron interaction. To understand superconductivity, it is important to realize that a weak attractive interaction between two fermions alone does not necessarily lead to a bound state. We can illustrate this fact by the following example. If we transform to center-of-mass and relative coordinates for the two particles under consideration, we obtain the problem of a single particle in an attractive potential. In three-dimensional space, this potential must have a certain minimum strength to lead to a bound state. A thorough discussion on the connection between density-of-states, dimensionality of space and the appearance of bound states can be found in Economou [10]. As a model, we consider a three-dimensional potential well with a characteristic length R of the range of the potential, and an effective depth V_0. The spatial extent of the wavefunction is characterized by a length a. The potential energy is approximately

$$E_{\text{pot}} \cong \begin{cases} -\left[\frac{R}{a}\right]^3 V_0 & \text{for } R < a \\ -V_0 & \text{for } a \leq R \end{cases}$$

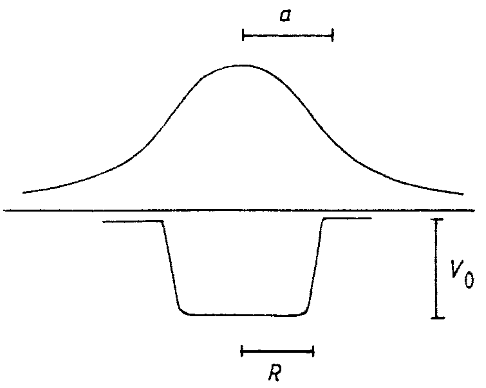


Figure 13.1 *A wavefunction of extent a/R in a potential well of depth V_0 and width R.*

and the kinetic energy is

$$E_{\text{kin}} \cong \left[\frac{\hbar}{a}\right]^2 \frac{1}{2m}.$$

The total energy is depicted as a function of a in figure 13.2.

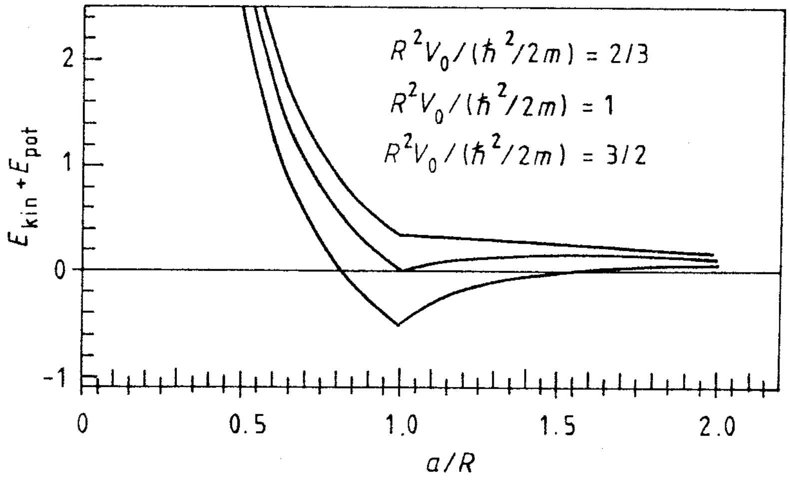


Figure 13.2 *Total energy as function of a for the simple model above.*

With this simple estimate we obtain a bound state, *i.e.*, $E_{\text{pot}}+E_{\text{kin}} < 0$, only for $V_0 > \hbar^2/(2mR^2)$. In this case the extent of the wavefunction is approximately equal to the extent of the well ($R \cong a$). Thus, for $V_0 < \hbar^2/(2mR^2)$ the reduction in interaction energy does not make up for the increase in kinetic energy, and it is energetically favorable for the two fermions to move independently in states with small kinetic energy.

We now consider two electrons on the Fermi surface. They would like to lower their energy by forming a bound state of a relatively large extent from the states available to them. Such states only have momenta at least of the order of k_F, because of the Pauli principle. This is a many-body effect in so far as the other electrons are necessary to occupy states with lower momenta. If the effective interaction is attractive even only over small distances, the two electrons will arrange their spins to be parallel (otherwise, they cannot come near each other) and form a spin singlet. The understanding of this so-called Cooper instability of the electron gas by the formation of pairs in the presence of a weak particle–particle interaction at low temperatures (we consider here $T = 0$ and start out from a sharp Fermi surface at ϵ_F) will of course not entirely clarify the question of the nature of the superconducting state. First of all, we have inadmissibly distinguished the two electrons from all the others. Secondly, we have extrapolated the concept that 'every two electrons form a Cooper pair' to the paradoxical situation that eventually no unperturbed electrons will remain within the Fermi surface, *i.e.*, below the Fermi energy. Therefore, the argument for the pair formation becomes questionable. However, from this discussion we can understand that the electrons tend to form singlet pairs in the presence of a weak attractive interaction. However, in a many-electron system, this picture is complicated by the fact that we have to consider how electron form pairs in the presence of other electrons, which also form pairs. Hence, the problem have to be solved self-consistently, with the electron pairing and the background of the other electrons determined simultaneously.

It is impossible to calculate the coupled electron–phonon system so precisely that we can obtain the tiny energy difference between superconducting and normal states as differences between total energies. (The energy scale of the transition temperature×Boltzmann's constant $\simeq 5 \times 10^{-4}$ eV, which sets the scale for the desired energy differences.) We are not interested in attempting to calculate details such as the dispersion relation ϵ_k of the Bloch electrons and the electron–phonon interaction to such an accuracy. Rather, it is important to understand the *difference* between the normal-conductor and the superconductor phases. For this, it suffices to consider the piece of the Hamiltonian which is responsible for the difference between these two phases. We investigate the situation which is associated with Cooper pairs at rest. We imagine that we can cast the phonon degrees of freedom in the form of an effective electron–electron interaction, and that we in this interaction only keep the part which contains two Cooper pairs:

$$\hat{H}_{\text{red}} \equiv \sum_{\mathbf{p}\sigma} \epsilon_p \hat{c}^\dagger_{\mathbf{p}\sigma} \hat{c}_{\mathbf{p}\sigma} + \sum_{\mathbf{p},\mathbf{q}} V_{pq} \hat{c}^\dagger_{\mathbf{p}\uparrow} \hat{c}^\dagger_{-\mathbf{p}\downarrow} \hat{c}_{-\mathbf{q}\downarrow} \hat{c}_{\mathbf{q}\uparrow}. \qquad (13.5)$$

We optimize the wavefunction of Bardeen, Cooper and Schrieffer with respect to this Hamiltonian. This wavefunction is written as

$$\mid \Psi_{\text{BCS}} \rangle \equiv \prod_{\mathbf{k}} \left(u_k + v_k \hat{c}^\dagger_{\mathbf{k}\uparrow} \hat{c}^\dagger_{-\mathbf{k}\downarrow} \right) \mid \text{vac} \rangle. \qquad (13.6)$$

We quickly see something new and surprising in this harmless-looking *ansatz.* The particle number is not a good quantum number for the general BCS function; parts with different particle numbers will be mixed. It should be remarked that the limiting case

$$\begin{array}{llll} |v_k| = 1 & \text{and} & u_k = 0 & \text{for } \epsilon_k < \epsilon_F \\ v_k = 0 & \text{and} & |u_k| = 1 & \text{otherwise} \end{array}$$

leads to the ground state of the unperturbed problem $\hat{H}_{\mathrm{e}}^{(0)}$ (*cf.* equation (13.1)).

We can determine the following expectation values by using the anti-commutation relations for fermions:

$$\begin{aligned} \langle \Psi_{\mathrm{BCS}} \mid \Psi_{\mathrm{BCS}} \rangle &= \prod_{\mathbf{p}} (u_p^* u_p + v_p^* v_p) \\ \langle \Psi_{\mathrm{BCS}} \mid \hat{N} \mid \Psi_{\mathrm{BCS}} \rangle &= 2 \sum_{\mathbf{k}} v_k^* v_k \times \prod_{\mathbf{p} \neq \mathbf{k}} (u_p^* u_p + v_p^* v_p) \\ \langle \Psi_{\mathrm{BCS}} \mid \hat{H}_{\mathrm{red}} \mid \Psi_{\mathrm{BCS}} \rangle &= 2 \sum_{\mathbf{k}} \epsilon_k v_k^* v_k \times \prod_{\mathbf{p} \neq \mathbf{k}} (u_p^* u_p + v_p^* v_p) \\ &\quad + \sum_{\mathbf{k},\mathbf{k}'} V_{kk'} u_{k'}^* v_k^* u_k v_{k'} \times \prod_{\substack{\mathbf{p} \neq \mathbf{k} \\ \mathbf{p} \neq \mathbf{k}'}} (u_p^* u_p + v_p^* v_p) \end{aligned}$$

The requirement of a determined particular particle number can only be satisfied on the average. This is accomplished as usual by the introduction of a chemical potential μ ($= \epsilon_F$). To normalize the state, we choose

$$|u_k|^2 + |v_k|^2 = 1$$

and u_k real and positive for all $\mathbf{k}$. This constraint can be satisfied by taking

$$u_k \equiv \sin\theta_k, \qquad v_k \equiv \mathrm{e}^{i\phi_k} \cos\theta_k$$

in the expression which is to be minimized:

$$\langle \Psi_{\mathrm{BCS}} \mid \hat{H}_{\mathrm{red}} - \mu \hat{N} \mid \Psi_{\mathrm{BCS}} \rangle .$$

The result is

$$\begin{aligned} & 2 \sum_{\mathbf{k}} (\epsilon_k - \mu) \cos^2\theta_k + \frac{1}{4} \sum_{\mathbf{k}} \sum_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'} (2 \sin\theta_k \cos\theta_k) \\ & \qquad \times (2 \sin\theta_{k'} \cos\theta_{k'}) \, \mathrm{e}^{i(\phi_{k'} - \phi_k)} \\ = & \quad \sum_{\mathbf{k}} (\epsilon_k - \mu)(1 + \cos(2\theta_k)) + \sum_{\mathbf{k}\mathbf{k}'} \frac{1}{4} V_{kk'} \sin(2\theta_k) \sin(2\theta_{k'}) \mathrm{e}^{i(\phi_{k'} - \phi_k)} . \end{aligned} \tag{13.7}$$

The condition of stationarity can be satisfied by

$$\phi_k = \alpha \tag{13.8}$$

with α an arbitrary constant, independent of k, and

$$\tan 2\theta_k = -\left(\mathrm{e}^{-i\alpha}\Delta_k\right)/(\epsilon_k - \mu) \tag{13.9}$$

where

$$\begin{aligned} \Delta_k &\equiv -\sum_{\mathbf{k}'} V_{kk'} u^*_{k'} v_{k'} \\ &= -\sum_{\mathbf{k}'} V_{kk'} \langle \Psi_{\mathrm{BCS}} \mid \hat{c}_{-\mathbf{k}'\downarrow} \hat{c}_{\mathbf{k}'\uparrow} \mid \Psi_{\mathrm{BCS}} \rangle . \end{aligned} \tag{13.10}$$

Hence, we have to investigate the equation

$$|\Delta_k| = \mathrm{e}^{-i\alpha}\Delta_k = -\frac{1}{2}\sum_{\mathbf{k}'} V_{kk'} \sin(2\theta_{k'})$$

where we have assumed that $V_{kk'} < 0$. This equation has the form of an integral equation in the continuum limit of $\mathbf{k}$ and $\mathbf{k}'$:

$$\begin{aligned} |\Delta_k| &= -\frac{1}{2}\sum_{\mathbf{k}'} V_{kk'} \sin\left\{\arctan\left[-\frac{|\Delta_{k'}|}{\epsilon_{k'} - \mu}\right]\right\} \\ &= -\frac{1}{2}\sum_{\mathbf{k}'} V_{kk'} \frac{|\Delta_{k'}|}{\sqrt{|\Delta_{k'}|^2 + (\epsilon_{k'} - \mu)^2}} \\ &= -\frac{1}{2}\sum_{\mathbf{k}'} V_{kk'} \frac{|\Delta_{k'}|}{E_{k'}}, \end{aligned} \tag{13.11}$$

with the abbreviation $E_k \equiv \sqrt{|\Delta_k|^2 + (\epsilon_k - \mu)^2}$. The solution of equation (13.11) is particularly simple if we take into consideration the fact that the effective interaction is particularly strong near the Fermi energy ($\epsilon_k \cong \mu$) and can be modeled by the simple approximation

$$V_{kk'} = \begin{cases} -V/\Omega & \text{if } |\epsilon_k - \mu| < \omega_D \text{ and } |\epsilon_{k'} - \mu| < \omega_D \\ 0 & \text{otherwise.} \end{cases} \tag{13.12}$$

Here ω_D is a cut-off parameter of the order of a typical phonon energy, a few meV. With this model interaction, the $\mathbf{k}$-dependence of Δ_k and θ_k simplifies:

$$\Delta_k = \begin{cases} \Delta & \text{for } |\epsilon_k - \mu| < \omega_D \\ 0 & \text{otherwise} \end{cases}, \tag{13.13}$$

$$\sin(2\theta_k) = \begin{cases} |\Delta|/E_k & \text{for } |\epsilon_k - \mu| < \omega_D \\ 0 & \text{otherwise} \end{cases}$$

$$|v_k|^2 = \frac{1}{2}\left[1+\cos(2\theta_k)\right] = \begin{cases} 1 & \text{for } \epsilon_k - \mu < -\omega_D \\ \frac{1}{2}\left[1 - \frac{\epsilon_k-\mu}{E_k}\right] & \text{for } |\epsilon_k - \mu < \omega_D \\ 0 & \text{for } \epsilon_k - \mu > \omega_D. \end{cases} \tag{13.14}$$

Then Δ is the solution of a *single* equation

$$1 = \frac{1}{2}\frac{V}{\Omega} \sum_{|\epsilon_k-\mu|<\omega_D} \frac{1}{\sqrt{(\epsilon_k-\mu)^2+|\Delta|^2}}. \tag{13.15}$$

The phase factor $\Delta/|\Delta| = \mathrm{e}^{i\alpha}$ remains undetermined.

In the so-called weak-coupling limit, which means that the product of the strength V of the effective interaction with the density-of-states at the Fermi energy $\nu(0) = \frac{1}{\Omega}\frac{\mathrm{d}N}{\mathrm{d}\epsilon}|_{\epsilon=\mu}$ is small compared to the Fermi energy, and that the denisty-of-states in the energy range of the integration can be taken to be $\nu(0)$, the sum in equation (13.15) can be replaced by an integral which yields

$$\begin{aligned} 1 &= \frac{1}{2}V\nu(0)\int_{\mu-\omega_D}^{\mu+\omega_D} \frac{\mathrm{d}\epsilon}{\sqrt{(\epsilon-\mu)^2+|\Delta|^2}} \\ &= V\nu(0)\sinh^{-1}(\omega_D/|\Delta|) \end{aligned}$$

or

$$|\Delta| = \frac{\omega_D}{\sinh\left[\frac{1}{\nu(0)V}\right]} \cong 2\omega_D \mathrm{e}^{-\frac{1}{(\nu(0)V)}}. \tag{13.16}$$

The difference in total energy (see equations (13.7), (13.1), and the definition (13.10)) between the BCS state and the normal state is then

$$\begin{aligned} \delta E &= \langle \Psi_{\mathrm{BCS}} \mid \hat{H}_{\mathrm{red}} - \mu\hat{N} \mid \Psi_{\mathrm{BCS}}\rangle - \langle \Psi_n \mid \hat{H}_{\mathrm{red}} - \mu N \mid \Psi_n\rangle \\ &= \sum_{\mathbf{k}} \left[(\epsilon_k - \mu)(1+\cos(2\theta_k)) - \frac{1}{2}\sin(2\theta_k)\,|\Delta_k|\right] - \sum_{\epsilon_k \le \mu} 2(\epsilon_k - \mu) \end{aligned}$$

which in weak-coupling limit becomes, with equations (13.10), (13.13), (13.14) and finally equation (13.16)

$$
\begin{aligned}
\frac{\delta E}{\Omega} &= 2\nu(0)\int_{\mu}^{\mu+\omega_D}(\epsilon-\mu)\mathrm{d}\epsilon \\
&\quad +\nu(0)\int_{\mu-\omega_D}^{\mu+\omega_D}(\epsilon-\mu)\frac{-(\epsilon-\mu)\mathrm{d}\epsilon}{\sqrt{(\epsilon-\mu)^2+|\Delta|^2}}-\nu(0)|\Delta|\frac{|\Delta|}{\nu(0)V} \\
&= \nu(0)\omega_D^2-2\nu(0)\frac{\omega_D}{2}\sqrt{\omega_d^2+|\Delta|^2}+2\nu(0)\frac{|\Delta|^2}{2}\sinh^{-1}\frac{\omega_D}{|\Delta|}-\frac{|\Delta|^2}{V} \\
&\cong 0-\frac{1}{2}\nu(0)|\Delta|^2+\nu(0)|\Delta|^2\frac{1}{\nu(0)V}-\frac{|\Delta|^2}{V} \\
&= -\frac{1}{2}\nu(0)|\Delta|^2. \qquad (13.17)
\end{aligned}
$$

In summary, we conclude that in the formation of the BCS-state

(1) energetically deep-lying states remain occupied,

$$|v_k|\cong 1 \quad \text{for} \quad \epsilon_k<\mu-|\Delta|;$$

(2) energetically high-lying states remain unoccupied,

$$v_k\cong 0 \quad \text{for} \quad \epsilon_k>\mu+|\Delta|.$$

Thus, the occupations differ appreciably from those of the normal-conducting state Ψ_n (see equation (13.1)) only in a very small region of order $|\Delta|$. This leads to a reduction in the total energy of the order of $\exp\{-2/(\nu(0)V)\}$, from equation (13.17) with equation (13.16). This expression is not analytic in the strength V of the potential and cannot be obtained from usual perturbation theory, *i.e.*, a power series in V. In view of this fact we will now make a digression and discuss this fact in some detail.

If we examine the calculations above in some detail, we will see that they lead to the following possible interpretation:

For each $\mathbf{k}$, $(u_k+v_k\hat{c}^\dagger_{\mathbf{k}\uparrow}\hat{c}^\dagger_{-\mathbf{k}\downarrow})$ is optimized with respect to the operator

$$\hat{H}(\mathbf{k})=\epsilon_k\left[\hat{c}^\dagger_{\mathbf{k}\uparrow}\hat{c}_{\mathbf{k}\uparrow}\hat{c}^\dagger_{-\mathbf{k}\downarrow}\hat{c}_{-\mathbf{k}\downarrow}\right]-\hat{c}^\dagger_{\mathbf{k}\uparrow}\hat{c}^\dagger_{-\mathbf{k}\downarrow}\Delta_k-\hat{c}_{-\mathbf{k}\downarrow}\hat{c}_{\mathbf{k}\uparrow}\Delta^*_k$$

and the expectation value

$$\Delta_k=-\sum_{\mathbf{k}'}V_{kk'}\langle\hat{c}_{-\mathbf{k}'\downarrow}\hat{c}_{\mathbf{k}'\uparrow}\rangle$$

is determined self-consistently.

This is analogous to the Hartree–Fock operator (here expressed through field operators in the shorthand $\hat{\psi}_x \equiv \hat{\psi}(x)$):

$$\hat{H}_{\mathrm{HF}} = \int \mathrm{d}x \hat{\psi}_x^\dagger \left[-\frac{\hbar^2}{2m}\nabla^2 + u(x) \right] \hat{\psi}_x + \int \mathrm{d}x \int \mathrm{d}y\, \rho(y,y) v(y,x) \hat{\psi}_x^\dagger \hat{\psi}_x - \int \mathrm{d}x \int \mathrm{d}y\, \rho(y,x) v(y,x) \hat{\psi}_y^\dagger \hat{\psi}_x$$

with a self-consistently determined expectation value

$$\rho(y,x) = \langle \hat{\psi}_x^\dagger \hat{\psi}_y \rangle .$$

Just as the direct Coulomb potential and the so-called exchange field of all other electrons enter as an effective potential in the Hartree–Fock approximation, the so-called *anomalous expectation values* of two creation or annihilation operators, *i.e.*, $\langle \hat{c}_{-\mathbf{k}\downarrow} \hat{c}_{\mathbf{k}\uparrow} \rangle$, plays the role of an effective mean-field in the theory of superconductivity . The similarity with the Hartree–Fock approximation becomes clearer if we form the following effective Hamiltonian by taking expectation values of the field operators above in the extremely short-ranged model interaction

$$\int\int (-V)\, \delta(\mathbf{r}-\mathbf{r}') \hat{\psi}_\uparrow^\dagger(\mathbf{r}) \hat{\psi}_\downarrow^\dagger(\mathbf{r}') \hat{\psi}_\downarrow(\mathbf{r}') \hat{\psi}_\uparrow(\mathbf{r}) \mathrm{d}^3 r\, \mathrm{d}^3 r'$$

(ordinary expectation values and constant terms will be ignored, since they are uninteresting). This yields

$$\begin{aligned} \hat{H}_{\mathrm{eff}} &= \sum_\sigma \int \mathrm{d}^3 r\, \hat{\psi}_\sigma^\dagger(\mathbf{r}) \left[\frac{-\hbar^2 \nabla^2}{2m} \right] \hat{\psi}_\sigma(\mathbf{r}) \\ &\quad - \int \mathrm{d}^3 r\, \Delta(\mathbf{r}) \hat{\psi}_\uparrow^\dagger(\mathbf{r}) \hat{\psi}_\downarrow^\dagger(\mathbf{r}) - \int \mathrm{d}^3 r\, \Delta^*(\mathbf{r}) \hat{\psi}_\downarrow(\mathbf{r}) \hat{\psi}_\uparrow(\mathbf{r}) \end{aligned}$$

with the expectation value

$$\Delta(\mathbf{r}) \equiv -(-V) \langle \hat{\psi}_\downarrow(\mathbf{r}) \hat{\psi}_\uparrow(\mathbf{r}) \rangle \tag{13.18}$$

to be determined self-consistently. It should be emphasized that the expectation value of $\hat{H}_{\mathrm{red}}$ in the state Ψ_{BCS} is not a simple sum of the expectation values of $\hat{H}(\mathbf{k})$. The relation between them is shown most quickly by rearranging (momentum- and spin-indices are suppressed):

$$\begin{aligned} \hat{c}^\dagger \hat{c}^\dagger \hat{c}\hat{c} &= \left(\hat{c}^\dagger \hat{c}^\dagger - \langle \hat{c}^\dagger \hat{c}^\dagger \rangle + \langle \hat{c}^\dagger \hat{c}^\dagger \rangle \right) \left(\hat{c}\hat{c} - \langle \hat{c}\hat{c} \rangle + \langle \hat{c}\hat{c} \rangle \right) \\ &= \hat{c}^\dagger \hat{c}^\dagger \langle \hat{c}\hat{c} \rangle + \langle \hat{c}^\dagger \hat{c}^\dagger \rangle \hat{c}\hat{c} - \langle \hat{c}^\dagger \hat{c}^\dagger \rangle \langle \hat{c}\hat{c} \rangle \\ &\quad + \left(\hat{c}^\dagger \hat{c}^\dagger - \langle \hat{c}^\dagger \hat{c}^\dagger \rangle \right) \left(\hat{c}\hat{c} - \langle \hat{c}\hat{c} \rangle \right) . \end{aligned}$$

The first two terms are the same as with the operator $\hat{H}(\mathbf{k})$. The third term is a real number: it is the ubiquitous term which must be present in the calculation of the total energy in order to avoid a double-counting of the interaction energy (*cf.* the discussion of the Hartree–Fock total energy in Chapter 7). The expectation value of the fourth term vanishes for the Ψ_{BCS}-*ansatz*; this term is bilinear in the difference of the expectation values and will henceforth be ignored.

We obtain a meaning of Δ as a 'gap-function', *i.e.*, the energy gap in the excitation spectrum, if we consider the elementary excitations in the BCS-state. This is most elegantly shown, if one convinces oneself that the operators defined by

$$\begin{array}{ll} \hat{\gamma}_{\mathbf{k}0} \equiv u_k \hat{c}_{\mathbf{k}\uparrow} - v_k \hat{c}^{\dagger}_{-\mathbf{k}\downarrow} & \hat{\gamma}^{\dagger}_{\mathbf{k}0} = u^*_k \hat{c}^{\dagger}_{\mathbf{k}\uparrow} - v^*_k \hat{c}_{-\mathbf{k}\downarrow} \\ \hat{\gamma}_{\mathbf{k}1} \equiv v_k \hat{c}^{\dagger}_{\mathbf{k}\uparrow} + u_k \hat{c}_{-\mathbf{k}\downarrow} & \hat{\gamma}^{\dagger}_{\mathbf{k}1} = v^*_k \hat{c}_{\mathbf{k}\uparrow} + u^*_k \hat{c}^{\dagger}_{-\mathbf{k}\downarrow} \end{array} \tag{13.19}$$

so that

$$\begin{array}{rcl} \hat{c}^{\dagger}_{\mathbf{k}\uparrow} & = & u_k \hat{\gamma}^{\dagger}_{\mathbf{k}0} + v^*_k \hat{\gamma}_{\mathbf{k}1} \\ \hat{c}^{\dagger}_{-\mathbf{k}\downarrow} & = & -v^*_k \hat{\gamma}_{\mathbf{k}0} + u_k \hat{\gamma}^{\dagger}_{\mathbf{k}1} \end{array} \tag{13.20}$$

satisfy

$$\begin{array}{rcl} \hat{\gamma}_{\mathbf{k}0} \mid \Psi_{\mathrm{BCS}}\rangle & = & 0 \\ \hat{\gamma}_{\mathbf{k}1} | \Psi_{\mathrm{BCS}}\rangle & = & 0 \end{array} \tag{13.21}$$

The newly introduced operators satisfy the usual anti-commutation relations, even though these operators are mixtures of fermion creation- and annihilation-operators:

$$\begin{array}{lcl} \left\{\hat{\gamma}^{\dagger}_{\mathbf{k}0}, \hat{\gamma}^{\dagger}_{\mathbf{k}'1}\right\} & = 0 = & \{\hat{\gamma}_{\mathbf{k}0}, \hat{\gamma}_{\mathbf{k}'1}\} \\ \left\{\hat{\gamma}_{\mathbf{k}0}, \hat{\gamma}^{\dagger}_{\mathbf{k}'1}\right\} & = 0 = & \left\{\hat{\gamma}_{\mathbf{k}1}, \hat{\gamma}^{\dagger}_{\mathbf{k}'0}\right\} \\ \left\{\hat{\gamma}_{\mathbf{k}0}, \hat{\gamma}^{\dagger}_{\mathbf{k}'0}\right\} & = \delta_{\mathbf{k},\mathbf{k}'} = & \left\{\hat{\gamma}_{\mathbf{k}1}, \hat{\gamma}^{\dagger}_{\mathbf{k}'1}\right\} \end{array} \tag{13.22}$$

By means of equation (13.21) and equation (13.22), these operators can then be interpreted as creation and annihilation operators of fermion quasi-particles on the ground state or on a new 'vacuum state', $\mid \Psi_{\mathrm{BCS}}\rangle$. Using the definitions equations (13.5), (13.19) and (13.20), one can easily calculate the result

$$\hat{H}_{\mathrm{red}} \cong E_{\mathrm{normal}} + \delta E + \sum_{\mathbf{k}} E_k \left(\hat{\gamma}^{\dagger}_{\mathbf{k}0} \hat{\gamma}_{\mathbf{k}0} + \hat{\gamma}^{\dagger}_{\mathbf{k}1} \hat{\gamma}_{\mathbf{k}1}\right).$$

[The relation is not exact in the absence on the right-hand side of the terms discussed above bilinear in the fluctuations $\left(\hat{c}^\dagger\hat{c}^\dagger - \langle\hat{c}^\dagger\hat{c}^\dagger\rangle\right)$ and $(\hat{c}\hat{c} - \langle\hat{c}\hat{c}\rangle)$, respectively.] The smallest possible excitation energy is for the simplified interaction equation (13.12) thus

$$\min_{\mathbf{k}}(E_k) = \min_{\mathbf{k}}\sqrt{|\Delta|^2 + (\epsilon_k - \mu)^2} = |\Delta|.$$

The excitation spectrum of the BCS-state thus exhibits a gap. The Hamiltonian which, for example, contains the interaction of one electron with an electromagnetic field has the structure

$$(\text{electromagnetic field})\,\underbrace{\hat{c}^\dagger_{\text{final state}}}_{(\ldots\hat{\gamma}^\dagger+\ldots\hat{\gamma})}\underbrace{\hat{c}_{\text{initial state}}}_{(\ldots\hat{\gamma}^\dagger+\ldots\hat{\gamma})}\,.$$

Since no quasi-particles are present in the ground state, the factors which contain at least one $\hat{\gamma}$ vanish when they act on $\mid \Psi_{\mathrm{BCS}}\rangle$, so the mean-field must then excite *two* quasi-particles; in experiments on optical absorption one finds stronger absorption only for photon energies larger than $2|\Delta|$. This absorption lies in the far infrared $(10^{10} - 10^{12}\mathrm{Hz})$.

The spatially homogeneous state $\mid \Psi_{\mathrm{BCS}}\rangle$, which we calculated within the approximation equation (13.12), is characterized by a complex order parameter, which is the expectation value

$$\Delta(\mathbf{r}) = V\langle\Psi_{\mathrm{BCS}} \mid \hat{\psi}_\downarrow(\mathbf{r})\hat{\psi}_\uparrow(\mathbf{r}) \mid \Psi_{\mathrm{BCS}}\rangle.$$

If we insert the transformation to momentum-annihilation operators and use the adjoint equation of equation (13.20), we obtain furthermore

$$\begin{aligned}
\Delta(\mathbf{r}) &= V\frac{1}{\Omega}\sum_{\mathbf{k}\mathbf{k}'} \mathrm{e}^{i(\mathbf{k}'-\mathbf{k})\cdot\mathbf{r}}\langle\Psi_{\mathrm{BCS}} \mid \hat{c}_{-\mathbf{k}\downarrow}\hat{c}_{\mathbf{k}'\uparrow} \mid \Psi_{\mathrm{BCS}}\rangle \\
&= V\frac{1}{\Omega}\sum_{\mathbf{k}\mathbf{k}'} \mathrm{e}^{-i(\mathbf{k}'-\mathbf{k})\cdot\mathbf{r}} u_k^* v_{k'}\underbrace{\langle\Psi_{\mathrm{BCS}} \mid \hat{\gamma}_{\mathbf{k}1}\hat{\gamma}^\dagger_{\mathbf{k}'1} \mid \Psi_{\mathrm{BCS}}\rangle}_{=\delta_{\mathbf{k}\mathbf{k}'}} \\
&= \sum_{\mathbf{k}} \frac{V}{\Omega}u_k^* v_k = \Delta = \mathrm{e}^{i\alpha}|\Delta|.
\end{aligned}$$

Different values of the phase factor $\mathrm{e}^{i\alpha}$ are degenerate in energy. It is obvious that we cannot start with a wavefunction for the normal state where $\langle\hat{\psi}_\downarrow\hat{\psi}_\uparrow\rangle = 0$ (in this state the symmetry of α is not broken) and do a perturbation expansion in an operator which is invariant under this symmetry and then obtain a state in which the symmetry *is* broken. This means that the perturbation series cannot converge for an arbitrary α. This clarifies the breakdown of usual perturbation theory when it is used to try to obtain the result equation (13.17) for the gain in energy. The problem of particle number conservation of the BCS wavefunction can be removed by superposing wavefunctions with fixed phases to obtain a wavefunction with a fixed particle number:

$$\begin{aligned} \mid \Psi\rangle_{N\ \mathrm{fixed}} &= \int_0^{2\pi} \mathrm{d}\alpha\, \mathrm{e}^{-\alpha N/2} \mid \Psi\rangle_{\alpha\ \mathrm{fixed}} \\ &= \int_0^{2\pi} \mathrm{d}\alpha\, \mathrm{e}^{-\alpha N/2} \prod_{\mathbf{k}} \left(|u_k| + |v_k| \mathrm{e}^{i\alpha} \hat{c}^{\dagger}_{\mathbf{k}\uparrow} \hat{c}^{\dagger}_{-\mathbf{k}\downarrow} \right) \mid \mathrm{vac}\rangle \end{aligned}$$

with $|u_k|$ and $|v_k|$ given by equation (13.14).

By this argument one does however easily overlook the following point, which is essential for a deeper understanding of superconductivity. For example, we can imagine a piece of copper cut into two pieces and our experience tells us that both pieces can be described by independent electron distribution. The number of electrons in one piece is not obtained exactly. The situation can be described in the grand canonical ensemble, calculated with a common electrochemical potential. In this way, density matrices of different particle numbers add. Correlations between electrons in the different pieces are restricted to at most a small boundary layer. If we apply an electrostatic potential, charge conservation will enforce a correlation between the two pieces: the total current through both pieces is the same. These long-range correlations thus originate in a conservation law, the law of charge conservation.

In the BCS theory, a new macroscopic variable emerges with the complex phase $\Delta(\mathbf{r})$. We cannot imagine simply cutting a homogeneous superconductor with a fixed phase into two independent pieces, since both pieces have the same phase. Besides conservation laws, breaking of a symmetry can thus also lead to long-range correlations. The situation is similar to a ferromagnet, in which a piece with homogeneous magnetization cannot be thought to be cut into two independent pieces, but in both pieces the full rotational symmetry is euqally broken by singling out a magnetization direction. Energetically, states with different magnetization directions are degenerate in the absence of external fields, just as the functions Ψ_{BCS} of different $\mathrm{e}^{i\alpha}$ are degenerate in energy.

All the above considerations concern the case associated with Cooper-pairs 'at rest'. We will here do without the discussion of 'moving' Cooper-pairs and the connected (rather tedious) proof of the statement that the BCS wavefunction really is a *superconducting* state. Another limitation of the discussion here was the restriction to spatially homogeneous systems. It is plausible that we can discuss a situation of a spatially inhomogeneous, but slowly varying, system through a local BCS-picture with a local, spatially slowly varying complex gap-parameter $\Delta(\mathbf{r})$ and that many phenomena produce macroscopic equations for $\Delta(\mathbf{r})$. This is preciesly what is done in the theory of Ginzburg and Landau [11] and Gorkov [12]. As a representative example of several other effects, we will discuss here the effects of the fact that $\hat{\psi}_\uparrow^\dagger(\mathbf{r})\hat{\psi}_\downarrow^\dagger(\mathbf{r})$ is closely related to fermion operators, but possesses a macroscopic expectation value. In the presence of a spatially slowly-varying vector potential $\mathbf{A}(\mathbf{r})$, the wavefunction of the electrons changes to lowest order only through a space-dependent phase factor:

$$\exp\left[-\frac{ie}{\hbar c}\int_{\mathbf{r}_0}^{\mathbf{r}} \mathbf{A}(\mathbf{r})\cdot \mathrm{d}\mathbf{s}\right].$$

This factor drops out of the density $n(\mathbf{r}) = \sum_\sigma \langle \hat{\psi}_\sigma^\dagger(\mathbf{r})\hat{\psi}_\sigma(\mathbf{r})\rangle$, but not from the order-parameter/gap function $\Delta(\mathbf{r}) \sim \langle \hat{\psi}_\downarrow(\mathbf{r})\hat{\psi}_\uparrow(\mathbf{r})\rangle$, where it enters twice. Thus, the order parameter Δ behaves in many ways like a macroscopic wavefunction. If we follow the wavefunction and Δ around a homogeneous superconducting ring, Δ can only change by a factor

$$1 = \exp[2\pi i\ell] = \exp\left[-2\frac{ie}{\hbar c}\oint \mathbf{A}(\mathbf{s})\cdot \mathrm{d}\mathbf{s}\right] \quad \text{with } \ell \in \mathcal{Z},$$

because of the single-valuedness of the expectation value. Thus, the line integral $\oint \mathbf{A}\cdot d\mathbf{s}$ and also the enclosed magnetic flux $\int\int \mathbf{B}\cdot d\mathbf{S}$ can only change by integral numbers of 'flux quanta' $(2\pi\hbar c/2e)$. This is the origin of the Josephson effect.

We will with this digression of the phenomenology of superconductivity end this part on the overview of the most important many-body effects and quasi-particles of solid state physics. Next, we will turn to the development of a systematic, and, above all, diagrammatic method of calculation of many-particle systems.

Part II

Green's Functions

Chapter 14

Pictures

The observables of a quantum mechanical system are characterized by linear operators in a Hilbert space. The fact that these operators themselves do not represent any measurable quantities is crucial to the definition of the so-called pictures. One can merely measure the expectation values of the operators in addition to the square of the absolute value of sums of transition amplitudes

$$\langle \psi \mid O \mid \phi \rangle.$$

(For ease of notation, we will hereafter only write operators with the caret when the context requires an unambiguous distinction.) Let $A(t)$ be in general a time-dependent operator, which is unitary at each time t:

$$A^{\dagger}(t)A(t) = 1 = A(t)A^{\dagger}(t).$$

We then have for a general matrix element

$$\begin{aligned} \langle \psi \mid O \mid \phi \rangle &= \langle \psi \mid A^{\dagger}(t)A(t)OA^{\dagger}(t)A(t) \mid \phi \rangle \\ &= \langle A(t)\psi \mid A(t)OA^{\dagger}(t) \mid A(t)\phi \rangle. \end{aligned}$$

Thus, if we transform *all* wavefunctions and *all* operators according to

$$\begin{aligned} \mid \psi(t)\rangle_A &\equiv A(t)|\psi\rangle \\ O(t)_A &\equiv A(t)OA^{\dagger}(t) \end{aligned}$$

all measurable quantities will remain unchanged:

$$\langle \psi \mid O \mid \phi \rangle = \langle \psi_A \mid O_A \mid \phi_A \rangle.$$

Such a transformation is called a picture transformation. Each time-dependent unitary operator defines a particular picture. In each picture, the 'normal' wavefunctions and operators have what we may call an additional artificial time-independence. However, the structure of the stationary Schrödinger equation as an eigenvalue equation is retained in every picture:

$$H(t)_A \mid \psi(t)\rangle_A = E \mid \psi(t)\rangle_A.$$

We now consider a few examples:

(1) The Schrödinger Picture: $A(t) \equiv 1$.

We denote by the Schrödinger picture the usual quantum mechanical picture in which the operators and wavefunctions have their 'natural' time-dependence. We will hereafter for the sake of clarity denote by a subscript S operators and wavefunctions in the Schrödinger picture. The time-dependent Schrödinger equation is in this notation

$$i\hbar\frac{\partial}{\partial t} \mid \Psi(t)\rangle_S = H_S \mid \Psi(t)\rangle_S.$$

We will now discuss the so-called time-evolution operator in the Schrödinger picture. This operator is defined by the equation

$$\mid \Psi(t)\rangle_S \equiv U(t,t_0)_S \mid \Psi(t_0)\rangle \tag{14.1}$$

for an arbitrary initial function $\mid \Psi(t_0)\rangle$ in the Hilbert space of the problem in question. Inserting equation (14.1) into the Schrödinger equation yields

$$i\hbar\frac{\partial}{\partial t}U(t,t_0)_S \mid \Psi(t_0)\rangle_S = H_S U(t,t_0)_S \mid \Psi(t_0)\rangle_S.$$

Since this holds for any initial function, the operator differential equation

$$i\hbar\frac{\partial}{\partial t}U(t,t_0)_S = H_S U(t,t_0)_S \tag{14.2}$$

together with the initial condition $U(t_0,t_0) = 1$ follows.

We will now prove that the operator $U(t,t_0)_S$ is unitary. If we use the defining equation (14.1) twice, we arrive at

$$\mid \Psi(t)\rangle_S = U(t,t')_S \mid \Psi(t')\rangle_S = U(t,t')_S U(t',t_0)_S \mid \Psi(t_0)\rangle_S.$$

It follows that

$$U(t,t_0)_S = U(t,t')_S U(t',t_0)_S.$$

For $t = t_0$ we have

$$1 = U(t_0,t')_S U(t',t_0)_S.$$

Hence

$$U(t,t_0)_S^{-1} = U(t_0,t)_S.$$

Furthermore, from the operator differential equation (14.2) and its adjoint equation

$$\begin{aligned}\frac{\partial U_S}{\partial t} &= -\frac{i}{\hbar} H_S U_S \\ \frac{\partial U_S^\dagger}{\partial t} &= \frac{i}{\hbar} U_S^\dagger H_S\end{aligned}$$

it follows that

$$\frac{\partial}{\partial t}\left[U_S^\dagger U_S\right] = \frac{\partial U_S^\dagger}{\partial t} U_S + U_S^\dagger \frac{\partial U_S}{\partial t} = 0$$

which implies that

$$U^\dagger(t,t_0)_S U(t,t_0)_S = \text{constant}.$$

Since $U(t_0,t_0)_S = 1$, we have $U^\dagger(t_0,t_0)_S = 1$, so $U^\dagger(t,t_0)_S U(t,t_0)_S = 1$. We already have shown that U_S is invertible; hence, the unitarity follows:

$$U^\dagger(t,t_0)_S = U^{-1}(t,t_0)_S.$$

If the Hamiltonian is explicitly time-independent in the Schrödinger picture, we can readily solve the operator differential equation (14.2). The solution is

$$U(t,t_0)_S = \exp\left[-\frac{i}{\hbar} H_S (t-t_0)\right]. \tag{14.3}$$

(2) The Heisenberg picture

This picture is defined by choosing

$$A(t) \equiv U^\dagger(t,t_0)_S = U(t_0,t)_S.$$

The wavefunctions are constant in time in the Heisenberg picture:

$$\mid \Psi(t)\rangle_H = A(t) \mid \Psi(t)\rangle_S = U(t_0,t)_S \mid \Psi(t)\rangle_S = \mid \Psi(t_0)\rangle_S = \text{ constant}. \tag{14.4}$$

The operators in the Heisenberg picture are given by

$$O(t)_H = U^\dagger(t,t_0)_S O(t)_S U(t,t_0)_S. \tag{14.5}$$

If H_S is explicitly time-independent, we have from equation (14.3) (if we also fix $t_0 = 0$)

$$O(t)_H = e^{+\frac{i}{\hbar} H_S t} O(t)_S e^{-\frac{i}{\hbar} H_S t}. \tag{14.6}$$

Since the wavefunctions are constant in the Heisenberg picture, the entire dynamics is contained in the operators. We now derive an equation of motion for operators in the Heisenberg picture.

$$\begin{aligned} i\hbar\frac{\mathrm{d}}{\mathrm{d}t}O(t)_H &= i\hbar\frac{\mathrm{d}}{\mathrm{d}t}\left(U_S^\dagger O_S U_S\right) \\ &= i\hbar\left(\frac{\partial U_S^\dagger}{\partial t}\right)O_S U_S + i\hbar U_S^\dagger\left(\frac{\partial O_S}{\partial t}\right)U_S + i\hbar U_S^\dagger O_S\left(\frac{\partial U_S}{\partial t}\right). \end{aligned}$$

If we then use

$$i\hbar\frac{\partial U_S}{\partial t} = H_S U_S$$

and

$$-i\hbar\frac{\partial U_S^\dagger}{\partial t} = U_S^\dagger H_S$$

we can write

$$\begin{aligned} & i\hbar\frac{\mathrm{d}}{\mathrm{d}t}O(t)_H \\ &= -U_S^\dagger H_S U_S U_S^\dagger O_S U_S + i\hbar U_S^\dagger\left(\frac{\partial O_S}{\partial t}\right)U_S + U_S^\dagger O_S U_S U_S^\dagger H_S U_S \\ &= -H_H O_H + O_H H_H + i\hbar U_S^\dagger\left(\frac{\partial O_S}{\partial t}\right)U_S. \end{aligned}$$

If we furthermore set

$$\left[\frac{\partial O}{\partial t}\right]_H \equiv U_S^\dagger\left(\frac{\partial O_S}{\partial t}\right)U_S$$

we finally obtain the so-called *Heisenberg equation of motion*:

$$i\hbar\frac{\mathrm{d}}{\mathrm{d}t}O(t)_H = [O_H, H_H] + i\hbar\left[\frac{\partial O}{\partial t}\right]_H. \tag{14.7}$$

The formulation of quantum mechanics in the Heisenberg picture formally resembles classical mechanics. To realize this, we consider two canonically conjugated variables $\mathbf{q}$ and $\mathbf{p}$. For these, we have

$$[q_j, p_k] = i\hbar\delta_{jk}.$$

It follows that

$$\begin{aligned} [q_j, p_k^n] &= q_j p_k^n - p_k^n q_j = (q_j p_k)p_k^{n-1} - p_k^n q_j \\ &= p_k q_j p_k^{n-1} + i\hbar\delta_{jk}p_k^{n-1} - p_k^n q_j \\ &= \ldots = p_k^n q_j + ni\hbar\delta_{jk}p_k^{n-1} - p_k^n q_j \\ &= i\hbar\delta_{jk}\frac{\partial}{\partial p_k}p_k^n. \end{aligned}$$

Analoguously, we obtain

$$[p_j, q_k^n] = -i\hbar\delta_{jk}\frac{\partial}{\partial q_k}q_k^n.$$

If an operator has the form of a general Laurent series

$$O(\mathbf{q},\mathbf{p}) = \sum_{\substack{n_1 n_2 n_3 \\ m_1 m_2 m_3}} a^{n_1 n_2 n_3}_{m_1 m_2 m_3} q_1^{n_1} q_2^{n_2} q_3^{n_3} p_1^{m_1} p_2^{m_2} p_3^{m_3}$$

it follows that

$$[q_j, O(\mathbf{q},\mathbf{p})] = i\hbar\frac{\partial}{\partial p_j}O(\mathbf{q},\mathbf{p})$$

and

$$[p_j, O(\mathbf{q},\mathbf{p})] = -i\hbar\frac{\partial}{\partial q_j}O(\mathbf{q},\mathbf{p}).$$

In particular, we have in the Heisenberg picture

$$i\hbar\frac{\mathrm{d}}{\mathrm{d}t}q_j(t)_H = [q_j(t)_H, H] + \underbrace{i\hbar\left[\frac{\partial}{\partial t}q_j(t)_H\right]}_{=0} = i\hbar\frac{\partial}{\partial p_j(t)_H}H$$

so that

$$\frac{\mathrm{d}q_j(t)_H}{\mathrm{d}t} = \frac{\partial H}{\partial p_j(t)_H}$$

and, analogously

$$\frac{\mathrm{d}p_j(t)_H}{\mathrm{d}t} = -\frac{\partial H}{\partial q_j(t)_H}.$$

Thus, Hamilton's equations of motion of classical mechanics hold formally for canonically conjugate Heisenberg operators.

(3) The interaction picture

Here, we start by partitioning the Hamiltonian according to

$$H_S = H_0 + V_S \quad H_0 \neq H_0(t)$$

where we assume that the time-independent problem given by H_0 is solved. We choose the unitary operator

$$A(t) \equiv \mathrm{e}^{\frac{i}{\hbar}H_0 t}$$

as the transformation to this picture. This yields

$$| \Psi(t)\rangle_I = e^{\frac{i}{\hbar}H_0 t} | \Psi(t)\rangle_S \tag{14.8}$$

and

$$O(t)_I = e^{\frac{i}{\hbar}H_0 t} O(t)_S e^{-\frac{i}{\hbar}H_0 t}. \tag{14.9}$$

In particular, the operator H_0 is the same in both the Schrödinger picture and the interaction picture:

$$[H_0]_I = e^{\frac{i}{\hbar}H_0 t} [H_0]_S \, e^{-\frac{i}{\hbar}H_0 t} = [H_0]_S \equiv H_0.$$

The partitioning of the full Hamiltonian into H_0 and V is in principle completely arbitrary (so long as H_0 is time-independent). We will, however, hereafter always let H_0 describe a system of *independent* particles (if necessary in an external potential), and V denote the interactions between the particles. As an example, we will now transform the creation and annihilation operators to the interaction picture. We assume that we have solved the problem given by H_0 and that $c_j^\dagger$ and c_j are the creation and annihilation operators in the Schrödinger picture of the corresponding single-particle states. We will show that only a phase-factor is added in the interaction picture:

$$\begin{aligned} c_j(t)_I &= c_j e^{-\frac{i}{\hbar}\epsilon_j t} \\ c_j^\dagger(t)_I &= c_j^\dagger e^{\frac{i}{\hbar}\epsilon_j t} \end{aligned} \tag{14.10}$$

For proof, we use the operator H_0 in diagonal form

$$H_0 = \sum_{i=1}^{\infty} \epsilon_i c_i^\dagger c_i$$

and then show that the usual representation of the operators in the interaction picture

$$\begin{aligned} c_j(t)_I &= e^{\frac{i}{\hbar}H_0 t} c_j e^{-\frac{i}{\hbar}H_0 t} \\ c_j^\dagger(t)_I &= e^{\frac{i}{\hbar}H_0 t} c_j^\dagger e^{-\frac{i}{\hbar}H_0 t} \end{aligned}$$

on the complete system of Slater determinants

$$| \phi_\alpha\rangle = \prod_{i=1}^{\infty} \left(c_i^\dagger\right)^{n_i^{(\alpha)}} | 0\rangle, \quad n_i^{(\alpha)} = 0 \text{ or } 1$$

leads to the result equation (14.10).

First of all, we have

$$H_0 \mid \phi_\alpha\rangle = W_\alpha \mid \phi_\alpha\rangle \quad \text{where} \quad W_\alpha = \sum_{i=1}^{\infty} n_i^{(\alpha)} \epsilon_i .$$

But $c_j \mid \phi_\alpha\rangle$ is of course also an eigenfunction of H_0 for arbitrary j and α:

$$H_0 c_j \mid \phi_\alpha\rangle = \sum_{i=1}^{\infty} \epsilon_i c_i^\dagger c_i c_j \mid \phi_\alpha\rangle .$$

From

$$c_i^\dagger c_i c_j = -c_i^\dagger c_j c_i = -\delta_{ij} c_i + c_j c_i^\dagger c_i$$

we obtain

$$\begin{aligned} H_0 c_j \mid \phi_\alpha\rangle &= -\epsilon_j c_j \mid \phi_\alpha\rangle + c_j H_0 \mid \phi_\alpha\rangle \\ &= \left(W_\alpha - \epsilon_j\right) c_j \mid \phi_\alpha\rangle . \end{aligned}$$

From this the statement to be proved follows:

$$\begin{aligned} c_j(t)_I \mid \phi_\alpha\rangle &= \mathrm{e}^{\frac{i}{\hbar} H_0 t} c_j \mathrm{e}^{-\frac{i}{\hbar} H_0 t} \mid \phi_\alpha\rangle \\ &= \mathrm{e}^{-\frac{i}{\hbar} W_\alpha t} \mathrm{e}^{\frac{i}{\hbar} H_0 t} c_j \mid \phi_\alpha\rangle \\ &= \mathrm{e}^{-\frac{i}{\hbar} W_\alpha t} \mathrm{e}^{\frac{i}{\hbar}(W_\alpha - \epsilon_j) t} c_j \mid \phi_\alpha\rangle \\ &= \mathrm{e}^{-\frac{i}{\hbar} \epsilon_j t} c_j \mid \phi_\alpha\rangle . \end{aligned}$$

The proof for $c_j^\dagger$ runs analogously.

Both the operators as well as the wavefunctions are time-dependent in the interaction picture. It follows that there are equations of motions for both quantities. For the operators, this equation is (the derivation is completely analogous to the derivation of the Heisenberg equation of motion):

$$i\hbar \frac{\mathrm{d}}{\mathrm{d}t} O(t)_I = [O(t)_I, H_0] + i\hbar \left[\frac{\partial O}{\partial t}\right]_I \tag{14.11}$$

with

$$\left[\frac{\partial O}{\partial t}\right]_I \equiv \mathrm{e}^{\frac{i}{\hbar} H_0 t} \left[\frac{\partial O_S}{\partial t}\right] \mathrm{e}^{-\frac{i}{\hbar} H_0 t} .$$

Next, we will derive the equation of motion for the wavefunction in the interaction picture. We start with the Schrödinger equation

$$\begin{aligned}
i\hbar\frac{\partial}{\partial t}\mid\Psi(t)\rangle_S &= H_S|\Psi(t)\rangle_S \\
\Rightarrow i\hbar\frac{\partial}{\partial t}\mathrm{e}^{-(i/\hbar)H_0 t}\mid\Psi(t)\rangle_I &= \mathrm{e}^{-(i/\hbar)H_0 t}\left[H_0\mid\Psi(t)\rangle_I + i\hbar\frac{\partial}{\partial t}|\Psi(t)\rangle_I\right] \\
&= H_S\mathrm{e}^{-(i/\hbar)H_0 t}\mid\Psi(t)\rangle_I \\
\Rightarrow i\hbar\frac{\partial}{\partial t}\mid\Psi(t)\rangle_I &= \mathrm{e}^{(i/\hbar)H_0 t}H_S\mathrm{e}^{-(i/\hbar)H_0 t}\mid\Psi(t)\rangle_I - H_0|\Psi(t)\rangle_I \\
&= [H(t)_I - H_0]\mid\Psi(t)\rangle_I \\
\Rightarrow i\hbar\frac{\partial}{\partial t}\mid\Psi(t)\rangle_I &= V(t)_I\mid\Psi(t)\rangle_I. \qquad (14.12)
\end{aligned}$$

The second-quantized representation of the particle–particle interaction is, with equation (14.9)

$$V(t)_I = \frac{1}{2}\sum_{ijk\ell}\langle ij\mid v\mid k\ell\rangle c_i^\dagger(t)_I c_j^\dagger(t)_I c_\ell(t)_I c_k(t)_I \qquad (14.13)$$

and with equation (14.10), this can be written

$$V(t)_I = \frac{1}{2}\sum_{ijk\ell}\langle ij\mid v\mid k\ell\rangle \mathrm{e}^{(i/\hbar)(\epsilon_i+\epsilon_j-\epsilon_\ell-\epsilon_k)t}c_i^\dagger c_j^\dagger c_\ell c_k.$$

Equation (14.12) is known as the *Tomonaga–Schwinger equation.* It is in its structure similar to the Schrödinger equation. The part due to the H_0-motion, which is assumed from the outset, is separated out so that only the particle–particle interaction is left (hence the name 'interaction picture'). Analogous to the Schrödinger picture, we now define a time-evolution operator in the interaction picture through

$$\mid\Psi(t)\rangle_I = U(t,t')\mid\Psi(t')\rangle_I. \qquad (14.14)$$

Just as for U_S, we can prove the following properties:

$$\begin{aligned}
U(t,t') &= U(t,t'')U(t'',t') \\
U^\dagger(t,t') &= U^{-1}(t,t') = U(t',t).
\end{aligned}$$

Furthermore, we have

$$\begin{aligned}
\mid\Psi(t)\rangle_I &= \mathrm{e}^{\frac{i}{\hbar}H_0 t}\mid\Psi(t)\rangle_S = \mathrm{e}^{\frac{i}{\hbar}H_0 t}U(t,t')_S\mid\Psi(t')\rangle_S \\
&= \mathrm{e}^{\frac{i}{\hbar}H_0 t}U(t,t')_S\mathrm{e}^{-\frac{i}{\hbar}H_0 t'}\mid\Psi(t')\rangle_I.
\end{aligned}$$

Consequently, we have the following relation between the time-evolution operators in the Schrödinger picture and in the interaction picture:

$$U(t,t') = \mathrm{e}^{(i/\hbar)H_0 t}U(t,t')_S\mathrm{e}^{-(i/\hbar)H_0 t'}. \qquad (14.15)$$

Here we have to be a little careful – a moment's thought shows that this is not a picture transformation, since the time arguments are different in the two exponential functions. Thus, $U(t,t')$ is not $U(t,t')_S$ transformed to the interaction picture. If H_S is explicitly time-dependent, we obtain from equation (14.3)

$$U(t,t') = \mathrm{e}^{(i/\hbar)H_0 t}\mathrm{e}^{-(i/\hbar)H_S(t-t')}\mathrm{e}^{-(i/\hbar)H_0 t'}.$$

Equation (14.15) yields a simple relation between operators in the interaction picture and in the Heisenberg picture: if we use equation (14.5) and set $t_0 = 0$ we obtain

$$\begin{aligned} O(t)_H &= U(0,t)_S O(t)_S U(t,0)_S \\ &= U(0,t_S)\mathrm{e}^{-(i/\hbar)H_0 t}O(t)_I \mathrm{e}^{(i/\hbar)H_0 t}U(t,0)_S \\ \Rightarrow O(t)_H &= U(0,t)O(t)_I U(t,0). \end{aligned} \tag{14.16}$$

We will now further investigate the time-evolution operator. If we insert the definition equation (14.14) in the Tomonaga–Schwinger equation, we obtain an equation of motion for U:

$$i\hbar\frac{\partial}{\partial t}U(t,t') = V(t)_I U(t,t') \tag{14.17}$$

with the initial condition $U(t',t') = 1$. This differential equation with its initial condition is equivalent to the following integral equation:

$$U(t,t') = 1 - \frac{i}{\hbar}\int_{t'}^{t} V(t_1)_I U(t_1,t')\,\mathrm{d}t_1 \tag{14.18}$$

which is readily shown by substitution. This integral equation is suitable for successive approximations:

$$\begin{aligned} U_0(t,t') &= 1 \\ U_1(t,t') &= 1 - \frac{i}{\hbar}\int_{t'}^{t} V(t_1)_I\,\mathrm{d}t_1 \\ U_2(t,t') &= 1 - \frac{i}{\hbar}\int_{t'}^{t} V(t_1)_I U_1(t_1,t')\,\mathrm{d}t_1 \\ &= 1 - \frac{i}{\hbar}\int_{t'}^{t} V(t_1)_I\,\mathrm{d}t_1 + \left(-\frac{i}{\hbar}\right)^2 \int_{t'}^{t} V(t_1)_I \int_{t'}^{t_1} V(t_2)_I\,\mathrm{d}t_2\mathrm{d}t_1. \end{aligned}$$

Correspondingly, we obtain for the N^{th} approximation

$$U_N(t,t') = 1 + \sum_{n=1}^{N} U^{(n)}(t,t')$$

where

$$U^{(n)}(t,t') = \left(\frac{i}{\hbar}\right)^n \int_{t'}^{t} \mathrm{d}t_1 \int_{t'}^{t_1} \mathrm{d}t_2 \ldots \int_{t'}^{t_{n-1}} \mathrm{d}t_n\, V(t_1)_I \ldots V(t_n)_I.$$

By construction, we always have

$$t' \le t_n \le t_{n-1} \le \ldots \le t_1 \le t.$$

If the successive approximations converge, we finally arrive at

$$U(t,t') = 1 + \sum_{n=1}^{\infty} U^{(n)}(t,t'). \tag{14.19}$$

This series can be interpreted as a perturbation expansion in the potential V. We will now make an additional simplification of the formula for $U^{(n)}$. We will show it here in detail for

$$U^{(2)}(t,t') = \left(-\frac{i}{\hbar}\right)^2 \int_{t'}^{t} \mathrm{d}t_1 \int_{t'}^{t_1} \mathrm{d}t_2 V(t_1)_I V(t_2)_I.$$

The simplification consists of removing the variable integration limit t_1 so that both integrations will run over the interval $[t',t]$. This clearly means that we will replace the triangular integration region shown in figure 14.1 by the entire square. If the $V(t_i)_I$ were *c*-numbers, we could without any problem evaluate the integral over the square and finally divide the result by 2. However, since we are dealing with functions of operators, the potentials at different times will in general not commute, *i.e.*,

$$V(t_1)_I V(t_2)_I \neq V(t_2)_I V(t_1)_I.$$

Hence, the evaluation of the integral is somewhat complicated. We start by setting

$$\begin{aligned}&\int_{t'}^{t} \mathrm{d}t_1 \int_{t'}^{t} \mathrm{d}t_2 V(t_1)_I V(t_2)_I \\ &\quad = \frac{1}{2}\int_{t'}^{t} \mathrm{d}t_1 \int_{t'}^{t_1} \mathrm{d}t_2 V(t_1)_I V(t_2)_I + \frac{1}{2}\int_{t'}^{t} \mathrm{d}t_2 \int_{t_2}^{t} \mathrm{d}t_1 V(t_1)_I V(t_2)_I.\end{aligned}$$

The two expression are identical, as one can see in figure 14.1. In the first expression, the integration over t_1 runs from t' to t, and for each t_1, t_2 runs from t' to the the bisectris ($t_2 = t_1$). In the second expression, on the other hand, only the sequence of points of the integration is changed. The integration over t_2 runs from t' to t and for each t_2, the integration over t_1 runs from the bisectris ($t_1 = t_2$) to t. By renaming the integration variables in the second expression, the integral can be written

$$\frac{1}{2}\int_{t'}^{t} \mathrm{d}t_1 \int_{t'}^{t_1} \mathrm{d}t_2 V(t_1)_I V(t_2)_I + \frac{1}{2}\int_{t'}^{t} \mathrm{d}t_2 \int_{t_1}^{t} \mathrm{d}t_1 V(t_2)_I V(t_1)_I.$$

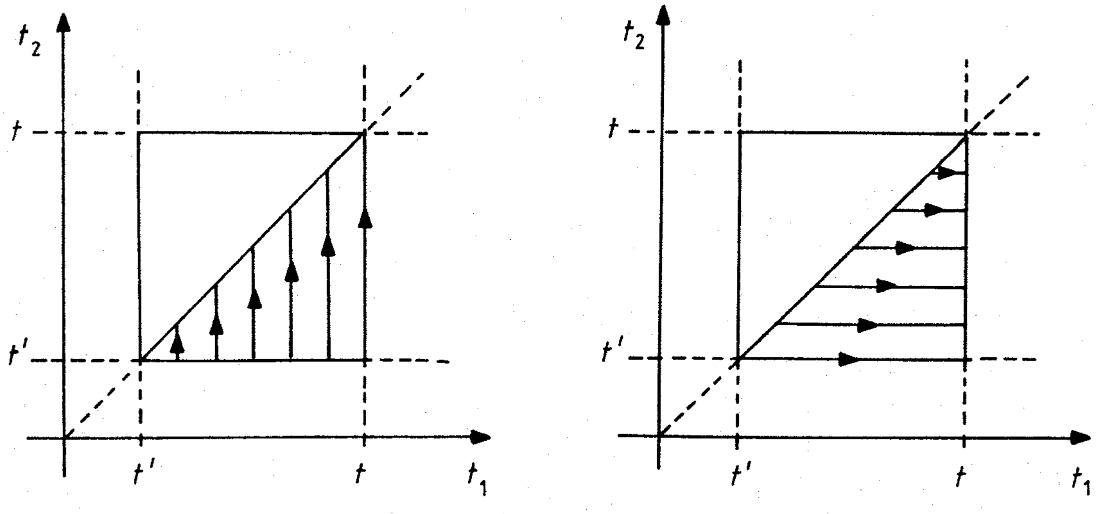


Figure 14.1 *The integrals in* $U^{(2)}$ *over* t_1 *and* t_2 *can be divided into two separate integrals; one over* t_1 *first, the other over* t_2 *first.*

For further formal simplification we define the time-ordered product of two operators through

$$T[A(t_1)B(t_2)] \equiv \begin{cases} A(t_1)B(t_2) & \text{if } t_1 > t_2 \\ B(t_2)A(t_1) & \text{if } t_2 > t_1. \end{cases}$$

Thus, we finally arrive at

$$U^{(2)}(t,t') = \frac{-(i/\hbar)^2}{2} \int_{t'}^{t} \mathrm{d}t_1 \int_{t'}^{t} \mathrm{d}t_2\, T[V(t_1)_I V(t_2)_I].$$

The time-ordered product is not defined for $t_1 = t_2$. However, this causes no problem in our case, since for $t_1 = t_2$ both operators are identical and thus commute with each other.

With an analogous definition of the time-ordered product of n operators we obtain

$$U^{(n)}(t,t') = \frac{(-i/\hbar)^n}{n!} \int_{t'}^{t} \mathrm{d}t_1 \int_{t'}^{t} \mathrm{d}t_2 \ldots \int_{t'}^{t} \mathrm{d}t_n T[V(t_1)_I \ldots V(t_n)_I]. \tag{14.20}$$

This is the central equation for perturbation calculations on many-particle systems. In all, we obtain for the time-evolution operator

$$\begin{aligned}
U(t,t') &= \sum_{n=0}^{\infty} \frac{(-i/\hbar)^n}{n!} \int_{t'}^{t} \mathrm{d}t_1 \ldots \int_{t'}^{n} \mathrm{d}t_n T[V(t_1)_I \ldots V(t_n)_I] \\
&= T \sum_{n=0}^{\infty} \frac{(-i/\hbar)^n}{n!} \int_{t'}^{t} \mathrm{d}t_1 \ldots \int_{t'}^{t} \mathrm{d}t_n V(t_1)_I \ldots V(t_n)_I \\
&= T \sum_{n=0}^{\infty} \frac{(-i/\hbar)^n}{n!} \left(\int_{t'}^{t} \mathrm{d}\tau V(\tau)_I \right)^n .
\end{aligned}$$

We can formally write the expression for $U(t,t')$ as

$$U(t,t') = T \exp\left[\frac{-i}{\hbar} \int_{t'}^{t} \mathrm{d}\tau V(\tau)_I \right] .$$

Chapter 15

The single-particle Green's function

Let $| \Psi_0\rangle$ denote the ground state in the Heisenberg picture of an interacting many-particle system. In particular, $| \Psi_0\rangle$ is then time-independent, and we have

$$H| \Psi_0\rangle = E_0| \Psi_0\rangle.$$

Furthermore, let $\psi(x,t)_H$ denote the field operator in the Heisenberg picture. This operator annihilates a field quantum at space–spin point x at time t, and $\psi^\dagger(x,t)$ is the corresponding creation operator. Occasionally, we will consider the spin-dependence separately, in which case we write

$$\psi(x,t)_H = \psi_s(\mathbf{r},t)_H$$

and

$$\psi^\dagger(x,t)_H = \psi_s^\dagger(\mathbf{r},t)_H.$$

The definition of the single-particle Green's function is

$$iG(xt,x't') \equiv \frac{1}{\langle\Psi_0| \Psi_0\rangle}\langle\Psi_0 \mid T[\psi(x,t)_H\psi^\dagger(x',t')_H]| \Psi_0\rangle \tag{15.1}$$

or, if we want to emphasize the spin-dependency

$$iG_{ss'}(\mathbf{r}t,\mathbf{r}'t') \equiv \frac{1}{\langle\Psi_0| \Psi_0\rangle}\langle\Psi_0 \mid T[\psi_s(\mathbf{r}t)_H\psi_{s'}^\dagger(\mathbf{r}'t')_H]| \Psi_0\rangle.$$

We define the time-ordered product of two creation or annihilation operators by

$$T[A(t)B(t')] = \begin{cases} A(t)B(t') & \text{for } t > t' \\ \pm B(t')A(t) & \text{for } t' > t \end{cases} \tag{15.2}$$

with plus-sign for bosons and minus-sign for fermions. This is an extension of the definition given in equation (14.20). The definition equation (15.2) contains an additional minus sign for fermions. However, this makes no difference in equation (14.20), since the interaction potential always is represented by an *even* number of creation and annihilation operators (*cf.* equation (14.13)).

The definition given here for the single-particle Green's function holds both for bosons and fermions. In the following considerations we will however restrict ourselves to fermions. The single-particle Green's function is in this case

$$\begin{aligned}
iG(xt, x't') &= \frac{1}{\langle\Psi_0|\,\Psi_0\rangle}\begin{cases} \langle\Psi_0 \mid \psi(x,t)_H\psi^\dagger(x't')_H|\,\Psi_0\rangle & t > t' \\ -\langle\Psi_0 \mid \psi^\dagger(x',t')_H\psi(x,t)_H|\,\Psi_0\rangle & t' > t \end{cases} \\
&= \frac{1}{\langle\Psi_0|\,\Psi_0\rangle}\Big[\theta(t-t')\langle\Psi_0 \mid \psi(x,t)_H\psi^\dagger(x',t')_H|\,\Psi_0\rangle \\
&\qquad -\theta(t'-t)\langle\Psi_0 \mid \psi^\dagger(x',t')_H\psi(x,t)_H|\,\Psi_0\rangle\Big] \qquad (15.3)
\end{aligned}$$

where

$$\theta(y) = \begin{cases} 1 & y > 0 \\ 0 & y < 0 \end{cases}$$

is the standard step-function.

Up to this point, we have only considered the Green's function in space–spin representation. If we transform to creation and annihilation operators of momentum eigenfunctions by a basis transformation (*cf.* equations (4.7) and (4.8))

$$\begin{aligned}
\psi_\alpha(\mathbf{r},t)_H &= \sum_{\mathbf{k}} \frac{1}{\sqrt{\Omega}} e^{i\mathbf{k}\cdot\mathbf{r}} c_{\mathbf{k}\alpha}(t)_H \\
\psi^\dagger_\beta(\mathbf{r}',t')_H &= \sum_{\mathbf{k}} \frac{1}{\sqrt{\Omega}} e^{-i\mathbf{k}'\cdot\mathbf{r}'} c^\dagger_{\mathbf{k}'\beta}(t')_H
\end{aligned}$$

the Green's function becomes

$$\begin{aligned}
iG_{\alpha\beta}(\mathbf{r}t, \mathbf{r}'t') &= \sum_{\mathbf{k},\mathbf{k}'} \frac{1}{\Omega} e^{i(\mathbf{k}\cdot\mathbf{r}-\mathbf{k}'\cdot\mathbf{r}')} \\
&\quad \times \frac{1}{\langle\Psi_0|\,\Psi_0\rangle}\langle\Psi_0 \mid T[c_{\mathbf{k}\alpha}(t)_H c^\dagger_{\mathbf{k}'\beta}(t')_H]|\,\Psi_0\rangle.
\end{aligned}$$

It is then natural to define the momentum Green's function by the quantity

$$iG_{\alpha\beta}(\mathbf{k}t, \mathbf{k}'t') \equiv \frac{1}{\langle\Psi_0|\,\Psi_0\rangle}\langle\Psi_0 \mid T[c_{\mathbf{k}\alpha}(t)_H c^\dagger_{\mathbf{k}'\beta}(t)_H]|\,\Psi_0\rangle. \qquad (15.4)$$

$H(x,t) \equiv H(x)$

In general, the Green's function in any single-particle basis representation is defined by

$$iG(\lambda t, \lambda' t') \equiv \frac{1}{\langle \Psi_0 | \Psi_0 \rangle} \langle \Psi_0 \mid T[c_\lambda(t)_H c^\dagger_{\lambda'}(t')_H] | \Psi_0 \rangle .$$

We will now derive a number of properties of the single-particle Green's function. First, we will prove that if the Hamiltonian is explicitly time-independent in the Schrödinger representation, and therefore also in the Heisenberg representation, the single-particle Green's function depends only on the time-difference $(t - t')$, *i.e.,*

wrong symbol

$$? \; \underline{H \neq H(t)} \quad \Rightarrow \quad G(\lambda t, \lambda' t') = G(\lambda(t - t'), \lambda' 0).$$

We will prove this only for the spatial Green's function, since the proof is quite similar for other representations. First, we transform the Heisenberg operators with equation (14.6) to the Schrödinger picture

$$\begin{aligned} \psi(xt)_H &= e^{iHt} \psi(x)_S e^{-iHt} \\ \psi^\dagger(xt)_H &= e^{iHt} \psi^\dagger(x)_S e^{-iHt}. \end{aligned}$$

(From here on, we will always use units in which $\hbar = 1$.) For $t > t'$ we then have

$$\underbrace{\langle \Psi_0 \mid e^{iHt}}_{\langle \Psi_0 | e^{iE_0 t}} \psi(x)_S e^{-iHt} e^{iHt'} \psi^\dagger(x')_S \underbrace{e^{-iHt'} | \Psi_0 \rangle}_{e^{-iE_0 t'} | \Psi_0 \rangle} .$$

Together with the corresponding expression for $t' > t$ we obtain in all for the Green's function:

$$\begin{aligned} & iG(xt, x't') \\ = \; & \frac{1}{\langle \Psi_0 | \Psi_0 \rangle} \Big[\theta(t - t') e^{iE_0(t-t')} \langle \Psi_0 \mid \psi(x)_S e^{-iH(t-t')} \psi^\dagger(x')_S | \Psi_0 \rangle \\ & - \theta(t' - t) e^{iE_0(t'-t)} \langle \Psi_0 \mid \psi^\dagger(x')_S e^{-iH(t'-t)} \psi(x)_S | \Psi_0 \rangle \Big] . \end{aligned}$$

From this expression, we see that the Green's function depends only on $(t - t')$ if H is time-independent. If we use the transformation of the ground state to the Schrödinger picture,

$$| \Psi_0 \rangle_S = e^{-iE_0 t} | \Psi_0 \rangle$$

we obtain

$$\begin{aligned} & iG(xt, x't') \\ = \; & \frac{1}{\langle \Psi_0 | \Psi_0 \rangle} \Big[\theta(t - t') \langle \Psi_0(t)_S \mid \psi(x)_S e^{-iH(t-t')} \psi^\dagger(x')_S \mid \Psi_0(t') \rangle_S \\ & - \theta(t' - t) \langle \Psi_0(t')_S \mid \psi^\dagger(x')_S e^{-iH(t'-t)} \psi(x)_S \mid \Psi_0(t) \rangle_S \Big] . \end{aligned} \tag{15.5}$$

This form of the Green's function allows for a clear interpretation: for $t > t'$, we add a particle at space–spin point x' to the ground state $\mid \Psi_0(t')\rangle_S$ by the action of $\psi^\dagger(x')_S$. The $(N+1)$-particle state created this way then propagates from t' to t under the influence of the Hamiltonian H (*cf.* equation (14.3)) and then forms the overlap with the $(N+1)$-particle state $\psi^\dagger(x')_S \mid \Psi_0(t)\rangle_S$. Thus, the Green's function for $t > t'$ is precisely the transition amplitude for the propagation from x' to x in the time interval $(t-t')$ of a test particle added to the many-particle ground state. Similarly, for $t' > t$ an $(N-1)$-particle state propagates. In other words: for $t' > t$ the Green's function describes a particle propagation and for $t > t'$ a hole propagation. The interpretation of a general Green's function $G(\lambda t, \lambda t')$ is completely analogous.

Next, we will prove that for systems for which the Hamiltonian commutes with the total-momentum operator

$$\hat{\mathbf{P}} = \sum_\alpha \int \mathrm{d}^3 r \, \hat{\psi}^\dagger_\alpha(\mathbf{r}) \, (-i\nabla) \, \hat{\psi}_\alpha(\mathbf{r})$$

the Green's function depends only on the difference $(\mathbf{r}-\mathbf{r}')$ between the space coordinates:

$$\left[\hat{H}, \hat{\mathbf{P}}\right] = 0 \quad \Rightarrow \quad G_{\alpha\beta}(\mathbf{r}t, \mathbf{r}'t') = G\left((\mathbf{r}-\mathbf{r}')t, 0\,t\right).$$

The translationally invariant systems discussed in Chapter 5 are examples of systems of this kind. It is clearly plausible that the Green's function, with the interpretation given above as a transition amplitude, should only depend on the coordinate difference for such systems. The explicit proof is nevertheless somewhat long. For the proof, we will use the following commutator identities, which we will also use later:

$$\begin{aligned} [A,BC] &= ABC - BCA \\ &= ABC + BAC - BAC - BCA \\ \Rightarrow \quad [A,BC] &= \{A,B\}C - B\{A,C\} \qquad (15.6) \\ [A,BC] &= [A,B]C - B[C,A] \qquad (15.7) \end{aligned}$$

and, similarly

$$\{A,BC\} = \{A,B\}C - B[A,C]. \qquad (15.8)$$

With the use of equation (15.6) and with $A = \hat{\psi}_\alpha(\mathbf{r})$, $B = \hat{\psi}^\dagger_\gamma(\mathbf{z})$, and $C = (-i\nabla_{\mathbf{z}})\,\hat{\psi}_\gamma(\mathbf{z})$, we readily obtain

$$\begin{aligned}
[\hat{\psi}_\alpha(\mathbf{r}), \hat{\mathbf{P}}] &= \sum_\gamma \int \mathrm{d}^3 z \left[\hat{\psi}_\alpha(\mathbf{r}), \hat{\psi}^\dagger_\gamma(\mathbf{z})\,(-i\nabla_\mathbf{z})\,\hat{\psi}_\gamma(\mathbf{z})\right] \\
&= \sum_\gamma \int \mathrm{d}^3 z \underbrace{\left\{\hat{\psi}_\alpha(\mathbf{r}), \hat{\psi}^\dagger_\gamma(\mathbf{z})\right\}}_{\delta_{\alpha\gamma}\delta(\mathbf{r}-\mathbf{z})}(-i\nabla_\mathbf{z})\,\hat{\psi}_\gamma(\mathbf{z}) \\
&\quad -\sum_\gamma \int \mathrm{d}^3 z\, \hat{\psi}^\dagger_\gamma(\mathbf{z}) \underbrace{\left\{\hat{\psi}_\alpha(\mathbf{r}), (-i\nabla_\mathbf{z})\,\hat{\psi}_\gamma(\mathbf{z})\right\}}_{-i\nabla_\mathbf{z}\{\hat{\psi}_\alpha(\mathbf{r}),\hat{\psi}_\gamma(\mathbf{z})\}=0}.
\end{aligned}$$

Thus

$$\left[\hat{\psi}_\alpha(\mathbf{r}), \hat{\mathbf{P}}\right] = -i\nabla_\mathbf{r}\hat{\psi}_\alpha(\mathbf{r}). \tag{15.9}$$

This equation represents an operator differential equation for $\hat{\psi}_\alpha(\mathbf{r})$. It can be formally integrated with the result

$$\hat{\psi}_\alpha(\mathbf{r}) = \mathrm{e}^{-i\hat{\mathbf{P}}\cdot\mathbf{r}}\hat{\psi}_\alpha(0)\mathrm{e}^{i\hat{\mathbf{P}}\cdot\mathbf{r}}. \tag{15.10}$$

This can be proved by inserting

$$\begin{aligned}
-i\nabla\hat{\psi}_\alpha(\mathbf{r}) &= -\hat{\mathbf{P}}\,\underbrace{\mathrm{e}^{-i\hat{\mathbf{P}}\cdot\mathbf{r}}\hat{\psi}_\alpha(0)\mathrm{e}^{i\hat{\mathbf{P}}\cdot\mathbf{r}}}_{\hat{\psi}_\alpha(\mathbf{r})} + \underbrace{\mathrm{e}^{-i\hat{\mathbf{P}}\cdot\mathbf{r}}\hat{\psi}_\alpha(0)\mathrm{e}^{i\hat{\mathbf{P}}\cdot\mathbf{r}}}_{\hat{\psi}_\alpha(\mathbf{r})}\hat{\mathbf{P}} \\
&= \left[\hat{\psi}_\alpha(\mathbf{r}), \hat{\mathbf{P}}\right].
\end{aligned}$$

We now return to the the expression equation (15.5) for the Green's function. To show that it depends only on the coordinate difference, we write the field operators in the Schrödinger picture:

$$\begin{aligned}
&iG_{\alpha\beta}(\mathbf{r}t, \mathbf{r}'t') \\
&= \frac{1}{\langle\Psi_0|\,\Psi_0\rangle}\Big[\theta(t-t')\mathrm{e}^{iE_0(t-t')}\langle\Psi_0\mid\hat{\psi}_\alpha(\mathbf{r})\mathrm{e}^{-i\hat{H}(t-t')}\hat{\psi}^\dagger_\beta(\mathbf{r}')|\,\Psi_0\rangle \\
&\quad -\theta(t'-t)\mathrm{e}^{-iE_0(t-t')}\langle\Psi_0\mid\hat{\psi}^\dagger_\beta(\mathbf{r}')\mathrm{e}^{i\hat{H}(t-t')}\hat{\psi}_\alpha(\mathbf{r})|\,\Psi_0\rangle\Big].
\end{aligned}$$

Here we insert the completeness relation in Fock space

$$1 = \mid\mathrm{vac}\rangle\langle\mathrm{vac}\mid + \sum_n \mid\Psi_n^{(1)}\rangle\langle\Psi_n^{(1)}\mid + \ldots + \sum_n \mid\Psi_n^{(N)}\rangle\langle\Psi_n^{(N)}\mid + \ldots \tag{15.11}$$

where $\mid\Psi_n^{(N)}\rangle$ denote the eigenfunctions of a system of N particles. This yields

$$
\begin{aligned}
iG_{\alpha\beta}(\mathbf{r}t,\mathbf{r}'t') = \frac{1}{\langle\Psi_0|\,\Psi_0\rangle}\Bigg[&\theta(t-t')\sum_n \mathrm{e}^{-i\left(E_n^{(N+1)}-E_0\right)(t-t')} \\
&\times\langle\Psi_0\mid\hat{\psi}_\alpha(\mathbf{r})\mid\Psi_n^{(N+1)}\rangle\langle\Psi_n^{(N+1)}\mid\hat{\psi}_\beta^\dagger(\mathbf{r}')|\,\Psi_0\rangle \\
&-\theta(t'-t)\sum_n \mathrm{e}^{-i\left(E_0-E_n^{(N-1)}\right)(t-t')} \\
&\times\langle\Psi_0\mid\hat{\psi}_\beta^\dagger(\mathbf{r}')\mid\Psi_n^{(N-1)}\rangle\langle\Psi_n^{(N-1)}\mid\hat{\psi}_\alpha(\mathbf{r})|\,\Psi_0\rangle\Bigg].
\end{aligned}
$$

The only non-vanishing contribution comes from the states with $(N \pm 1)$ particles, since the Fock space scalar product between wavefunctions with different particle numbers vanishes. Under the assumption that $\hat{H}$ and $\hat{\mathbf{P}}$ commute, we can choose $\mid\Psi_n^{(N\pm1)}\rangle$ as eigenfunctions of $\hat{\mathbf{P}}$:

$$
\hat{\mathbf{P}}\mid\Psi_n^{(N\pm1)}\rangle = \mathbf{P}_n^{(N\pm1)}\mid\Psi_n^{(N\pm1)}\rangle.
$$

If we then insert equation (15.10) and also choose the coordinate system so that $\hat{\mathbf{P}}|\,\Psi_0\rangle = 0$, it finally follows that

$$
\begin{aligned}
&iG_{\alpha\beta}(\mathbf{r}t,\mathbf{r}'t') \\
&= \frac{1}{\langle\Psi_0|\,\Psi_0\rangle}\Bigg[\theta(t-t')\sum_n \mathrm{e}^{-i\left(E_n^{(N+1)}-E_0\right)(t-t')}\mathrm{e}^{i\mathbf{P}_n^{(N+1)}\cdot(\mathbf{r}-\mathbf{r}')} \\
&\quad\times\langle\Psi_0\mid\hat{\psi}_\alpha(0)\mid\Psi_n^{(N+1)}\rangle\langle\Psi_n^{(N+1)}\mid\hat{\psi}_\beta^\dagger(0)|\,\Psi_0\rangle \\
&\quad-\theta(t'-t)\sum_n \mathrm{e}^{-\left(E_0-E_n^{(N-1)}\right)(t-t')}\mathrm{e}^{-i\mathbf{P}_n^{(N-1)}\cdot(\mathbf{r}-\mathbf{r}')} \\
&\quad\times\langle\Psi_0\mid\hat{\psi}_\beta^\dagger(0)\mid\Psi_n^{(N-1)}\rangle\langle\Psi_n^{(N-1)}\mid\hat{\psi}_\alpha(0)|\,\Psi_0\rangle\Bigg].
\end{aligned}
$$

This equation proves the statement that the single-particle Green's function only depends on the coordinate difference if $[\hat{H},\hat{\mathbf{P}}] = 0$. We can then form the Fourier transform with respect to this coordinate difference:

$$
G_{\alpha\beta}(\mathbf{k},t,t') = \int \mathrm{d}^3(\mathbf{r}-\mathbf{r}')\mathrm{e}^{-i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')}G_{\alpha\beta}(\mathbf{r}t,\mathbf{r}'t').
$$

The inverse transformation is

$$
G_{\alpha\beta}(\mathbf{r}t,\mathbf{r}'t') = \int \frac{\mathrm{d}^3k}{(2\pi)^3}\mathrm{e}^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')}G_{\alpha\beta}(\mathbf{k},t,t'). \tag{15.12}
$$

We will now show that for translationally invariant systems, the momentum Green's function defined earlier in equation (15.4) is diagonal and that the diagonal elements correspond to the simple Fourier transform of the space Green's function:

$$\left[\hat{H}, \hat{\mathbf{P}}\right] = 0 \quad \Rightarrow \quad G_{\alpha\beta}(\mathbf{k}t, \mathbf{k}'t') = \delta_{\mathbf{k},\mathbf{k}'} G_{\alpha\beta}(\mathbf{k}, t, t'). \tag{15.13}$$

To prove this, we insert the explicit Heisenberg transformation into the definition of the momentum Green's function

$$iG_{\alpha\beta}(\mathbf{k}t, \mathbf{k}'t') = \frac{1}{\langle \Psi_0 |\, \Psi_0 \rangle} \langle \Psi_0 \mid T[c_{\mathbf{k}\alpha}(t)_H c^\dagger_{\mathbf{k}'\beta}(t')_H] |\, \Psi_0 \rangle$$

and insert the completeness relation equation (15.11) of the exact system of eigenfunctions of $\hat{H}$. This yields

$$\begin{aligned} & iG_{\alpha\beta}(\mathbf{k}t, \mathbf{k}'t') \\ = & \frac{1}{\langle \Psi_0 |\, \Psi_0 \rangle} \left[\theta(t-t') \sum_n \mathrm{e}^{-i\left(E_n^{(N+1)} - E_0\right)(t-t')} \right. \\ & \times \langle \Psi_0 \mid c_{\mathbf{k}\alpha} \mid \Psi_n^{(N+1)} \rangle \langle \Psi_n^{(N+1)} \mid c^\dagger_{\mathbf{k}'\beta} |\, \Psi_0 \rangle \\ & - \theta(t'-t) \sum_n \mathrm{e}^{-i\left(E_0 - E_n^{(N-1)}\right)(t-t')} \\ & \left. \times\, \langle \Psi_0 \mid c^\dagger_{\mathbf{k}'\beta} \mid \Psi_n^{(N-1)} \rangle \langle \Psi_n^{(N-1)} \mid c_{\mathbf{k}\alpha} |\, \Psi_0 \rangle \right]. \end{aligned}$$

Since $c^\dagger_{\mathbf{k}'\beta} |\, \Psi_0 \rangle$ is an eigenfunction of $\hat{\mathbf{P}}$ with eigenvalue $\mathbf{k}'$, and furthermore $\langle \Psi_n^{(N+1)} |$ can be chosen as eigenfunctions of $\hat{\mathbf{P}}$ with eigenvalue $\mathbf{P}_n^{(N+1)}$, the overlap vanishes:

$$\langle \Psi_n^{(N+1)} \mid c^\dagger_{\mathbf{k}'\beta} |\, \Psi_0 \rangle = 0 \quad \text{for} \quad \mathbf{k}' \neq \mathbf{P}_n^{(N+1)}.$$

Correspondingly, we have

$$\langle \Psi_0 \mid c_{\mathbf{k}\alpha} \mid \Psi_n^{N+1)} \rangle = \langle c^\dagger_{\mathbf{k}\alpha} \Psi_0 \mid \Psi_n^{(N+1)} \rangle = 0 \quad \text{for} \quad \mathbf{k} \neq \mathbf{P}_n^{(N+1)}.$$

Furthermore, $c_{\mathbf{k}\alpha} |\, \Psi_0 \rangle$ is an eigenfunction of $\hat{\mathbf{P}}$ with eigenvalue $-\mathbf{k}$. Hence, the overlap

$$\langle \Psi_n^{(N-1)} \mid c_{\mathbf{k}\alpha} |\, \Psi_0 \rangle$$

vanishes for $-\mathbf{k} \neq \mathbf{P}_n(N-1)$, and the corresponding overlap

$$\langle \Psi_0 \mid c^\dagger_{\mathbf{k}'\beta} | \Psi_n^{(N-1)} \rangle$$

vanishes for $-\mathbf{k}' \neq \mathbf{P}_n^{(N-1)}$. Altogether, all the terms for which $\mathbf{k} \neq \mathbf{k}'$ vanish, which yields

$$G_{\alpha\beta}(\mathbf{k}t, \mathbf{k}'t') = \delta_{\mathbf{k}\mathbf{k}'} G_{\alpha\beta}(\mathbf{k}t, \mathbf{k}t').$$

It is then only left to show that these diagonal elements correspond precisely to the above Fourier transform of the spatial Green's function. This follows from the construction of the momentum Green's function by a basis transformation:

$$\begin{aligned} G_{\alpha\beta}(\mathbf{r}t, \mathbf{r}'t') &= \frac{1}{\Omega}\sum_{\mathbf{k}}\sum_{\mathbf{k}'} \mathrm{e}^{i(\mathbf{k}\cdot\mathbf{r}-\mathbf{k}'\cdot\mathbf{r}')} G_{\alpha\beta}(\mathbf{k}t, \mathbf{k}'t') \\ &= \frac{1}{\Omega}\sum_{\mathbf{k}} \mathrm{e}^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')} G_{\alpha\beta}(\mathbf{k}t, \mathbf{k}t'). \end{aligned}$$

Thus, in the continuum limit

$$\frac{1}{\Omega}\sum_{\mathbf{k}} \to \int \frac{\mathrm{d}^3k}{(2\pi)^3}$$

we obtain

$$G_{\alpha\beta}(\mathbf{r}t, \mathbf{r}'t') = \int \frac{\mathrm{d}^3k}{(2\pi)^3} \mathrm{e}^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')} G_{\alpha\beta}(\mathbf{k}t, \mathbf{k}t').$$

In comparison with equation (15.12) and the uniqueness of the Fourier transform, the relation

$$iG_{\alpha\beta}(\mathbf{k}, t, t') = iG_{\alpha\beta}(\mathbf{k}t, \mathbf{k}t') = \frac{1}{\langle \Psi_0 | \Psi_0 \rangle} \langle \Psi_0 \mid T[c_{\mathbf{k}\alpha}(t)_H c^\dagger_{\mathbf{k}\beta}(t')_H] | \Psi_0 \rangle$$

follows. The procedures which have led us here to the *diagonal* momentum Green's function in a translationally invariant system is typical of the use of symmetries: one makes an effort to choose a representation in which the Green's function is diagonal. Hence, the Green's function is sometimes in the literature defined in its symmetric form

$$iG(\lambda, t, t') = \frac{1}{\langle \Psi_0 | \Psi_0 \rangle} \langle \Psi_0 \mid T[c_\lambda(t)_H c^\dagger_\lambda(t')_H] | \Psi_0 \rangle.$$

If the Hamiltonian commutes with the total momentum, and is in addition explicitly time-independent, we have for the spatial Green's function

$$G_{\alpha\beta}(\mathbf{r}t, \mathbf{r}'t') = G_{\alpha\beta}\left((\mathbf{r}-\mathbf{r}')(t-t'), 0\,0\right).$$

In this case, we can form the four-dimensional Fourier transform

$$G_{\alpha\beta}(\mathbf{k}\omega) = \int \mathrm{d}^3(\mathbf{r}-\mathbf{r}') \int \mathrm{d}(t-t') \mathrm{e}^{-i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')} \mathrm{e}^{i\omega(t-t')} G_{\alpha\beta}(\mathbf{r}t, \mathbf{r}'t').$$

A formalism which is manifestly covariant can be constructed with this Green's function. This formalism has obvious special importance for relativistic many-particle systems (see Chapter 24). The inverse transformation is

$$G_{\alpha\beta}(\mathbf{r}t,\mathbf{r}'t') = \frac{1}{(2\pi)^4}\int \mathrm{d}^3k \int \mathrm{d}\omega\, \mathrm{e}^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')}\mathrm{e}^{-i\omega(t-t')}G_{\alpha\beta}(\mathbf{k}\omega).$$

The single-particle Green's function contains a great deal of information about the system under consideration. We will prove that with the help of the Green's function we can calculate

(1) the ground state expectation value of any single-particle operator,

(2) the ground state energy of the system,

(3) the excitation energies of the system.

Thus, given a single-particle Green's function of a system, we can obtain the most important physical properties of the system. We will first show property (1). For the sake of simplicity, we will show this property for a single-particle operator which is *local* in the space-coordinates, but non-diagonal with respect to the spin-coordinates (thus, the most common cases are included). Such an operator is in second quantization

$$A = \int \mathrm{d}^3r \sum_{\beta\alpha} \psi_\beta^\dagger(\mathbf{r})A_{\beta\alpha}(\mathbf{r})\psi_\alpha(\mathbf{r})$$

and the ground state expectation value is

$$\langle A\rangle = \frac{1}{\langle\Psi_0|\,\Psi_0\rangle}\int \mathrm{d}^3r \sum_{\alpha\beta}\langle\Psi_0\mid \psi_\beta^\dagger(\mathbf{r})A_{\alpha\beta}(\mathbf{r})\psi_\alpha(\mathbf{r})|\,\Psi_0\rangle.$$

If $A_{\beta\alpha}(\mathbf{r})$ is a differential operator, it will also act on the space-dependence of the field operators. In order for such a case not to complicate the expectation value, we use the trick of writing the expectation value as

$$\langle A\rangle = \frac{1}{\langle\Psi_0|\,\Psi_0\rangle}\int \mathrm{d}^3r \lim_{\mathbf{r}'\to\mathbf{r}} \sum_{\alpha\beta} A_{\beta\alpha}\langle\Psi_0|\psi_\beta^\dagger(\mathbf{r}')\psi_\alpha(\mathbf{r})|\,\Psi_0\rangle$$

where it is understood that $A_{\alpha\beta}(\mathbf{r})$ acts *before* we perform the limit. We then transform the field operators to the Heisenberg picture

$$
\begin{aligned}
&\langle\Psi_0 \mid \psi^\dagger_\beta(\mathbf{r}')\psi_\alpha(\mathbf{r})|\ \Psi_0\rangle \\
&= \lim_{t'\to t} \mathrm{e}^{-iE_0(t-t')}\langle\Psi_0 \mid \Psi^\dagger_\beta(\mathbf{r}')\mathrm{e}^{iH(t-t')}\psi_\alpha(\mathbf{r})|\ \Psi_0\rangle \\
&= \lim_{t'\to t}\langle\Psi_0 \mid \psi^\dagger_\beta(\mathbf{r}'t')_H\psi_\alpha(\mathbf{r}t)_H|\ \Psi_0\rangle \\
&= -\lim_{\substack{t'\to t\\ t'>t}}\langle\Psi_0 \mid T[\psi_\alpha(\mathbf{r}t)_H\psi^\dagger_\beta(\mathbf{r}'t')_H]|\ \Psi_0\rangle \\
&= -\lim_{t'\to t+} iG_{\alpha\beta}(\mathbf{r}t,\mathbf{r}'t')\langle\Psi_0|\ \Psi_0\rangle.
\end{aligned}
$$

Thus, the statement follows:

$$
\begin{aligned}
\langle A\rangle &= -i\int \mathrm{d}^3r \lim_{\mathbf{r}'\to\mathbf{r}}\lim_{t'\to t+}\left[\sum_{\alpha\beta} A_{\beta\alpha}(\mathbf{r})G_{\alpha\beta}(\mathbf{r}t,\mathbf{r}'t')\right] \\
&= -i\int \mathrm{d}^3r \lim_{\mathbf{r}'\to\mathbf{r}} \mathrm{Tr}\left(A(\mathbf{r})G(\mathbf{r}t,\mathbf{r}'t^+)\right). \qquad (15.14)
\end{aligned}
$$

In the short-hand notation of the last part, 'Tr' means the trace over the spin variables, and t^+ implies the limit $t'\to t^+$.

We will now consider a few examples.

(i) The kinetic energy is in first quantization

$$T = \sum_{i=1}^{N} -\frac{\nabla_i^2}{2m}.$$

According to the formula above, we then have

$$\langle T\rangle = -i\int \mathrm{d}^3r \lim_{\mathbf{r}'\to\mathbf{r}}\left(-\frac{\nabla_r^2}{2m}\right)\mathrm{Tr}\left(G(\mathbf{r}t,\mathbf{r}'t^+)\right).$$

(ii) The density operator (see Chapter 6) is in first quantization

$$\hat\rho(\mathbf{R}) = \sum_{i=1}^{N}\delta(\mathbf{R}-\mathbf{r}_i).$$

From the formula above, it follows that the ground state density of the system is

$$
\begin{aligned}
\rho(\mathbf{R}) = \langle\hat\rho(\mathbf{R})\rangle &= -i\int \mathrm{d}^3r \lim_{\mathbf{r}'\to\mathbf{r}}\delta(\mathbf{R}-\mathbf{r})\mathrm{Tr}\left(G(\mathbf{r}t,\mathbf{r}'t^+)\right) \\
&= -i\int \mathrm{d}^3r\, \delta(\mathbf{R}-\mathbf{r})\mathrm{Tr}\left(G(\mathbf{r}t,\mathbf{r}'t^+)\right) \\
&= -i\mathrm{Tr}\left(G(\mathbf{R}t,\mathbf{R}t^+)\right).
\end{aligned}
$$

Similarly, we obtain

(iii) The kinetic energy density $\hat{\tau}(\mathbf{R}) = \sum_{i=1}^{N} \delta(\mathbf{R}-\mathbf{r}_i)\left(-\frac{\nabla_i^2}{2m}\right)$:

$$\tau(\mathbf{R}) = \langle\hat{\tau}(\mathbf{R})\rangle = -i \lim_{\mathbf{r}'\to\mathbf{r}} \left(-\frac{\nabla_R^2}{2m}\right) \mathrm{Tr}\left(G(\mathbf{R}t, \mathbf{r}'t')\right),$$

and

(iv) the spin density $\vec{\sigma}(\mathbf{R}) = \sum_{i=1}^{N} \delta(\mathbf{R}-\mathbf{r}_i)\sigma_i$, where $\vec{\sigma}$ denotes the vector whose components are the three Pauli spin matrices:

$$\langle\vec{\sigma}(\mathbf{R})\rangle = -i\mathrm{Tr}\left(\vec{\sigma}G(\mathbf{R}t, \mathbf{R}t^+)\right).$$

We conclude this discussion by investigating the relation between the single-particle Green's function and the density matrix discussed in Chapter 6. The general space–spin density matrix is in second quantization (see equation (6.5)):

$$\rho(x, x') = \psi^\dagger(x')\psi(x) \quad (x = (\mathbf{r}, s)).$$

Thus, the ground state density matrix is obtained by

$$\begin{aligned}
\rho(x, x') &= \frac{1}{\langle\Psi_0|\,\Psi_0\rangle}\langle\Psi_0 \mid \rho(x, x')|\,\Psi_0\rangle \\
&= \frac{1}{\langle\Psi_0|\,\Psi_0\rangle}\langle\Psi_0 \mid \psi^\dagger(x')\psi(x)|\,\Psi_0\rangle \\
&= \lim_{t'\to t} \frac{1}{\langle\Psi_0|\,\Psi_0\rangle}\langle\Psi_0 \mid \psi^\dagger(x't')_H\psi(xt)_H|\,\Psi_0\rangle \\
&= -iG(xt, x't^+)
\end{aligned}$$

where we have omitted the individual steps in the proof. For Hamiltonians which in addition are explicitly time independent, so that

$$G(xt, x't') = G(x0, x'(t'-t))$$

the ground state density matrix expresses precisely the Green's function at the origin of time:

$$\rho(x, x') = -iG(x0, x'0^+). \tag{15.15}$$

Hence, the Green's function can be interpreted as a time-dependent extension of the density matrix. Indeed, this time-dependence contains a great deal of information, since one cannot calculate the exact ground state energy from the single-particle density matrix – for this, the two-particle density matrix is required. According to the statement (2) above, which we will now prove, the ground state energy can nevertheless be calculated from the single-particle Green's function. We will carry out the proof for the case of a particle–particle interaction which is local in space, but non-diagonal with respect to the spin indices, so that it does have a genuine spin-dependence. The Hamiltonian is then

$$\begin{aligned} H &= T+V=\sum_{\alpha}\int \mathrm{d}^3r\,\psi^{\dagger}_{\alpha}(\mathbf{r})\left(-\frac{\nabla^2_r}{2m}\right)\psi_{\alpha} \\ &\quad +\frac{1}{2}\sum_{\substack{\alpha\alpha'\\ \beta\beta'}}\int\!\!\int \mathrm{d}^3r\,\mathrm{d}^3r'\,\psi^{\dagger}_{\alpha}(\mathbf{r})\psi^{\dagger}_{\beta}(\mathbf{r}')V_{\substack{\alpha\alpha'\\ \beta\beta'}}(\mathbf{r},\mathbf{r}')\psi_{\beta'}(\mathbf{r}')\psi_{\alpha'}(\mathbf{r}). \end{aligned} \tag{15.16}$$

For the kinetic energy contribution, we have

$$[\psi_{\alpha}(\mathbf{r}),T]=-\frac{\nabla^2_r}{2m}\psi_{\alpha}(\mathbf{r}).$$

The proof runs completely analogously to the proof of equation (15.9). For the commutator of the field operators with the interaction potential

$$\begin{aligned} &[\psi_{\alpha}(\mathbf{r}),V] \\ &= \frac{1}{2}\sum_{\substack{\gamma\alpha'\\ \beta\beta'}}\int \mathrm{d}^3z\int \mathrm{d}^3y\left[\underbrace{\psi_{\alpha}(\mathbf{r})}_{A},\underbrace{\psi^{\dagger}_{\gamma}(\mathbf{z})}_{B}\underbrace{\psi^{\dagger}_{\beta}(\mathbf{y})V_{\substack{\gamma\alpha'\\ \beta\beta'}}(\mathbf{z},\mathbf{y})\psi_{\beta'}(\mathbf{y})\psi_{\alpha'}(\mathbf{z})}_{C}\right] \end{aligned}$$

we obtain with equation (15.6)

$$\begin{aligned} &\frac{1}{2}\sum_{\substack{\gamma\alpha'\\ \beta\beta'}}\int \mathrm{d}^3z\int \mathrm{d}^3y\Big[\underbrace{\left\{\psi_{\alpha}(\mathbf{r}),\psi^{\dagger}_{\gamma}(\mathbf{z})\right\}}_{=\delta_{\alpha\gamma}\delta(\mathbf{r}-\mathbf{z})}C \\ &\qquad -\psi^{\dagger}_{\gamma}(\mathbf{z})\left\{\psi_{\alpha}(\mathbf{r}),\psi^{\dagger}_{\beta}(\mathbf{y})V_{\substack{\gamma\alpha'\\ \beta\beta'}}(\mathbf{z},\mathbf{y})\psi_{\beta'}(\mathbf{y})\psi_{\alpha'}(\mathbf{z})\right\}\Big] \\ &= \frac{1}{2}\sum_{\alpha'\beta\beta'}\int \mathrm{d}^3y\,\psi^{\dagger}_{\beta}(\mathbf{y})V_{\substack{\alpha\alpha'\\ \beta\beta'}}(\mathbf{r},\mathbf{y})\psi_{\beta'}(\mathbf{y})\psi_{\alpha'}(\mathbf{r})+Z \end{aligned}$$

where, with equation (15.8), we furthermore have

$$\begin{aligned} Z &= \frac{1}{2}\sum_{\substack{\gamma\alpha'\\ \beta\beta'}}\int \mathrm{d}^3z\int \mathrm{d}^3y\left(-\psi^{\dagger}_{\gamma}(\mathbf{z})\right) \\ &\quad\times\underbrace{\left\{\psi_{\alpha}(\mathbf{r}),\psi^{\dagger}_{\beta}(\mathbf{y})\right\}}_{=\delta_{\alpha\beta}\delta(\mathbf{r}-\mathbf{y})}V_{\substack{\gamma\alpha'\\ \beta\beta'}}(\mathbf{z},\mathbf{y})\;\underbrace{\psi_{\beta'}(\mathbf{y})\psi_{\alpha'}(\mathbf{z})}_{=-\psi_{\alpha'}(\mathbf{z})\psi_{\beta'}(\mathbf{y})} \end{aligned}$$

$$
\begin{aligned}
&+\psi_\gamma^\dagger(\mathbf{z})\psi_\beta^\dagger(\mathbf{y})V_{\substack{\gamma\alpha'\\ \beta\beta'}}(\mathbf{z},\mathbf{y})\underbrace{\left[\psi_\alpha(\mathbf{r}),\psi_{\beta'}(\mathbf{y})\psi_{\alpha'}(\mathbf{z})\right]}_{=0,\ \text{by (15.6)}}\\
=\ &\frac{1}{2}\sum_{\gamma\alpha'\beta'}\int \mathrm{d}^3z\,\psi_\gamma^\dagger(\mathbf{z})V_{\substack{\gamma\alpha'\\ \alpha\beta'}}(\mathbf{z},\mathbf{r})\psi_{\alpha'}(\mathbf{z})\psi_{\beta'}(\mathbf{r}).
\end{aligned}
$$

We then rename the summation indices according to $\mathbf{z}\to\mathbf{y},\gamma\to\beta,\alpha'\leftrightarrow\beta'$, which leads to

$$
Z=\frac{1}{2}\sum_{\beta\beta'\alpha'}\int \mathrm{d}^3y\,\psi_\beta^\dagger(\mathbf{y})V_{\substack{\beta\beta'\\ \alpha\alpha'}}(\mathbf{y},\mathbf{r})\psi_{\beta'}(\mathbf{y})\psi_{\alpha'}(\mathbf{r}).
$$

Because of the indistinguishability of the microscopic particles of the system, we can assume that the potential is symmetric under interchange of the coordinates:

$$
V_{\substack{\gamma\gamma'\\ \delta\delta'}}(\mathbf{r},\mathbf{r}')=V_{\substack{\delta\delta'\\ \gamma\gamma'}}(\mathbf{r}',\mathbf{r})
$$

(non-symmetric parts leave no contributions to equation (15.16)). This yields

$$
Z=\frac{1}{2}\sum_{\alpha'\beta\beta'}\int \mathrm{d}^3y\,\psi_\beta^\dagger(\mathbf{y})V_{\substack{\alpha\alpha'\\ \beta\beta'}}(\mathbf{r},\mathbf{y})\psi_{\beta'}(\mathbf{y})\psi_{\alpha'}(\mathbf{r}).
$$

The total result for the commutator is thus twice the contribution of the potential energy

$$
[\psi_\alpha(\mathbf{r}),H]=-\frac{\nabla_r^2}{2m}\psi_\alpha(\mathbf{r})+\sum_{\alpha'\beta\beta'}\int \mathrm{d}^3y\,\psi_\beta^\dagger(\mathbf{y})V_{\substack{\alpha\alpha'\\ \beta\beta'}}(\mathbf{r},\mathbf{y})\psi_{\beta'}(\mathbf{y})\psi_{\alpha'}(\mathbf{r}).
\tag{15.17}
$$

We then insert this result in the Heisenberg equation of motion for the field operators

$$
\begin{aligned}
i\frac{\partial}{\partial t}\psi_\alpha(\mathbf{r}t)_H &= [\psi_\alpha(\mathbf{r}t)_H,H]=\mathrm{e}^{iHt}\,[\psi_\alpha(\mathbf{r})_S,H]\,\mathrm{e}^{-iHt}\\
&= \left[-\frac{\nabla_r^2}{2m}\right]\psi_\alpha(\mathbf{r}t)_H\\
&\quad+\sum_{\alpha'\beta\beta'}\int \mathrm{d}^3y\,\psi_\beta^\dagger(\mathbf{y}t)_H V_{\substack{\alpha\alpha'\\ \beta\beta'}}(\mathbf{r},\mathbf{y})\psi_{\beta'}(\mathbf{y}t)_H\psi_{\alpha'}(\mathbf{r}t)_H.
\end{aligned}
\tag{15.18}
$$

We multiply this equation on the left with $\psi_\alpha^\dagger(\mathbf{r}'t')_H$ and divide by $\langle\Psi_0\mid\Psi_0\rangle$ to form the ground state expectation value. This yields

$$\left[i\frac{\partial}{\partial t} - \left(-\frac{\nabla_r^2}{2m}\right)\right] \frac{\langle\Psi_0 \mid \psi_\alpha^\dagger(\mathbf{r}'t')_H \psi_\alpha(\mathbf{r}t)_H \mid \Psi_0\rangle}{\langle\Psi_0 \mid \Psi_0\rangle}$$
$$= \sum_{\alpha'\beta\beta'} \int \mathrm{d}^3y \frac{1}{\langle\Psi_0 \mid \Psi_0\rangle}$$
$$\times \langle\Psi_0 \mid \psi_\alpha^\dagger(\mathbf{r}'t')_H \psi_\beta^\dagger(\mathbf{y}t)_H V_{\substack{\alpha\alpha' \\ \beta\beta'}}(\mathbf{r},\mathbf{y}) \psi_{\beta'}(\mathbf{y}t)_H \psi_{\alpha'}(\mathbf{r}t)_H \mid \Psi_0\rangle .$$

We now take the limits $\mathbf{r}' \to \mathbf{r}$ and $t' \to t$ in this equation, then integrate over d^3r and sum over α. From the definition of the single-particle Green's function it then follows that

$$\int \mathrm{d}^3r \lim_{t'\to t^+} \lim_{\mathbf{r}'\to\mathbf{r}} \left(i\frac{\partial}{\partial t} + \frac{\nabla_r^2}{2m}\right) \mathrm{Tr}\left[-iG_{\alpha\beta}(\mathbf{r}t,\mathbf{r}'t')\right] = 2\langle\Psi_0 \mid V \mid \Psi_0\rangle . \tag{15.19}$$

With the help of this equation can we eliminate the potential energy from the ground state energy

$$E_0 = \langle\Psi_0 \mid T \mid \Psi_0\rangle + \langle\Psi_0 \mid V \mid \Psi_0\rangle$$

to obtain the final result

$$E_0 = -\frac{i}{2}\int \mathrm{d}^3r \lim_{t'\to t} \lim_{\mathbf{r}'\to\mathbf{r}} \left(i\frac{\partial}{\partial t} - \frac{\nabla_r^2}{2m}\right) \mathrm{Tr}\left[G_{\alpha\beta}(\mathbf{r}t,\mathbf{r}'t')\right] . \tag{15.20}$$

For translationally invariant, explicitly time-independent systems we obtain a particularly simple equation if we use the four-dimensional Fourier transform of the Green's function :

$$E_0 = -\frac{i}{2}\frac{\Omega}{(2\pi)^4} \lim_{\tau\to 0+} \int \mathrm{d}^3k \int \mathrm{d}\omega\, \mathrm{e}^{i\omega\tau} \left(\frac{k^2}{2m} + \omega\right) \mathrm{Tr}\left[G(\mathbf{k},\omega)\right] . \tag{15.21}$$

Before we can prove statement (3) above, we will first discuss the Green's function of a system of free, non-interacting fermions, *i.e.*, $H_0 = T$ and $V \equiv 0$. In this case, the Heisenberg picture and the interacting picture are identical, so that we can calculate the Green's function from

$$iG^{(0)}_{\alpha\beta}(\mathbf{r}t,\mathbf{r}'t') = \langle\Phi_0 \mid T[\psi_\alpha(\mathbf{r}t)_I \psi_\beta^\dagger(\mathbf{r}'t')_I] \mid \Phi_0\rangle .$$

We transform to creation and annihilation operators of the momentum eigenfunctions and use the representation equation (14.10) in the interaction picture:

$$\psi_\alpha(\mathbf{r}t)_I = \sum_{\mathbf{k}} \frac{1}{\sqrt{\Omega}} \mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}} c_{\mathbf{k}\alpha}(t)_I = \sum_{\mathbf{k}} \frac{1}{\sqrt{\Omega}} \mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}} \mathrm{e}^{-i\epsilon_k t} c_{\mathbf{k}\alpha}$$

and

$$\psi_\beta^\dagger(\mathbf{r}'t')_I = \sum_{\mathbf{k}'} \frac{1}{\sqrt{\Omega}} \mathrm{e}^{-i\mathbf{k}'\cdot\mathbf{r}'} \mathrm{e}^{i\epsilon_{k'}t'} c^\dagger_{\mathbf{k}'\beta}$$

where

$$\epsilon_k = \frac{k^2}{2m}.$$

This yields

$$iG^{(0)}_{\alpha\beta}(\mathbf{r}t, \mathbf{r}'t') = \frac{1}{\Omega}\sum_{\mathbf{k}\mathbf{k}'} \mathrm{e}^{i(\mathbf{k}\cdot\mathbf{r}-\mathbf{k}'\cdot\mathbf{r}')}\mathrm{e}^{-i(\epsilon_k t-\epsilon_{k'}t')}$$
$$\times \left[\theta(t-t')\langle\Phi_0 \mid c_{\mathbf{k}\alpha}c^\dagger_{\mathbf{k}'\beta} \mid \Phi_0\rangle - \theta(t'-t)\langle\Phi_0 \mid c^\dagger_{\mathbf{k}'\beta}c_{\mathbf{k}\alpha} \mid \Phi_0\rangle\right].$$

Here $\mid \Phi_0\rangle$ is the ground state wavefunction of $H_0 = T$, *i.e.*, a Slater-determinant of all plane waves of momentum less than k_F. Consequently, the matrix elements vanish unless the created state $(\mathbf{k}'\beta)$ is identical to the annihilated state $(\mathbf{k}\alpha)$. This yields

$$iG^{(0)}_{\alpha\beta}(\mathbf{r}t, \mathbf{r}'t') = \frac{\delta_{\alpha\beta}}{\Omega}\sum_{\mathbf{k}} \mathrm{e}^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')}\mathrm{e}^{-i\epsilon_k(t-t')}$$
$$\times \left[\theta(t-t')\langle\Phi_0 \mid c_{\mathbf{k}\alpha}c^\dagger_{\mathbf{k}\alpha} \mid \Phi_0\rangle - \theta(t'-t)\langle\Phi_0 \mid c^\dagger_{\mathbf{k}\alpha}c_{\mathbf{k}\alpha} \mid \Phi_0\rangle\right].$$

If we now also use

$$\begin{aligned}\langle\Phi_0 \mid c_{\mathbf{k}\alpha}c^\dagger_{\mathbf{k}\alpha} \mid \Phi_0\rangle &= \langle c^\dagger_{\mathbf{k}\alpha}\Phi_0 \mid c^\dagger_{\mathbf{k}\alpha}\Phi_0\rangle \left\{\begin{array}{ll} 1: & k > k_F \\ 0: & k \le k_F \end{array}\right\} = \theta(k-k_F) \\ \langle\Phi_0 \mid c^\dagger_{\mathbf{k}\alpha}c_{\mathbf{k}\alpha} \mid \Phi_0\rangle &= \langle c_{\mathbf{k}\alpha}\Phi_0 \mid c_{\mathbf{k}\alpha}\Phi_0\rangle = \left\{\begin{array}{ll} 1: & k \le k_F \\ 0: & k > k_F \end{array}\right\} = \theta(k_F-k)\end{aligned}$$

we finally obtain in the continuum limit

$$\begin{aligned}iG^{(0)}_{\alpha\beta}(\mathbf{r}t, \mathbf{r}'t') &= \delta_{\alpha\beta}\int \frac{\mathrm{d}^3k}{(2\pi)^3}\mathrm{e}^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')}\mathrm{e}^{-i\epsilon_k(t-t')} \\ &\quad \times \left[\theta(t-t')\theta(k-k_F) - \theta(t'-t)\theta(k_F-k)\right].\end{aligned} \tag{15.22}$$

By definition, it follows that the momentum Green's function is

$$iG^{(0)}_{\alpha\beta}(\mathbf{k}, t-t') = \delta_{\alpha\beta}\mathrm{e}^{-i\epsilon_k(t-t')}\left[\theta(t-t')\theta(k-k_F) - \theta(t'-t)\theta(k_F-k)\right]. \tag{15.23}$$

For the derivation of the four-dimensional Fourier transform, we will first show that the step function has the following representation:

$$\theta(\tau) = \lim_{\eta\to 0^+} -\frac{1}{2\pi i}\int_{-\infty}^{\infty} \mathrm{d}\omega \frac{\mathrm{e}^{-i\omega\tau}}{\omega + i\eta}. \tag{15.24}$$

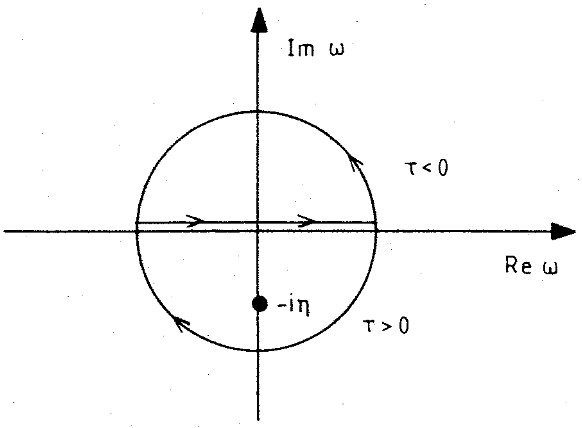


Figure 15.1 *Integration paths for $\tau < 0$ and $\tau > 0$.*

The integrand has a simple pole at $\omega = -i\eta$ and the residue leaves a contribution of

$$\mathrm{Res}\frac{\mathrm{e}^{-i\omega\tau}}{\omega + i\eta} = \lim_{\omega\to -i\eta}(\omega + i\eta)\frac{\mathrm{e}^{-i\omega\tau}}{(\omega + i\eta)} = \mathrm{e}^{-\eta\tau}.$$

If we want to calculate the integral with the help of the theorem of residues, we have to close the integration path with a semi-circle. To ensure that the integration over the arc in the limit of an infinitely large radius leaves a vanishing contribution, we must, because of

$$\mathrm{e}^{-i\omega\tau} = \mathrm{e}^{-i(\mathrm{Re}\,\omega)\tau}\mathrm{e}^{(\mathrm{Im}\,\omega)\tau}$$

close the arc in the lower half-plane for $\tau > 0$ and in the upper half-plane for $\tau < 0$. Since there are no singularities enclosed by the semi-circle, the integral over the closed path vanishes according to Cauchy's theorem. Thus, for $\tau < 0$ the integral leaves a null result, which we had to show. For $\tau > 0$ we obtain, by using the theorem of residues

$$\begin{aligned}\int_{-\infty}^{\infty} \mathrm{d}\omega \frac{\mathrm{e}^{-i\omega\tau}}{\omega + i\eta} &= \oint \mathrm{d}\omega \frac{\mathrm{e}^{-i\omega\tau}}{\omega + i\eta} \\ &= -2\pi i \times (\text{sum of residues}) \\ &= -2\pi i \mathrm{e}^{-\eta\tau}.\end{aligned}$$

The minus sign comes from the negative orientation of the integration path. For $\tau > 0$ the statement then follows:

$$\lim_{\eta\to 0+} -\frac{1}{2\pi i}\int_{-\infty}^{\infty} \mathrm{d}\omega \frac{\mathrm{e}^{-i\omega\tau}}{\omega + i\eta} = 1.$$

One can analogously show that

$$\theta(-\tau) = \lim_{\eta\to 0+} = +\frac{1}{2\pi i}\int_{-\infty}^{\infty} \mathrm{d}\omega \frac{\mathrm{e}^{-i\omega\tau}}{\omega - i\eta}. \tag{15.25}$$

If we insert these into the above expression equation (15.22) for the Green's function, we obtain

$$\begin{aligned} iG^{(0)}_{\alpha\beta}(\mathbf{r}t, \mathbf{r}'t') &= i \lim_{\eta\to 0+} \delta_{\alpha\beta} \int \frac{\mathrm{d}^3k}{(2\pi)^3} \mathrm{e}^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')} \\ &\times \int_{-\infty}^{\infty} \frac{\mathrm{d}w}{2\pi} \mathrm{e}^{-i(\epsilon_k + w)(t-t')} \left[\frac{\theta(k-k_F)}{w+i\eta} + \frac{\theta(k_F-k)}{w-i\eta}\right]. \end{aligned}$$

With the substitution $\omega \equiv \epsilon_k + w$ it finally follows that

$$\begin{aligned} G^{(0)}_{\alpha\beta}(\mathbf{r}t, \mathbf{r}'t') &= \lim_{\eta\to 0+} \delta_{\alpha\beta} \int \frac{\mathrm{d}^3k}{(2\pi)^3} \int \frac{\mathrm{d}\omega}{2\pi} \\ &\times \mathrm{e}^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')} \mathrm{e}^{-i\omega(t-t')} \left[\frac{\theta(k-k_F)}{\omega - \epsilon_k + i\eta} + \frac{\theta(k_F-k)}{\omega-\epsilon_k - i\eta}\right] \end{aligned}$$

so that

$$G^{(0)}_{\alpha\beta}(\mathbf{k}\omega) = \lim_{\eta\to 0+} \delta_{\alpha\beta} \left[\frac{\theta(k-k_F)}{\omega - \epsilon_k + i\eta} + \frac{\theta(k_F-k)}{\omega-\epsilon_k - i\eta}\right]. \tag{15.26}$$

This function has for $k > k_F$, *i.e.*, for $\epsilon_k = \frac{k^2}{2m} > \frac{k_F^2}{2m} = \epsilon_F$, a simple pole at

$$\omega = \epsilon_k - i\eta,$$

and for $k < k_F$, *i.e.*, for $\epsilon_k < \epsilon_F$, a simple pole at

$$\omega = \epsilon_k + i\eta.$$

It is essential to note that we only obtain discrete poles so long as we are only considering a *finite* system. In the continuum limit, the analytical structure of the Green's function changes, and we obtain a branch cut along the real axis.

We will now test the this formalism by using the Green's function that we have just determined together with equation (15.21) to calculate the well-known ground state energy of the free non-interacting electron gas:

$$\begin{aligned} E_0 &= -\frac{i}{2}\frac{\Omega}{(2\pi)^4} \int \mathrm{d}^3k \lim_{\tau\to 0+} \int_{-\infty}^{\infty} \mathrm{d}\omega \mathrm{e}^{i\omega\tau} (\epsilon_k + \omega) \operatorname{Tr}\left\{G^{(0)}(\mathbf{k},\omega)\right\} \\ &= -\frac{i}{2}\frac{\Omega}{(2\pi)^4} \int_0^{\infty} 4\pi k^2 \mathrm{d}k \lim_{\substack{\tau\to 0+ \\ \eta\to 0+}} \int_{-\infty}^{\infty} \mathrm{d}\omega\, \mathrm{e}^{i\omega\tau} \\ &\times 2\left[\theta(k-k_F)\frac{\epsilon_k+\omega}{\omega-\epsilon_k+i\eta} + \theta(k_F-k)\frac{\epsilon_k+\omega}{\omega-\epsilon_k-i\eta}\right]. \end{aligned}$$

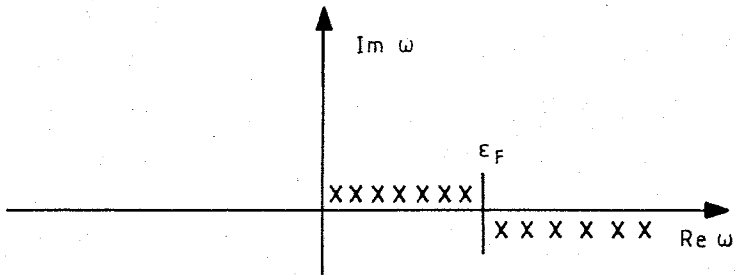


Figure 15.2 *The locations of the poles of the Green's function are just above the real axis for* $\epsilon_k < \epsilon_F$*, and just below the real axis for* $\epsilon_k > \epsilon_F$*.*

Since $\tau > 0$ we choose an integration path Γ which closes with a counter-clockwise semi-circle in the *upper* half-plane:

$$\int_{-\infty}^{\infty} \mathrm{d}\omega = \int_{\Gamma} \mathrm{d}\omega.$$

The first term ($k > k_F$) of the integrand does not leave any contribution, since this term has no singularities in the upper half-plane. This leaves only the contribution from the second term:

$$E_0 = -i\frac{\Omega}{(2\pi)^4}\int_0^{k_F} 4\pi k^2 \mathrm{d}k \lim_{\substack{\tau\to 0+\\ \eta\to 0+}} \int_{\Gamma} \mathrm{d}\omega\, \mathrm{e}^{i\omega\tau}\frac{\epsilon_k+\omega}{\omega-\epsilon_k-i\eta}.$$

The calculation of the integral over the closed path yields, with the help of the residue theorem

$$\begin{aligned}
&\lim_{\substack{\tau\to 0+\\ \eta\to 0+}} \int_{\Gamma} \mathrm{d}\omega\, \mathrm{e}^{i\omega\tau}\frac{\epsilon_k+\omega}{\omega-\epsilon_k-i\eta}\\
=\;& \lim_{\substack{\tau\to 0+\\ \eta\to 0+}} (2\pi i) \lim_{\omega\to\epsilon_k+i\eta}\left[\mathrm{e}^{i\omega\tau}(\epsilon_k+\omega)\right]\\
=\;& \lim_{\substack{\tau\to 0+\\ \eta\to 0+}} (2\pi i)\mathrm{e}^{i(\epsilon_k+i\eta)\tau}(\epsilon_k+\epsilon_k+i\eta)\\
=\;& (2\pi i)2\epsilon_k = (2\pi i)\frac{k^2}{m}.
\end{aligned}$$

Thus, we obtain the familiar expression

$$E_0 = \frac{\Omega}{2\pi^2}\int_0^{k_F} k^2 \mathrm{d}k \frac{k^2}{m} = \frac{\Omega}{10m\pi^2}k_F^5$$

for the total energy.

We will now for later purposes write the Green's function of a non-interacting Fermi gas in yet another way. To do so, we first consider a system with $(N+1)$ particles. The ground state energy of this system is obtained by adding a particle at the Fermi level to the N-particle system, so that

$$E_0^{(N+1)} = \sum_{k\leq k_F} \epsilon_k + \epsilon_F.$$

We obtain an excited state of the $(N+1)$-particle system by adding a particle with momentum $\mathbf{K}$ such that $K > k_F$ to the N-particle system. The energy of this state is then

$$E_{\mathbf{K}}^{(N+1)} = \sum_{k\leq k_F} \epsilon_k + \epsilon_K.$$

Hence the different excitation energies of the $(N+1)$-particle system are

$$w_{\mathbf{K}}^{(N+1)} \equiv E_{\mathbf{K}}^{(N+1)} - E_0^{(N+1)} = \epsilon_K - \epsilon_F > 0.$$

We obtain the ground state energy of a system with $(N-1)$ particles by removing one particle from the Fermi level

$$E_0^{(N-1)} = \sum_{k\leq k_F} \epsilon_k - \epsilon_F.$$

On the other hand, an excited state of the $(N-1)$-particle system is obtained by removing any particle with momentum $\mathbf{K}$ and energy $\epsilon_K < \epsilon_F$ from the ground state of the N-particle system. The entire system has then a momentum $-\mathbf{K}$ (since the previously fully occupied Fermi sphere had zero momentum) and energy

$$E_{-\mathbf{K}}^{(N-1)} = \sum_{k\leq k_F} \epsilon_k - \epsilon_K.$$

Thus, the excitation energies of the $(N-1)$-particle system are given by

$$w_{-\mathbf{K}}^{(N-1)} \equiv E_{-\mathbf{K}}^{(N-1)} - E_0^{(N-1)} = -\epsilon_K + \epsilon_F > 0.$$

We can now write the Green's function of the non-interacting N-particle system as a function of the excitation energies of the $(N-1)$- and the

$(N+1)$-particle systems:

$$\begin{aligned} & G^{(0)}_{\alpha\beta}(\mathbf{k},\omega) \\ = & \lim_{\eta\to 0^+} \delta_{\alpha\beta} \left[\frac{\theta(k-k_F)}{\omega-\epsilon_F-(\epsilon_k-\epsilon_F)+i\eta} + \frac{\theta(k_F-k)}{\omega-\epsilon_F+(\epsilon_F-\epsilon_k)-i\eta} \right] \\ = & \lim_{\eta\to 0^+} \delta_{\alpha\beta} \left[\frac{\theta(k-k_F)}{\omega-\epsilon_F-w^{(N+1)}_{\mathbf{k}}+i\eta} + \frac{\theta(k_F-k)}{\omega-\epsilon_F+w^{(N-1)}_{-\mathbf{k}}-i\eta} \right] . \end{aligned} \tag{15.27}$$

Thus, the Green's functions has its poles at the exact excitation energies relative to the Fermi level of the

$$(N+1)\text{-particle system:} \qquad \omega = \epsilon_F + w^{(N+1)}_{\mathbf{k}} - i\eta$$

and of the

$$(N-1)\text{-particle system:} \qquad \omega = \epsilon_F - w^{(N-1)}_{-\mathbf{k}} + i\eta .$$

We will now show that this statement also holds for the exact Green's function of an interacting system, which proves statement (3).

For the sake of simplicity, we will restrict ourselves to explicitly time-independent, translationally invariant systems. It then suffices to consider the (diagonal) momentum Green's functions. We will furthermore also restrict ourselves to spin-independent interactions, so that we have

$$G_{\alpha\beta}(\mathbf{k},t-t') = \delta_{\alpha\beta}G(\mathbf{k},t-t')$$

with

$$\begin{aligned} iG(\mathbf{k},t-t') = & \frac{1}{\langle\Psi_0|\,\Psi_0\rangle}\langle\Psi_0\mid T[c_{\mathbf{k}}(t)_H c^\dagger_{\mathbf{k}}(t')_H]|\,\Psi_0\rangle \\ = & \frac{1}{\langle\Psi_0|\,\Psi_0\rangle}\left[\theta(t-t')\sum_n \mathrm{e}^{-i\left(E^{(N+1)}_n-E^{(N)}_0\right)(t-t')}\right. \\ & \times\langle\Psi_0\mid c_{\mathbf{k}}\mid\Psi^{(N+1)}_n\rangle\langle\Psi^{(N+1)}_n\mid c^\dagger_{\mathbf{k}}|\,\Psi_0\rangle \\ & -\theta(t'-t)\sum_n \mathrm{e}^{-i\left(E^{(N)}_0-E^{(N-1)}_n\right)(t-t')} \\ & \left.\times\,\langle\Psi_0\mid c^\dagger_{\mathbf{k}}\mid\Psi^{(N-1)}_n\rangle\langle\Psi^{(N-1)}_n\mid c_{\mathbf{k}}|\,\Psi_0\rangle\right] . \end{aligned}$$

We have here performed the transformation of the Heisenberg operators to the Schrödinger picture and inserted the completeness relation equation

(15.11). With the representation equations (15.24) and (15.25) of the step function, we obtain

$$
\begin{aligned}
&iG(\mathbf{k},t-t') \\
&= i \lim_{\eta\to 0^+} \left\{ \int_{-\infty}^{\infty} \frac{\mathrm{d}w}{2\pi} \sum_n \frac{\mathrm{e}^{-i\left(w+E_n^{(N+1)}-E_0^N\right)(t-t')}}{w+i\eta} \frac{\left|\langle \Psi_n^{(N+1)} \mid c_{\mathbf{k}}^{\dagger} \mid \Psi_0\rangle\right|^2}{\langle \Psi_0 \mid \Psi_0\rangle} \right. \\
&\qquad \left. + \int_{-\infty}^{\infty} \frac{\mathrm{d}w}{2\pi} \sum_n \frac{\mathrm{e}^{-i\left(w+E_0^N-E_n^{(N-1)}\right)(t-t')}}{w-i\eta} \frac{\left|\langle \Psi_n^{(N-1)} \mid c_{\mathbf{k}} \mid \Psi_0\rangle\right|^2}{\langle \Psi_0 \mid \Psi_0\rangle} \right\}.
\end{aligned}
$$

With the substitutions $\omega \equiv w + E_n^{(N+1)} - E_0^N$ in the first integral, and $\omega \equiv w - E_n^{(N-1)} + E_0^N$ in the second integral, this expression becomes

$$
\begin{aligned}
&i \lim_{\eta\to 0^+} \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{2\pi} \mathrm{e}^{-i\omega(t-t')} \frac{1}{\langle \Psi_0 \mid \Psi_0\rangle} \left\{ \sum_n \frac{\left|\langle \Psi_n^{(N+1)} \mid c_{\mathbf{k}}^{\dagger} \mid \Psi_0\rangle\right|^2}{\omega - E_n^{(N+1)} + E_0^N + i\eta} \right. \\
&\qquad \left. + \sum_n \frac{\left|\langle \Psi_n^{(N-1)} \mid c_{\mathbf{k}} \mid \Psi_0\rangle\right|^2}{\omega + E_n^{(N-1)} - E_0^N - i\eta} \right\}.
\end{aligned}
$$

We now look a little closer at the denominators that appear in this expression. In the first term we have

$$
\omega - E_n^{(N+1)} + E_0^N + i\eta = \omega - \left(E_n^{(N+1)} - E_0^{(N+1)}\right) - \left(E_0^{(N+1)} - E_0^N\right) + i\eta.
$$

The difference

$$
w_n^{(N+1)} \equiv E_n^{(N+1)} - E_0^{(N+1)} > 0
$$

is precisely an excitation energy of the $(N+1)$-particle system. Hence

$$
\left(E_0^{(N+1)} - E_0^N\right) \cong \left.\frac{\partial E_0}{\partial N}\right|_N = \mu^{(N)}
$$

is the change of the ground state energy in adding one particle, which is precisely the chemical potential.

The second denominator is

$$
\omega + E_n^{(N-1)} - E_0 - i\eta = \omega + \left(E_n^{(N-1)} - E_0^{(N-1)}\right) - \left(E_0^N - E_0^{(N-1)}\right) - i\eta.
$$

The difference

$$
w_n^{(N-1)} \equiv E_n^{(N-1)} - E_0^{(N-1)} > 0
$$

is this time an excitation energy of the $(N-1)$-particle system, and

$$E_0^{(N)} - E_0^{(N-1)} = \mu^{(N-1)}$$

is furthermore the chemical potential. For very large systems, we can set

$$\mu^{(N)} \cong \mu^{(N-1)} \equiv \mu.$$

(However, we have to be careful in the case of systems for which the ground state energy E_0 is discontinuous as a function of the quasi-continuous variable N, so that there are gaps in the ground state energy, such as the band gap in isolators. In such cases, $\mu^{(N)} \neq \mu^{(N-1)}$.) Finally, we take into consideration that the matrix element $\langle \Psi_n^{(N+1)} \mid c_{\mathbf{k}}^\dagger \mid \Psi_0 \rangle$ vanishes unless $\Psi_n^{(N-1)}$ is a state with total momentum $\mathbf{P}_n = \mathbf{k}$, and similarly the matrix element $\langle \Psi_n^{(N-1)} \mid c_{\mathbf{k}} \mid \Psi_0 \rangle$ vanishes unless $\Psi_n^{(N-1)}$ is a state with total momentum $\mathbf{P}_n = -\mathbf{k}$. Hence, we can restrict the sum over the intermediate states and the final result is the so-called *Lehmann representation* of the Green's function:

$$\begin{aligned} G(\mathbf{k},\omega) &= \lim_{\eta\to 0^+} \frac{1}{\langle \Psi_0 \mid \Psi_0 \rangle} \left\{ \sum_n \frac{\left| \langle \Psi_n^{(N+1)}(\mathbf{k}) \mid c_{\mathbf{k}}^\dagger \mid \Psi_0 \rangle \right|^2}{\omega - \mu - w_{n,\mathbf{k}}^{(N+1)} + i\eta} \right. \\ & \left. \qquad + \sum_n \frac{\left| \langle \Psi_n^{(N-1)}(-\mathbf{k}) \mid c_{\mathbf{k}} \mid \Psi_0 \rangle \right|^2}{\omega - \mu + w_{n,-\mathbf{k}}^{(N-1)} - i\eta} \right\}. \end{aligned} \tag{15.28}$$

Thus, the Green's function of an interacting many-particle system has its poles at the exact excitation energies, relative to the chemical potential, of

$$\begin{aligned} &\text{an} \quad (N+1)\text{-particle systems:} \quad \omega = \mu + w_{n,\mathbf{k}}^{(N+1)} - i\eta \\ &\text{and of an} \quad (N-1)\text{-particle systems:} \quad \omega = \mu - w_{n,-\mathbf{k}}^{(N-1)} + i\eta. \end{aligned}$$

We can also write $G(\mathbf{k},\omega)$ in the form

$$G(\mathbf{k},\omega) = \lim_{\eta\to 0^+} \int_0^\infty \mathrm{d}\epsilon \left[\frac{A(\mathbf{k},\epsilon)}{\omega - \mu - \epsilon + i\eta} + \frac{B(\mathbf{k},\epsilon)}{\omega - \mu + \epsilon - i\eta} \right] \tag{15.29}$$

where

$$A(\mathbf{k},\epsilon) = \sum_n \frac{\left| \langle \Psi_n^{(N+1)}(\mathbf{k}) \mid c_{\mathbf{k}}^\dagger \mid \Psi_0 \rangle \right|^2}{\langle \Psi_0 \mid \Psi_0 \rangle} \delta(\epsilon - w_{n,\mathbf{k}}^{(N+1)})$$

and

$$B(\mathbf{k},\epsilon) = \sum_n \frac{\left| \langle \Psi_n^{(N-1)}(-\mathbf{k}) \mid c_{\mathbf{k}} \mid \Psi_0 \rangle \right|^2}{\langle \Psi_0 \mid \Psi_0 \rangle} \delta(\epsilon - w_{n,-\mathbf{k}}^{(N-1)})$$

The *spectral functions* defined in this way are by construction real and positive:

$$
\begin{aligned}
A^*(\mathbf{k},\epsilon) = A(\mathbf{k},\epsilon) &\geq 0 \\
B^*(\mathbf{k},\epsilon) = B(\mathbf{k},\epsilon) &\geq 0.
\end{aligned}
\qquad (15.30)
$$

Because $w_n^{(N\pm1)} > 0$, it furthermore follows that

$$A(\mathbf{k},\epsilon) = 0 = B(\mathbf{k},\epsilon) \text{ for } \epsilon < 0. \qquad (15.31)$$

and we obtain the sum rule

$$\int_0^\infty \mathrm{d}\epsilon\,(A(\mathbf{k},\epsilon) + B(\mathbf{k},\epsilon)) = 1. \qquad (15.32)$$

To prove this last equation we simply integrate:

$$
\begin{aligned}
\int \mathrm{d}\epsilon\, A(\mathbf{k},\epsilon) &= \sum_n \frac{1}{\langle\Psi_0|\,\Psi_0\rangle}\langle\Psi_0\mid c_{\mathbf{k}}\mid\Psi_n^{(N+1)}\rangle\langle\Psi_n^{(N+1)}\mid c_{\mathbf{k}}^\dagger|\,\Psi_0\rangle \\
&= \frac{\langle\Psi_0\mid c_{\mathbf{k}}c_{\mathbf{k}}^\dagger|\,\Psi_0\rangle}{\langle\Psi_0|\,\Psi_0\rangle} = \frac{\langle\Psi_0\mid 1 - c_{\mathbf{k}}^\dagger c_{\mathbf{k}}|\,\Psi_0\rangle}{\langle\Psi_0|\,\Psi_0\rangle} = 1 - \langle n_{\mathbf{k}}\rangle.
\end{aligned}
$$

Similarly, we obtain

$$\int \mathrm{d}\epsilon\, B(\mathbf{k},\epsilon) = \langle n_{\mathbf{k}}\rangle$$

and the sum rule is proved.

For the case of non-interacting Fermions it follows from equation (15.27) that

$$
\begin{aligned}
A(\mathbf{k},\epsilon) &= \theta(k-k_F)\delta(\epsilon - w_{\mathbf{k}}^{(N+1)}) &&= (1-\langle n_{\mathbf{k}}\rangle)\,\delta(\epsilon - w_{\mathbf{k}}^{(N+1)}) \\
B(\mathbf{k},\epsilon) &= \theta(k_F-k)\delta(\epsilon - w_{-\mathbf{k}}^{(N-1)}) &&= \langle n_{\mathbf{k}}\rangle\delta(\epsilon - w_{-\mathbf{k}}^{(N-1)}).
\end{aligned}
$$

In this case the sum rule is trivially satisfied.

We can now express the time-dependent Green's function using the spectral functions:

$$
\begin{aligned}
iG(\mathbf{k},t-t') &= \theta(t-t')\int_0^\infty \mathrm{d}\epsilon\, A(\mathbf{k},\epsilon)\mathrm{e}^{-i(\epsilon+\mu)(t-t')} \\
&\quad -\theta(t'-t)\int_0^\infty \mathrm{d}\epsilon\, B(\mathbf{k},\epsilon)\mathrm{e}^{-i(\mu-\epsilon)(t-t')}.
\end{aligned}
\qquad (15.33)
$$

From this it readily follows that

$$
\begin{aligned}
\lim_{\tau\to0^+} iG(\mathbf{k},\tau) &= \int_0^\infty \mathrm{d}\epsilon\, A(\mathbf{k},\epsilon) = 1 - \langle n_{\mathbf{k}}\rangle \\
\lim_{\tau\to0^-} iG(\mathbf{k},\tau) &= -\int_0^\infty \mathrm{d}\epsilon\, B(\mathbf{k},\epsilon) = -\langle n_{\mathbf{k}}\rangle.
\end{aligned}
\qquad (15.34)
$$

Hence the Green's function has a discontinuity at the point $\tau = 0$:

$$\lim_{\tau \to 0^+} G(\mathbf{k}, \tau) - \lim_{\tau \to 0^-} G(\mathbf{k}, \tau) = -i.$$

Equation (15.34) is for practical reasons a very important representation of the momentum distribution $\langle n_{\mathbf{k}} \rangle$. With the help of this representation, we will prove in Chapter 26 that the function $\langle n_{\mathbf{k}} \rangle$ has a discontinuity at $k = k_F$, *i.e.,* a Fermi edge, also for interacting systems.

We will now conclude this chapter by further investigating the analytical structure of the Green's function. From the general formula

$$\lim_{\eta \to 0^+} \frac{1}{x - x_0 \pm i\eta} = P \frac{1}{x - x_0} \mp i\pi\delta(x - x_0),$$

it follows that

$$\begin{aligned}
&G(\mathbf{k}, \omega) \\
&= \lim_{\eta \to 0^+} \left\{ -\int_0^\infty \mathrm{d}\epsilon \frac{A(\mathbf{k}, \epsilon)}{\epsilon - (\omega - \mu) - i\eta} + \int_0^\infty \mathrm{d}\epsilon \frac{B(\mathbf{k}, \epsilon)}{\epsilon - (\mu - \omega) - i\eta} \right\} \\
&= P \int_0^\infty \mathrm{d}\epsilon \frac{A(\mathbf{k}, \epsilon)}{\omega - \mu - \epsilon} + P \int_0^\infty \mathrm{d}\epsilon \frac{B(\mathbf{k}, \omega)}{\omega - \mu + \epsilon} \\
&\quad -i\pi A(\mathbf{k}, \omega - \mu) + i\pi B(\mathbf{k}, \mu - \omega).
\end{aligned}$$

Since A and B are real (equation (15.30)), we have

$$\mathrm{Re}\, G(\mathbf{k}, \omega) = P \int_0^\infty \mathrm{d}\epsilon \frac{A(\mathbf{k}, \epsilon)}{\omega - \mu\epsilon} + P \int_0^\infty \mathrm{d}\epsilon \frac{B(\mathbf{k}, \epsilon)}{\omega - \mu + \epsilon} \tag{15.35}$$

$$\mathrm{Im}\, G(\mathbf{k}, \omega) = -\pi A(\mathbf{k}, \omega - \mu) + \pi B(\mathbf{k}, \mu - \omega) = \left\{ \begin{array}{ll} -\pi A(\mathbf{k}, \omega - \mu) & \omega > \mu \\ +\pi B(\mathbf{k}, \mu - \omega) & \omega < \mu \end{array} \right. \tag{15.36}$$

This last identity, which follows from equation (15.31), shows that $\mathrm{Im}\, G(\mathbf{k}, \omega)$ changes sign at $\omega = \mu$, since both A and B are positive according to equation (15.30). We can also re-write equation (15.36) as

$$\begin{aligned}
A(\mathbf{k}, \epsilon) &= -\frac{1}{\pi} \mathrm{Im}\, G(\mathbf{k}, \epsilon + \mu) \\
B(\mathbf{k}, \omega) &= +\frac{1}{\pi} \mathrm{Im}\, G(\mathbf{k}, \mu - \epsilon)
\end{aligned} \tag{15.37}$$

(for $\epsilon > 0$). If we insert equation (15.37) in equation (15.35), we obtain

$$\mathrm{Re}\, G(\mathbf{k}, \omega) = -\frac{1}{\pi} P \int_0^\infty \mathrm{d}\epsilon \frac{\mathrm{Im}\, G(\mathbf{k}, \epsilon + \mu)}{\omega - \mu - \epsilon} + \frac{1}{\pi} P \int_0^\infty \mathrm{d}\epsilon \frac{\mathrm{Im}\, G(\mathbf{k}, \mu - \epsilon}{\omega - \mu + \epsilon}.$$

With the subsitutions $\epsilon_{new} = \mu+\epsilon_{old}$ in the first integral, and $\epsilon_{new} = \mu-\epsilon_{old}$ in the second integral, we finally obtain the dispersion relation

$$\operatorname{Re} G(\mathbf{k},\omega) = -\frac{1}{\pi} P \int_{\mu}^{\infty} \mathrm{d}\epsilon \, \frac{\operatorname{Im} G(\mathbf{k},\epsilon)}{\omega-\epsilon} + \frac{1}{\pi} P \int_{-\infty}^{\mu} \mathrm{d}\epsilon \, \frac{\operatorname{Im} G(\mathbf{k},\epsilon)}{\omega-\epsilon}. \quad (15.38)$$

Here we see a possible application of the spectral function. Let us assume that we have calculated the single-particle Green's function within some particular approximation (for example the diagrammatic method which we will discuss shortly). In this approximation, the Green's function will in general not have the correct analytic properties; we could for example see that the dispersion relation derived above is not satisfied. In this case, we could for example only use the imaginary part of the approximate Green's function and from this then calculate the spectral function by using equation (15.37) and then finally determine anew the real part of the Green's function from equation (15.35). The Green's function corrected in this way will by construction satisfy the dispersion relation. One can also attempt to introduce further corrections so that, for example, the sum rule equation (15.32) is satisfied.

We will close this chapter with a remark on the theory of superconducting systems. The single-particle Green's function is the expectation value $\langle\psi^\dagger\psi\rangle$ and $\langle\psi\psi^\dagger\rangle$, respectively. In superconductors, on the other hand, expectations values of the type $\langle\psi^\dagger(\mathbf{r}'t')\psi^\dagger(\mathbf{r}t)\rangle$ and $\langle\psi(\mathbf{r}'t')\psi(\mathbf{r}t)\rangle$, the so-called anomalous propagators, are of fundamental importance. The order parameter Δ is for example an expectation value of this sort. The properties of the single-particle Green's function discussed here and in what follows (analytic structure, equation of motion and diagrammatic expansion) can easily be carried over to the anomalous propagators.

Chapter 16

The polarization propagator, the two-particle Green's function and the hierarchy of equations of motion

As we have seen, the single-particle Green's function contains a large amount of interesting physical information of a system. However, there are quantities which cannot be calculated from this Green's function. One example is the correlation between the observables A and B, which is usually defined by

$$f_{AB} = \langle (A - \langle A \rangle)(B - \langle B \rangle) \rangle = \langle AB \rangle - \langle A \rangle \langle B \rangle .$$

This quantity gives a measure of the mutual dependence of the fluctuations of A and B on one another. If the deviation of the quantity A from its mean value $\langle A \rangle$ is somehow coupled to the deviation of the quantity B from its mean value $\langle B \rangle$, then f_{AB} will have a non-zero value. If, on the other hand, $f_{AB} = 0$, the observables A and B are said to be statistically independent.

If A and B are local operators in the space–spin representation, so that

$$\begin{aligned} A &= \int \mathrm{d}x\, A(x) \psi^\dagger(x) \psi(x) \\ B &= \int \mathrm{d}x'\, B(x') \psi^\dagger(x') \psi(x') \end{aligned}$$

then their ground state expectation values are given by

$$\begin{aligned} \langle A \rangle &= \frac{1}{\langle \Psi_0 \mid \Psi_0 \rangle} \int \mathrm{d}x\, A(x) \langle \Psi_0 | \psi^\dagger(x) \psi(x) | \Psi_0 \rangle \\ \langle B \rangle &= \frac{1}{\langle \Psi_0 \mid \Psi_0 \rangle} \int \mathrm{d}x'\, B(x') \langle \Psi_0 | \psi^\dagger(x') \psi(x') | \Psi_0 \rangle . \end{aligned}$$

Hence, the correlation function is

$$
\begin{aligned}
f_{AB} = & \frac{1}{\langle \Psi_0 \mid \Psi_0 \rangle} \int\int \mathrm{d}x\mathrm{d}x'\, A(x)B(x') \\
& \times \langle \Psi_0 \mid \left[\psi^\dagger(x)\psi(x) - \frac{\langle \Psi_0 \,|\psi^\dagger(x)\psi(x)|\, \Psi_0 \rangle}{\langle \Psi_0 \mid \Psi_0 \rangle} \right] \\
& \times \left[\psi^\dagger(x')\psi(x') - \frac{\langle \Psi_0 \,|\psi^\dagger(x')\psi(x')|\, \Psi_0 \rangle}{\langle \Psi_0 \mid \Psi_0 \rangle} \right] \mid \Psi_0 \rangle .
\end{aligned}
$$

If we also introduce

$$
\widetilde{\rho}(x) \equiv \rho(x) - \langle \rho(x) \rangle = \psi^\dagger(x)\psi(x) - \frac{\langle \Psi_0 \,|\psi^\dagger(x)\psi(x)|\, \Psi_0 \rangle}{\langle \Psi_0 \mid \Psi_0 \rangle} \tag{16.1}
$$

the correlation function f_{AB} can be written

$$
f_{AB} = \frac{1}{\langle \Psi_0 \mid \Psi_0 \rangle} \int \mathrm{d}x \int \mathrm{d}x' A(x)B(x') \langle \Psi_0 \,|\widetilde{\rho}(x)\widetilde{\rho}(x')|\, \Psi_0 \rangle .
$$

If we furthermore are only interested in correlations of quantities at different times, it is natural to define a time-ordered density correlation function in the following way:

$$
\begin{aligned}
i\Pi(xt, x't') &= \frac{1}{\langle \Psi_0 \mid \Psi_0 \rangle} \langle \Psi_0 \,| T[\widetilde{\rho}(xt)_H \widetilde{\rho}(x't')_H] |\, \Psi_0 \rangle \\
&= \frac{\langle \Psi_0 \,| T[\psi^\dagger(xt)_H \psi(xt)_H \psi^\dagger(x't')_H \psi(x't')_H] |\, \Psi_0 \rangle}{\langle \Psi_0 \mid \Psi_0 \rangle} - \langle \rho(x) \rangle \langle \rho(x') \rangle .
\end{aligned} \tag{16.2}
$$

For reasons that will become clear later, Π is also known as the *polarization propagator.* By using this quantity, we can calculate the ground state expectation value of a local (in space–spin representation), but otherwise arbitrary, two-particle potential,

$$
\langle v \rangle = \frac{1}{2} \frac{1}{\langle \Psi_0 \mid \Psi_0 \rangle} \int \mathrm{d}x \int \mathrm{d}x' v(x, x') \langle \Psi_0 \,|\psi^\dagger(x)\psi^\dagger(x')\psi(x')\psi(x)|\, \Psi_0 \rangle .
$$

To show how this is done, we use the fermion anti-commutation relations and obtain

$$
\begin{aligned}
&\frac{\langle\Psi_0\,|\psi^\dagger(x)\psi^\dagger(x')\psi(x')\psi(x)|\,\Psi_0\rangle}{\langle\Psi_0\mid\Psi_0\rangle}\\
&= -\frac{\langle\Psi_0\,|\psi^\dagger(x)\psi^\dagger(x')\psi(x)\psi(x')|\,\Psi_0\rangle}{\langle\Psi_0\mid\Psi_0\rangle}\\
&= \frac{\langle\Psi_0\,|\psi^\dagger(x)\psi(x)\psi^\dagger(x')\psi(x')|\,\Psi_0\rangle - \delta_{xx'}\langle\Psi_0\,|\psi^\dagger(x)\psi(x')|\,\Psi_0\rangle}{\langle\Psi_0\mid\Psi_0\rangle}\\
&= \frac{\langle\Psi_0\,|\rho(x)\rho(x')|\,\Psi_0\rangle - \delta_{xx'}\langle\Psi_0\,|\rho(x)|\,\Psi_0\rangle}{\langle\Psi_0\mid\Psi_0\rangle}\\
&= \frac{\langle\Psi_0\,|\widetilde{\rho}(x)\widetilde{\rho}(x')|\,\Psi_0\rangle}{\langle\Psi_0\mid\Psi_0\rangle} + \langle\rho(x)\rangle\langle\rho(x')\rangle - \delta_{xx'}\langle\rho(x)\rangle.
\end{aligned}
$$

If we then use the definition of the polarization propagator, we obtain in total

$$
\langle v\rangle = \frac{1}{2}\int \mathrm{d}x \int \mathrm{d}x' v(x,x')\left[i\Pi(x0,x'0) + \langle\rho(x)\rangle\langle\rho(x')\rangle - \delta_{xx'}\langle\rho(x)\rangle\right]. \tag{16.3}
$$

If we want to continue to calculate the correlation between two non-local observables

$$
\begin{aligned}
A &= \int \mathrm{d}x_1 \int \mathrm{d}x_2 A(x_1,x_2)\psi^\dagger(x_1)\psi(x_2)\\
B &= \int \mathrm{d}x_3 \int \mathrm{d}x_4 B(x_3,x_4)\psi^\dagger(x_3)\psi(x_4)
\end{aligned}
$$

we arrive at

$$
\begin{aligned}
f_{AB} &= \langle AB\rangle - \langle A\rangle\langle B\rangle\\
&= \int \mathrm{d}x_1 \int \mathrm{d}x_2 \int \mathrm{d}x_3 \int \mathrm{d}x_4 A(x_1,x_2)B(x_3,x_4)\\
&\quad\times\left[\frac{\langle\Psi_0\,|\psi^\dagger(x_1)\psi(x_2)\psi^\dagger(x_3)\psi(x_4)|\,\Psi_0\rangle}{\langle\Psi_0\mid\Psi_0\rangle}\right.\\
&\quad\left.-\frac{\langle\Psi_0\,|\psi^\dagger(x_1)\psi(x_2)|\,\Psi_0\rangle}{\langle\Psi_0\mid\Psi_0\rangle}\frac{\langle\Psi_0\,|\psi^\dagger(x_3)\psi(x_4)|\,\Psi_0\rangle}{\langle\Psi_0\mid\Psi_0\rangle}\right].
\end{aligned}
$$

Hence, the function Π defined earlier is not sufficient to calculate such a correlation function – a generalization is necessary. This leads us for time-dependent extensions of Π to the definition of the two-particle Green's function, which in space–spin representation is

$$
\begin{aligned}
&i^2 G(x_1 t_1, x_2 t_2, x_3 t_3, x_4 t_4) \\
&\equiv \frac{1}{\langle \Psi_0 \mid \Psi_0 \rangle} \langle \Psi_0 \, | T[\psi(x_1 t_1)_H \psi(x_2 t_2)_H \psi^\dagger(x_3 t_3)_H \psi^\dagger(x_4 t_4)_H] | \, \Psi_0 \rangle .
\end{aligned}
\tag{16.4}
$$

Here, the time-ordered product of several Fermion creation or annihilation operators is defined as

$$
\begin{aligned}
T\left[A_1(t_1) A_2(t_2) \ldots A_n(t_n)\right] &= \operatorname{sgn}(P) A_{P(1)}(t_{P(1)}) A_{P(2)}(t_{P(2)}) \cdots \\
&\quad \cdots A_{P(n)}(t_{P(n)}),
\end{aligned}
\tag{16.5}
$$

where the permutations $P \in S_n$ are chosen such that

$$t_{P(1)} > t_{P(2)} > \ldots > t_{P(n)} .$$

From this definition of the time-ordered product we obtain the identity

$$G(1234) = -G(2134) = -G(1243) = G(2143). \tag{16.6}$$

Equation (16.6) is proved by, for example,

$$G(2134) = -\langle T[\psi_2 \psi_1 \psi_3^\dagger \psi_4^\dagger] \rangle = +\langle T[\psi_1 \psi_2 \psi_3^\dagger \psi_4^\dagger] \rangle = -G(1234).$$

For the single-particle Green's function, we needed to examine only the two cases $t > t'$ and $t' > t$. For the two-particle Green's function there are 24 distinct cases to examine, corresponding to the possible permutations of the times t_1, t_2, t_3, t_4. Due to the symmetries given by equation (16.6), this number is fortunately reduced to six:

(1) $t_1 > t_2 > t_3 > t_4$: $i^2 G(1234) = \langle \psi_1 \psi_2 \psi_3^\dagger \psi_4^\dagger \rangle$. Because of equation (16.6), this time ordering includes the cases

$$
\begin{aligned}
t_2 > t_1 > t_3 > t_4 \\
t_1 > t_2 > t_4 > t_3 \\
t_2 > t_1 > t_4 > t_3
\end{aligned}
$$

[as to the sign, see equation (16.6)]. The basic structure is

$$G = \langle \psi \psi \psi^\dagger \psi^\dagger \rangle$$

with all possible indices.

(2) $t_3 > t_4 > t_1 > t_2$: $i^2 G(1234) = \langle \psi_3^\dagger \psi_4^\dagger \psi_1 \psi_2 \rangle$. Here the cases

$$
\begin{aligned}
t_4 > t_3 > t_1 > t_2 \\
t_3 > t_4 > t_2 > t_1 \\
t_4 > t_3 > t_2 > t_1
\end{aligned}
$$

are included. The basic structure is $G = \langle \psi^\dagger \psi^\dagger \psi \psi \rangle$.

(3) $t_1 > t_3 > t_2 > t_4$: $G(1234) = -\langle \psi_1 \psi_3^\dagger \psi_2 \psi_4^\dagger \rangle$, and all other indexings with the structure $G = \langle \psi\psi^\dagger\psi\psi^\dagger \rangle$.

We will only give the three basic structures for the remaining 12 possibilities. Each basic structure includes four cases, just as above.

(4) $G = \langle \psi^\dagger\psi\psi^\dagger\psi \rangle$

(5) $G = \langle \psi^\dagger\psi\psi\psi^\dagger \rangle$

(6) $G = \langle \psi\psi^\dagger\psi^\dagger\psi \rangle$.

The polarization propagator, equation (16.2) (without the prefactor and the additional term $\langle \rho(x) \rangle \langle \rho(x') \rangle$) is obviously a special case of case (4).

The interpretation of the two-particle Green's function is analogous to that of the single-particle Green's function: In case (1) the two-particle Green's function describes the propagation of two additional particles and gives the transition amplitude for finding the particles at $(x_1 t_1)$ and $(x_2 t_2)$ if they were added to the system at $(x_3 t_3)$ and $(x_4 t_4)$. Case (2) similarly describes the propagation of a hole-pair, whereas cases (3) – (6) treat the propagation of particle–hole pairs.

We will here refrain from a thorough discussion of the analytical properties of the two-particle Green's function. Instead, we conclude this chapter by deriving the equation of motion for the single-particle Green's function, which will turn out to contain the two-particle Green's function.

First, we calculate the time derivative of the time-ordered product of two field operators in the Heisenberg representation:

$$
\begin{aligned}
& \frac{\partial}{\partial t} T[\psi(xt)\psi^\dagger(x't')] \\
& \quad = \frac{\partial}{\partial t}\left[\theta(t-t')\psi(xt)\psi^\dagger(x't') - \theta(t'-t)\psi^\dagger(x't')\psi(xt)\right] \\
& \quad = \delta(t-t')\psi(xt)\psi^\dagger(x't') + \delta(t'-t)\psi^\dagger(x't')\psi(xt) \\
& \qquad +\theta(t-t')\frac{\partial\psi(xt)}{\partial t}\psi^\dagger(x't') - \theta(t'-t)\psi^\dagger(x't')\frac{\partial\psi(x)}{\partial t} \\
& \quad = \delta(t-t')\delta_{xx'} + T\left[\frac{\partial\psi(xt)}{\partial t}\psi^\dagger(x't')\right] \\
\Rightarrow i\frac{\partial}{\partial t}G(xt,x't') & \quad = \frac{\partial}{\partial t}\langle T[\psi(x)\psi^\dagger(x't')]\rangle \\
& \quad = \delta(t-t')\delta_{xx'} - i\langle T[i\left(\frac{\partial}{\partial t}\psi(xt)\right)\psi^\dagger(x't')]\rangle .
\end{aligned}
$$

We then use equation (15.18) for a potential which is local in space and spin:

$$
i\frac{\partial}{\partial t}\psi(xt) = -\frac{\nabla^2}{2m}\psi(xt) + \int \mathrm{d}y\, v(x,y)\psi^\dagger(yt)\psi(yt)\psi(xt).
$$

This yields

$$\begin{aligned} i\frac{\partial}{\partial t}G(xt,x't') &= \delta(t-t')\delta_{xx'} - \frac{\nabla_r^2}{2m}(-i)\langle T[\psi(xt)\psi^\dagger(x't')]\rangle \\ &\quad -i\int \mathrm{d}y\, v(x,y)\langle T[\psi^\dagger(yt)\psi(yt)\psi(xt)\psi^\dagger(x't')]\rangle . \end{aligned}$$

The ambiguity of the time-ordered product for operators with the same time argument can in this case be easily overcome. The product $\psi^\dagger(yt)\psi(yt)\psi(xt)$ originates from a single operator, namely $\partial\psi(xt)/\partial t$. For this reason, the product must remain together *in this sequence* and regarded as one unit. Hence, the only possible ways of time-ordering are

$$\langle T\left[\psi^\dagger(yt)\psi(yt)\psi(xt)\psi^\dagger(x't')\right]\rangle \equiv \begin{cases} \langle\psi^\dagger(yt)\psi(yt)\psi(xt)\psi^\dagger(x't')\rangle & t>t' \\ -\langle\psi^\dagger(x't')\psi^\dagger(yt)\psi(yt)\psi(xt)\rangle & t'>t \end{cases}$$

which furthermore can be written as

$$\lim_{\tau\to t^+}\langle T[\psi(yt)\psi(xt)\psi^\dagger(y\tau)\psi^\dagger(x't')]\rangle .$$

Finally, if we use the anti-commutation relation $\psi(yt)\psi(xt) = -\psi(xt)\psi(yt)$ (which holds only for Heisenberg operators at *equal* times), it follows that this expression becomes

$$-\lim_{\tau\to t^+}\langle T[\psi(xt)\psi(yt)\psi^\dagger(y\tau)\psi^\dagger(x't')]\rangle = G(xt,yt,yt^+,x't').$$

We then obtain the equation of motion for the single-particle Green's function:

$$\left[i\frac{\partial}{\partial t}+\frac{\nabla_r^2}{2m}\right]G(xt,x't') = \delta(t-t')\delta_{xx'} - i\int \mathrm{d}y\, v(x,y)G(xt,yt,yt^+,x't'). \tag{16.7}$$

In particular, for a non-interacting system we have

$$\left[i\frac{\partial}{\partial t}+\frac{\nabla_r^2}{2m}\right]G^{(0)}(xt,x't') = \delta(t-t')\delta_{xx'}. \tag{16.8}$$

In this case, the Green's function is a true Green's function in the mathematical sense, whereas the name is strictly not correct for interacting systems.

The derivation of equations (16.7) and (16.8) assumed a system *without* an external potential — only in this case is the use of equation (15.18) valid. If there is an external potential $u(x)$, the operator on the left hand side of equations (16.7) and (16.8) must be replaced according to

$$\left[i\frac{\partial}{\partial t}+\frac{\nabla_r^2}{2m}\right] \to \left[i\frac{\partial}{\partial t}+\frac{\nabla_r^2}{2m}-u(x)\right]. \tag{16.9}$$

The equation of motion, equation (16.7), contains the two-particle Green's function for interacting systems. Hence, if we wish to calculate the single-particle Green's function from this equation, we must first have an expression for the two-particle Green's function. This raises the question of an equation of motion for the two-particle Green's function, which will in turn contain a three-particle Green's function, and so on. We can define an n-particle Green's function by

$$\begin{aligned}
&(i)^n G_n(x_1t_1,\ldots x_nt_n;x'_1t'_1\ldots x'_nt'_n)\\
&\equiv \frac{1}{\langle\Psi_0\mid\Psi_0\rangle}\langle\Psi_0\;|T[\psi(x_1t_1)\ldots\psi(x_nt_n)\psi^\dagger(x'_1t'_1)\ldots\psi^\dagger(x'_nt'_n)]|\;\Psi_0\rangle.
\end{aligned}$$

For each n, these functions contain information about higher order correlations. Analogous to the previous derivation, we then obtain an equation of motion for the n-particle Green's function:

$$\begin{aligned}
&\left[i\frac{\partial}{\partial t_1}+\frac{\nabla_1^2}{2m}\right]G_n(x_1t_1,\ldots,x_nt_n;x'_1t'_1,\ldots,x'_nt'_n)\\
&= \sum_{j=1}^{n}\delta_{x_1,x'_j}\delta(t_1-t'_j)(-1)^{n-j}\\
&\quad G_{n-1}(x_2t_2,\ldots,x_nt_n;x'_1t'_1,\ldots,x'_{j-1}t'_{j-1},x'_{j+1}t'_{j+1},\ldots,x'_nt'_n)\\
&\quad -i\int \mathrm{d}y\,v(x_1,y)G_{n+1}x_1t_1,\ldots,x_nt_n,yt_1;yt_1^+,x'_1t'_1,\ldots,x'_nt'_n)
\end{aligned} \tag{16.10}$$

which always contains the next higher Green's function. In this way, we obtain a system of coupled equations for the different Green's function. This system is just as impossible to solve exactly as it is to calculate the exact many-particle wavefunction. However, the advantage of the Green's function lies precisely in this partitioning of the full problem into a hierarchy of simple equations. The exact wavefunction of an interacting many-particle system is an enormously complicated structure which contains information on arbitrarily high correlations. Even if this function were given to us, it would be practically impossible to calculate physically relevant information, such as the ground state energy, for macroscopic systems (*i.e.*, with 10^{23} particles). For that reason, it is more favorable to work with quantities such as the Green's function, which indeed contain much less information, but are more intimately related to measurable quantities. If the hierarchy is broken at any point by assuming an approximate Greens' function, all Green's functions of *lower* order can in principle be calculated from the equation of motion equation (16.10).

Part III

Perturbation Theory

Chapter 17

Time-independent perturbation theory

We begin by separating the complete Hamiltonian

$$H = H_0 + v$$

into an 'unperturbed' part H_0 and a 'perturbation' v, which in most of the problems discussed here will represent the particle–particle interactions. We assume that the eigenvalue problem associated with H_0

$$H_0 \mid \Phi_n\rangle = W_n \mid \Phi_n\rangle$$

has been solved. We separate out a coupling constant from the perturbing potential

$$v = g\overline{v}$$

and interpret the eigenvalues and wavefunctions of the complete problem as functions of this coupling constant. The basic idea of perturbation theory is simply to expand each quantity in a power series in g. One expands about $g = 0$, *i.e.,* in some sense about the unperturbed problem. If g is small, so that the potential really is a weak perturbation, one can hope that only a few terms in the series will be adequate. However, it is often necessary to sum either the entire series, or at least the dominant terms of the series, to infinity.

In this chapter, we will briefly review the traditional methods of stationary perturbation theory. Our goal is to obtain an expression for the ground state of the complete problem

$$H|\,\Psi_0\rangle = E_0|\,\Psi_0\rangle.$$

First of all

$$\begin{aligned} v|\,\Psi_0\rangle &= (H - H_0)|\,\Psi_0\rangle = (E_0 - H_0|\,\Psi_0\rangle \\ \Rightarrow \langle\Phi_0 \mid v|\,\Psi_0\rangle &= \langle\Phi_0 \mid E_0 - H_0|\,\Psi_0\rangle = (E_0 - W_0)\langle\Phi_0|\,\Psi_0\rangle. \end{aligned}$$

From this we obtain the general equation

$$\Delta E \equiv E_0 - W_0 = \frac{\langle \Phi_0 \mid v \mid \Psi_0 \rangle}{\langle \Phi_0 \mid \Psi_0 \rangle}. \tag{17.1}$$

We denote the projection operator onto the ground state of the unperturbed problem as

$$P \equiv \mid \Phi_0 \rangle \langle \Phi_0 \mid \tag{17.2}$$

and the projection operator on the remainder of the Hilbert space as

$$Q \equiv 1 - P = \sum_{n=0}^{\infty} \mid \Phi_n \rangle \langle \Phi_n \mid - \mid \Phi_0 \rangle \langle \Phi_0 \mid = \sum_{n=1}^{\infty} \mid \Phi_n \rangle \langle \Phi_n \mid . \tag{17.3}$$

This operator commutes with H_0:

$$\begin{aligned} H_0 Q &= H_0 - H_0 \mid \Phi_0 \rangle \langle \Phi_0 \mid = H_0 - W_0 \mid \Phi_0 \rangle \langle \Phi_0 \mid = H_0 - \mid \Phi_0 \rangle \langle \Phi_0 \mid H_0 \\ &= Q H_0. \end{aligned}$$

Thus, for any number E, Q commutes with the operator $(E - H_0)$, and we can write

$$(E - H_0)\, Q \mid \Psi_0 \rangle = Q\,(E - H_0) \mid \Psi_0 \rangle = Q\,(E - E_0 + v) \mid \Psi_0 \rangle .$$

Hence

$$Q \mid \Psi_0 \rangle = \frac{1}{E - H_0} Q\,(E - E_0 + v) \mid \Psi_0 \rangle = \mid \Psi_0 \rangle - \mid \Phi_0 \rangle \langle \Phi_0 \mid \Psi_0 \rangle . \tag{17.4}$$

If we define

$$\mid \xi \rangle \equiv \frac{\mid \Psi_0 \rangle}{\langle \Phi_0 \mid \Psi_0 \rangle} \tag{17.5}$$

equation (17.4) can be written as

$$\mid \xi \rangle = \mid \Phi_0 \rangle + \frac{1}{E - H_0} Q\,(E - E_0 + v) \mid \xi \rangle . \tag{17.6}$$

If we iterate this equation, we obtain

$$\begin{aligned} \mid \xi \rangle &= \mid \Phi_0 \rangle + \frac{1}{E - H_0} Q\,(E - E_0 + v) \mid \Phi_0 \rangle + \ldots \\ \mid \xi \rangle &= \sum_{n=0}^{\infty} \left[\frac{1}{E - H_0} Q\,(E - E_0 + v) \right]^n \mid \Phi_0 \rangle . \end{aligned} \tag{17.7}$$

We have found a general equation from which we can in principle calculate the solution of the complete problem from the ground state of the unperturbed problem. If we insert equation (17.7) into equation (17.1), we obtain for the energy shift

$$\Delta E = \langle \Phi_0 \mid v \mid \xi \rangle = \sum_{n=0}^{\infty} \langle \Phi_0 \mid v \left[\frac{1}{E - H_0} Q \, (E - E_0 + v) \right]^n \mid \Phi_0 \rangle . \quad (17.8)$$

We obtain the *Rayleigh–Schrödinger* version of stationary perturbation theory by setting $E = W_0$. This yields

$$\begin{aligned} \mid \xi \rangle &= \sum_{n=0}^{\infty} \left[\frac{1}{W_0 - H_0} Q \, (W_0 - E_0 + v) \right]^n \mid \Phi_0 \rangle & (17.9) \\ \Delta E &= \sum_{n=0}^{\infty} \langle \Phi_0 v \left[\frac{1}{W_0 - H_0} Q \, (v - \Delta E) \right]^n \mid \Phi_0 \rangle . & (17.10) \end{aligned}$$

Next, we separate out from equation (17.10) all terms of different orders in the coupling constant g. We do so explicitly for the first term of the energy shift. The first terms of the series above are

$$\begin{aligned} n = 0 : \quad & \langle \Phi_0 \mid v \mid \Phi_0 \rangle \sim g \\ n = 1 : \quad & \langle \Phi_0 \mid v \frac{1}{W_0 - H_0} Q \, (v - \Delta E) \mid \Phi_0 \rangle \\ &= \langle \Phi_0 \mid v \frac{1}{W_0 - H_0} Q v \mid \Phi_0 \rangle \\ &= \langle \Phi_0 \mid v \frac{1}{W_0 - H_0} \sum_{n=1}^{\infty} \mid \Phi_n \rangle \langle \Phi_n \mid v \mid \Phi_0 \rangle \\ &= \sum_{n=1}^{\infty} \frac{\langle \Phi_0 \mid v \mid \Phi_n \rangle \langle \Phi_n \mid v \mid \Phi_0 \rangle}{W_0 - W_n} \sim g^2 \\ n = 2 : \quad & \langle \Phi_0 \mid v \frac{1}{W_0 - H_0} Q \, (v - \Delta E) \, \frac{1}{W_0 - H_0} Q \, (v - \Delta E) \mid \Phi_0 \rangle \\ &= \sum_{n=1}^{\infty} \frac{1}{W_0 - W_n} \langle \Phi_0 \mid v \frac{1}{W_0 - H_0} Q \, (v - \Delta E) \mid \Phi_n \rangle \langle \Phi_n \mid v \mid \Phi_0 \rangle \\ &= \sum_{n=1}^{\infty} \sum_{m=1}^{\infty} \underbrace{\frac{\langle \Phi_0 \mid v \mid \Phi_m \rangle \langle \Phi_m \mid v \mid \Phi_n \rangle \langle \Phi_n \mid v \mid \Phi_0 \rangle}{(W_0 - W_n) \, (W_0 - W_m)}}_{\sim g^3} \\ & \quad - \Delta E \sum_{n=1}^{\infty} \frac{\langle \Phi_0 \mid v \Phi_n \rangle \langle \Phi_n \mid v \mid \Phi_0 \rangle}{(W_0 - W_n)^2} . \end{aligned}$$

If we arrange the contributions according to their orders in g, the result is

$$\Delta E = \Delta E^{(1)} + \Delta E^{(2)} + \Delta E^{(3)} + \ldots$$

where

$$\begin{aligned} \Delta E^{(1)} &= \langle \Phi_0 \mid v \mid \Phi_0 \rangle \\ \Delta E^{(2)} &= \sum_{n=1}^{\infty} \frac{\langle \Phi_0 \mid v \mid \Phi_n \rangle \langle \Phi_n \mid v \mid \Phi_0 \rangle}{W_0 - W_n}. \end{aligned} \tag{17.11}$$

Initially, the terms in the Rayleigh–Schrödinger series run in parallel to their orders in g. However, this pattern changes at the $n = 2$ term, at which point arbitrarily high orders in g are included. We observe that the terms in the Rayleigh–Schrödinger series, with $n \geq 3$, are of at least fourth order in g. Hence, the third-order correction $\Delta E^{(3)}$ is obtained from the $n = 2$ term above, with ΔE replaced by $\Delta E^{(1)} = \langle \Phi_0 \mid v \mid \Phi_0 \rangle$:

$$\begin{aligned} \Delta E^{(3)} &= \sum_{m=1}^{\infty} \sum_{n=1}^{\infty} \frac{\langle \Phi_0 \mid v \mid \Phi_m \rangle \langle \Phi_m \mid v \mid \Phi_n \rangle \langle \Phi_n \mid v \mid \Phi_0 \rangle}{(W_0 - W_m)(W_0 - W_n)} \\ &\quad - \langle \Phi_0 \mid v \mid \Phi_0 \rangle \sum_{n=1}^{\infty} \frac{\langle \Phi_0 \mid v \mid \Phi_n \rangle \langle \Phi_n \mid v \mid \Phi_0 \rangle}{(W_0 - W_n)^2}. \end{aligned} \tag{17.12}$$

As the order in g increases, it becomes correspondingly difficult to sort out the terms for each order.

The *Brillouin–Wigner* version of stationary perturbation theory possibly provides a more systematic approach. In it, we set $E = E_0$ in the general formulas, equations (17.7) and (17.8). This yields

$$\mid \xi \rangle = \sum_{n=0}^{\infty} \left[\frac{1}{E_0 - H_0} QV \right]^n \mid \Phi_0 \rangle \tag{17.13}$$

$$\Delta E = \sum_{n=0}^{\infty} \langle \Phi_0 v \left[\frac{1}{E_0 - H_0} QV \right]^n \mid \Phi_0 \rangle. \tag{17.14}$$

As in the Rayleigh–Schrödinger series, the first term of the Brillouin–Wigner series for the energy shift corresponds to the first-order term in g:

$$\Delta E^{(1)} = \langle \Phi_0 \mid v \mid \Phi_0 \rangle.$$

However, the second term of the Brillouin–Wigner series

$$\langle \Phi_0 \mid v \frac{1}{E_0 - H_0} Qv \mid \Phi_0 \rangle = \sum_{n=1}^{\infty} \frac{\langle \Phi_0 \mid v \mid \Phi_n \rangle \langle \Phi_n \mid v \mid \Phi_0 \rangle}{E_0 - W_n}$$

already contains terms of arbitrarily high orders in g:

$$\begin{aligned}\frac{1}{E_0 - W_n} &= \frac{1}{W_0 + (E_0 - W_0) - W_n} = \frac{1}{W_0 - W_n + \Delta E(g)} \\ &= \left.\frac{1}{W_0 - W_n + \Delta E(g)}\right|_{g=0} + g\left.\left(\frac{\mathrm{d}}{\mathrm{d}g}\frac{1}{W_0 - W_n + \Delta E(g)}\right)\right|_{g=0} \pm \dots \\ &= \frac{1}{W_0 - W_n} - \frac{\Delta E^{(1)}}{(W_0 - W_n)^2} \pm \dots\end{aligned}$$

When we separate the powers of g, we obtain the same result as in the Rayleigh–Schrödinger expansion:

$$\Delta E^{(2)} = \sum_{n=1}^{\infty} \frac{\langle \Phi_0 \mid v \mid \Phi_n \rangle \langle \Phi_n \mid v \mid \Phi_0 \rangle}{W_0 - W_n}.$$

The expressions for each order of the energy shift, derived from the Brillouin–Wigner series, are identical to those from the Rayleigh–Schrödinger series because the expansion in powers of g is unique. However, separating the powers of g from the Brillouin–Wigner series is at least as difficult as in the Rayleigh–Schrödinger series.

In conclusion, whereas both the Rayleigh–Schrödinger and the Brillouin–Wigner methods of stationary perturbation theory formally give exact expansions of the complete problem, separating the orders in the perturbing potential (*i.e.*, the powers of g) becomes rather tedious. This limits their usefulness to the first few of orders in g. If we want to sum the series in g to infinity, it will be necessary to have a perturbation expansion that will directly give us the individual orders in g.

Chapter 18

Time-dependent perturbation theory with adiabatic turning-on of the interaction

The series derived in Chapter 14 for the time evolution operator in the interaction picture (*cf.* equations (14.19) and (14.20)) is a direct expansion in orders of the potential:

$$U(t,t') = \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \int_{t'}^{t} \mathrm{d}t_1 \int_{t'}^{t} \mathrm{d}t_2 \ldots \int_{t'}^{t} \mathrm{d}t_n \, T\left[v(t_1)_I \ldots v(t_n)_I\right]. \quad (18.1)$$

In this chapter, we are going to construct a fictitious time-dependent problem such the wavefunction of the complete problem can be obtained by applying the time evolution operator to the unperturbed wavefunction

$$\mid \Psi_0\rangle = U(0,-\infty) \mid \Phi_0\rangle.$$

The series for U given in equation (18.1) then gives a direct method for expansion in orders of the potential. We will now discuss in detail how and under what general conditions such an expansion can be constructed.

We define an explicitly time-dependent Hamiltonian in the Schrödinger picture by

$$H_\epsilon(t)_S \equiv H_0 + \mathrm{e}^{-\epsilon|t|}\, v \quad \text{with } \epsilon > 0.$$

This Hamiltonian has the following properties:

$$\begin{aligned} H_\epsilon(t \to \pm\infty) &= H_0 \\ H_\epsilon(t \to 0) &= H. \end{aligned}$$

Thus, we will slowly turn on the potential at $t = \pm\infty$ to the unperturbed problem H_0, and at $t = 0$ the potential is completely turned on. The time-dependent Schrödinger equation

$$i\frac{\partial}{\partial t}|\,\Psi_\epsilon(t)\rangle_S = H_\epsilon(t)_S|\,\Psi_\epsilon(t)\rangle_S \tag{18.2}$$

at $t = \pm\infty$ goes over to the asymptotic equation

$$i\frac{\partial}{\partial t}|\,\Psi_\epsilon(t)\rangle_S = H_0|\,\Psi_\epsilon(t)\rangle_S.$$

The required initial conditions for equation (18.2) at $t = -\infty$ is that the interacting ground state evolves from the non-interacting one:

$$|\,\Psi_\epsilon(t \to -\infty)\rangle_S \equiv \mathrm{e}^{-iW_0 t}|\,\Phi_0\rangle. \tag{18.3}$$

The equation of motion is in the interaction picture

$$i\frac{\partial}{\partial t}|\,\Psi_\epsilon(t)\rangle_I = \mathrm{e}^{-\epsilon|t|}v(t)_I|\,\Psi_\epsilon(t)\rangle_I. \tag{18.4}$$

Since the right-hand side vanishes for $t \to \pm\infty$

$$\lim_{t\to\pm\infty} i\frac{\partial}{\partial t}|\,\Psi_\epsilon(t)\rangle_I = 0$$

the state vector in the interaction picture becomes time-independent in this limit:

$$|\,\Psi_\epsilon(t \to \pm\infty)\rangle_I = \text{constant}.$$

For $t \to -\infty$ we obtain from equation (18.3) the initial condition

$$\lim_{t\to\pm\infty}|\,\Psi_\epsilon(t)\rangle_I = \lim_{t\to\pm\infty}\mathrm{e}^{iH_0 t}|\,\Psi_\epsilon(t)\rangle_S = \mathrm{e}^{iH_0 t}\mathrm{e}^{-iW_0 t}|\,\Phi_0\rangle = |\,\Phi_0\rangle. \tag{18.5}$$

The formal solution of the equation of motion, equation (18.4), with the initial condition equation (18.5), is

$$|\,\Psi_\epsilon(t)\rangle_I = U_\epsilon(t, -\infty)|\,\Phi_0\rangle.$$

The potential has reached its full strength at the time $t = 0$. The question then arises in which sense the state

$$|\,\Psi_\epsilon(0)\rangle = U_\epsilon(0, -\infty)|\,\Phi_0\rangle$$

is related to the exact ground state $|\,\Psi_0\rangle$. (We will from now on drop the index I at $t = 0$, since at this time all pictures are identical). Clearly, $|\,\Psi_\epsilon(0)\rangle$ depends on the magnitude of ϵ, *i.e.*, how fast the potential is turned on. If the potential is turned on sufficiently slowly ('adiabatically'), we can hope that at each point in time, the ground state has adjusted to the potential strength at that time, and that we obtain the exact ground state from

$$| \Psi_0\rangle = \lim_{\epsilon \to 0} | \Psi_\epsilon(0)\rangle. \tag{18.6}$$

This question is not answered trivially, since we explicitly used $\epsilon > 0$ when we established the initial condition equation (18.5). The question if and under what conditions such a limit gives sensible results is answered by the Gell-Mann–Low theorem [13]:

(1) If the quantity $| \xi\rangle = \lim_{\epsilon\to 0} \frac{| \Psi_\epsilon(0)\rangle}{\langle\Phi_0 | \Psi_\epsilon(0)\rangle}$ exists to all orders in perturbation theory (*i.e.*, if in the perturbation expansion

$$\frac{| \Psi_\epsilon(0)\rangle}{\langle\Phi_0 | \Psi_\epsilon(0)\rangle} = \sum_{n=0}^{\infty} | \xi_\epsilon^{(n)}\rangle g^n$$

the limit $\lim_{\epsilon\to 0} | \xi\rangle^{(n)}$ exists for each n), then $| \xi\rangle$ is an exact eigenfunction H. (The theorem does not guarantee that this state is the ground state!)

(2) The limit $\lim_{\epsilon\to 0} | \Psi_\epsilon(0)\rangle$ does not exists; in fact

$$| \Psi_\epsilon(0)\rangle \sim e^{-iC(g)/\epsilon}$$

as $\epsilon \to 0$ under the conditions in 1.

The infinite phase that appears in (2) will obviously cancel with the denominator in (1).

If we pause for a while to consider the Gell-Mann–Low theorem, we realize that it is a fairly weak theorem. We would rather have a confirmation that the limit $\epsilon \to 0$ indeed exists, or at least know the conditions under which it does exist. However, the theorem does guarantee the desired final result, equation (18.7), if we only can calculate the limit $\epsilon \to 0$ using perturbation theory. This guarantee is of course also very valuable.

We now proceed with the proof of the statements of the theorem. We have

$$\begin{aligned}
&(H_0 - W_0) | \Psi_\epsilon(0)\rangle \\
&= (H_0 - W_0) U_\epsilon(0, -\infty) | \Phi_0\rangle \\
&= [H_0, U_\epsilon(0, -\infty)] | \Phi_0\rangle \\
&= \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \int_{-\infty}^{0} \mathrm{d}t_1 \ldots \int_{-\infty}^{0} \mathrm{d}t_n \\
&\quad \times e^{-\epsilon(|t_1|+\ldots+|t_n|)} [H_0, T(v(t_1)_I \ldots v(t_n)_I)] \Phi_0\rangle.
\end{aligned} \tag{18.7}$$

For each fixed n-tuple $(t_1, \ldots, t_n)$, we obtain the time ordering in equation (18.7) by expanding:

$$\begin{aligned}
&[H_0, T(v(t_1)\ldots v(t_n))] \\
&\quad= [H_0, v(t_i)v(t_j)\ldots v(t_k)] \\
&\quad= H_0 v(t_i)v(t_j)\ldots v(t_k) - v(t_i)H_0 v(t_j)\ldots v(t_k) \\
&\qquad +v(t_i)H_0 v(t_j)\ldots v(t_k) + \ldots - v(t_i)v(t_j)H_0\ldots v(t_k) \\
&\qquad +\ldots - v(t_i)v(t_j)\ldots v(t_k)H_0 \\
&\quad= [H_0, v(t_i)]\, v(t_j)\ldots v(t_k) + v(t_i)\left[H_0, v(t_j)\right]\ldots v(t_k) + \ldots \\
&\qquad \ldots + v(t_i)v(t_j)\ldots [H_0, v(t_k)]\,,
\end{aligned}$$

where $1 \leq i, j, k \leq n$. If we now use the equation of motion, equation (14.11), for the interaction potential

$$-i\frac{\partial}{\partial t}v(t)_I = [H_0, v(t)_I]$$

(the contribution from the explicit time dependence is omitted, since $v(t)_I$ denotes the interaction representation of the potential which is time *in*dependent in the Schrödinger picture; the time dependent prefactor $\mathrm{e}^{-\epsilon|t|}$ will be negligible in equation (18.7)), we obtain

$$\begin{aligned}
&[H_0, T(v(t_1)\ldots v(t_n))] \\
&\quad= -i\left(\frac{\partial}{\partial t_1} + \frac{\partial}{\partial t_2} + \ldots + \frac{\partial}{\partial t_n}\right) v(t_i)v(t_j)\ldots v(t_k) \\
&\quad= -i\left[\sum_{j=1}^{n}\frac{\partial}{\partial t_j}\right] T(v(t_1)\ldots v(t_n))\,.
\end{aligned}$$

This identity is independent of the particular sequence in which the operators $v(t_1)\ldots v(t_n)$ are ordered with respect to time. The following integrals in equation (18.7) then remain to be performed:

$$\begin{aligned}
&\int_{-\infty}^{0} \mathrm{d}t_1 \ldots \int_{-\infty}^{0} \mathrm{d}t_n\, \mathrm{e}^{-\epsilon(|t_1|+\ldots+|t_n|)}(-i)\sum_{j=1}^{n}\frac{\partial}{\partial t_j}T(v(t_1)\ldots v(t_n)) \\
&= -i\sum_{j=1}^{n}\int_{-\infty}^{0}\mathrm{d}t_1\ldots\int_{-\infty}^{0}\mathrm{d}t_n\,\mathrm{e}^{-\epsilon(|t_1|+\ldots+|t_n|)}\frac{\partial}{\partial t_j}T(v(t_1)\ldots v(t)_n)) \\
&= -in\int_{-\infty}^{0}\mathrm{d}t_1\ldots\int_{-\infty}^{0}\mathrm{d}t_n\,\mathrm{e}^{-\epsilon(|t_1|+\ldots+|t_n|)}\frac{\partial}{\partial t_1}T(v(t_1)\ldots v(t_n))\,.
\end{aligned}$$

But

$$\begin{aligned}
&\int_{-\infty}^{0} \mathrm{d}t_1\, \mathrm{e}^{+\epsilon t_1} \frac{\partial}{\partial t_1} T\left(v(t_1)\dots v(t_n)\right) \\
&= \left[\mathrm{e}^{\epsilon t_1} T\left(v(t_1)\dots v(t_n)\right)\right]_{-\infty}^{0} - \epsilon \int_{-\infty}^{0} \mathrm{d}t_1\, \mathrm{e}^{\epsilon t_1} T\left(v(t_1)\dots v(t_n)\right) \\
&= v(0) T\left(v(t_2)\dots v(t_n)\right) - \epsilon \int_{-\infty}^{0} \mathrm{d}t_1\, \mathrm{e}^{-\epsilon |t_1|} T\left(v(t_1)\dots v(t_n)\right).
\end{aligned}$$

It follows that

$$\begin{aligned}
&(H_0 - W_0) \mid \Psi_\epsilon(0)\rangle \\
&= \sum_{n=0}^{\infty} \frac{(-i)^{n+1}}{(n-1)!} \\
&\quad \times \left[v_S \int_{-\infty}^{0} \mathrm{d}t_2 \dots \int_{-\infty}^{0} \mathrm{d}t_n\, \mathrm{e}^{-\epsilon(|t_2|+\dots+|t_n|)} T\left(v(t_2)\dots v(t_n)\right) \right. \\
&\quad \left. -\epsilon \int_{-\infty}^{0} \mathrm{d}t_1 \dots \int_{-\infty}^{0} \mathrm{d}t_n\, \mathrm{e}^{-\epsilon(|t_1|+\dots+|t_n|)} T\left(v(t_1)\dots v(t_n)\right) \right] \mid \Phi_0\rangle \\
&= -v_S \mid \Psi_\epsilon(0)\rangle + \epsilon \sum_{n=0}^{\infty} \frac{(-i)^{n-1}}{(n-1)!} \int_{-\infty}^{0} \mathrm{d}t_1 \dots \int_{-\infty}^{0} \mathrm{d}t_n \\
&\quad \times \mathrm{e}^{-\epsilon(|t_1|+\dots+|t_n|)} T\left(v(t_1)\dots v(t_n)\right) \mid \Phi_0\rangle.
\end{aligned}$$

Each factor $v(t)$ contains one factor g; thus

$$T\left(v(t_1)\dots v(t_n)\right) \sim g^n$$

and

$$\frac{(-i)^{n-1}}{(n-1)!} g^n = ig \frac{\partial}{\partial g} \frac{(-i)^n}{n!} g^n .$$

We then finally arrive at

$$\begin{aligned}
(H_0 - W_0) \mid \Psi_\epsilon(0)\rangle &= -v_S \mid \Psi_\epsilon(0)\rangle + i\epsilon g \frac{\partial}{\partial g} \mid \Psi_\epsilon(0)\rangle \\
\Rightarrow (H - W_0) \mid \Psi_\epsilon(0)\rangle &= i\epsilon g \frac{\partial}{\partial g} \mid \Psi_\epsilon(0)\rangle .
\end{aligned}$$

Hence

$$\begin{aligned}
&\left(H - W_0 - i\epsilon g \frac{\partial}{\partial g}\right) \frac{\mid \Psi_\epsilon(0)\rangle}{\langle \Phi_0 \mid \Psi_\epsilon(0)\rangle} \\
&= \frac{1}{\langle \Phi_0 \mid \Psi_\epsilon(0)\rangle} \underbrace{\left(H - W_0 - i\epsilon g \frac{\partial}{\partial g} \mid \Psi_\epsilon(0)\rangle\right)}_{=0}
\end{aligned}$$

$$
\begin{aligned}
&+\frac{|\Psi_\epsilon(0)\rangle}{\langle\Phi_0|\Psi_\epsilon(0)\rangle^2}\langle\Phi_0\,|\,i\epsilon g\frac{\partial}{\partial g}|\,\Psi_\epsilon(0)\rangle \\
&= \frac{|\Psi_\epsilon(0)\rangle}{\langle\Phi_0|\Psi_\epsilon(0)\rangle}\frac{\langle\Phi_0\,|\,H-W_0|\,\Psi_\epsilon(0)\rangle}{\langle\Phi_0|\Psi_\epsilon(0)\rangle}.
\end{aligned}
$$

The terms on the right-hand and left-hand sides with prefactor W_0 are identical, which leaves

$$
\left(H - i\epsilon g\frac{\partial}{\partial g}\right)\frac{|\Psi_\epsilon(0)\rangle}{\langle\Phi_0|\Psi_\epsilon(0)\rangle} = \langle\Phi_0\,|\,H\frac{|\Psi_\epsilon(0)\rangle}{\langle\Phi_0|\Psi_\epsilon(0)\rangle}\frac{|\Psi_\epsilon(0)\rangle}{\langle\Phi_0|\Psi_\epsilon(0)\rangle}.
$$

By assumption, the quantity $|\Psi_\epsilon(0)\rangle/\langle\Phi_0|\Psi_\epsilon(0)\rangle$ exists to all orders in perturbation theory in the limit $\epsilon \to 0$. The contribution from $i\epsilon g\frac{\partial}{\partial g}$ then vanishes as $\epsilon \to 0$, and what remains is

$$
H\,|\,\xi\rangle = \langle\Phi_0\,|\,H\,|\,\xi\rangle\,|\,\xi\rangle.
$$

Thus, statement (1) of the Gell-Mann–Low theorem is proved.

To prove statement (2), we consider the quantity

$$
\begin{aligned}
&\lim_{\epsilon\to 0} i\epsilon g\frac{\partial}{\partial g}\ln\langle\Phi_0|\Psi_\epsilon(0)\rangle \\
&= \lim_{\epsilon\to 0}\frac{1}{\langle\Phi_0|\Psi_\epsilon(0)\rangle}\langle\Phi_0\,|\,i\epsilon g\frac{\partial}{\partial g}|\,\Psi_\epsilon(0)\rangle \\
&= \lim_{\epsilon\to 0}\frac{\langle\Phi_0\,|\,H-W_0|\,\Psi_\epsilon(0)\rangle}{\langle\Phi_0|\Psi_\epsilon(0)\rangle} \\
&= \lim_{\epsilon\to 0}\frac{\langle\Phi_0\,|\,v|\,\Psi_\epsilon(0)\rangle}{\langle\Phi_0|\Psi_\epsilon(0)\rangle} = \lim_{\epsilon\to 0}\langle\Phi_0\,|\,v\,|\,\xi\rangle = \Delta E(g).
\end{aligned}
$$

Here we have used hypothesis (1) and the general formula equation (17.1) for the energy shift. It follows that

$$
\begin{aligned}
\lim\nolimits_{\epsilon\to 0}\frac{\partial}{\partial g}\ln\langle\Phi_0|\Psi_\epsilon(0)\rangle &\sim -i\frac{\Delta E(g)}{g}\frac{1}{\epsilon} \\
\Rightarrow \qquad \lim\nolimits_{\epsilon\to 0}\ln\langle\Phi_0|\Psi_\epsilon(0)\rangle &\sim -i\frac{C(g)}{\epsilon} \\
\Rightarrow \qquad \lim\nolimits_{\epsilon\to 0}\langle\Phi_0|\Psi_\epsilon(0)\rangle &\sim e^{-iC(g)/\epsilon}.
\end{aligned}
$$

This proves statement (2).

We will now derive a formula for the energy shift ΔE. To do so, we first consider the quantity

$$
i\frac{\partial}{\partial t}\ln\langle\Phi_0|U_\epsilon(t,-\infty)|\,\Phi_0\rangle\Big|_{t=0}
$$

and use the equation of motion equation (14.17):

$$\begin{aligned}
&i\frac{\partial}{\partial t}\ln\langle\Phi_0\mid U_\epsilon(t,-\infty)|\,\Phi_0\rangle\bigg|_{t=0}\\
&\quad=\left.\frac{\langle\Phi_0\mid \mathrm{e}^{-\epsilon|t|}v(t)_I U_\epsilon(t,-\infty)|\,\Phi_0\rangle}{\langle\Phi_0\mid U_\epsilon(t,-\infty)|\,\Phi_0\rangle}\right|_{t=0}\\
&\quad=\frac{\langle\Phi_0\mid v(0)_I U_\epsilon(0,-\infty)|\,\Phi_0\rangle}{\langle\Phi_0\mid U_\epsilon(0,-\infty)|\,\Phi_0\rangle}=\langle\Phi_0\mid v_S\mid\frac{\mid\Psi_\epsilon(0)\rangle}{\langle\Phi_0|\,\Psi_\epsilon(0)\rangle}.
\end{aligned}$$

Under the assumptions of the Gell-Mann–Low theorem we obtain for $\epsilon\to 0$:

$$\lim_{\epsilon\to 0} i\frac{\partial}{\partial t}\ln\langle\Phi_0\mid U_\epsilon(t,-\infty)|\,\Phi_0\rangle\bigg|_{t=0}=\langle\Phi_0\mid v_S\mid\xi\rangle=\Delta E. \tag{18.8}$$

Hence, we have arrived at our goal, at least as far as the energy shift is concerned. We have found a formula, which together with the series expansion for the time-evolution operator, make possible a direct perturbation expansion in the coupling constant g. In addition, this formula allows for a diagrammatic analysis with Feynman diagrams, which we will discuss in later chapters. If we are interested in properties other than the ground state energy of the system, we express these in terms of single-particle Green's functions through the time-evolution operator. To do so, we first show the identity

$$\begin{aligned}
&\frac{\langle\Psi_0\mid O(t)_H|\,\Psi_0\rangle}{\langle\Psi_0|\,\Psi_0\rangle}\\
&\quad=\lim_{\epsilon\to 0}\frac{1}{\langle\Phi_0\mid S_\epsilon|\,\Phi_0\rangle}\langle\Phi_0\mid\sum_{\nu=0}^{\infty}\frac{(-i)^\nu}{\nu!}\int_{-\infty}^{\infty}\mathrm{d}t_1\ldots\int_{-\infty}^{\infty}\mathrm{d}t_\nu\\
&\qquad\times\mathrm{e}^{-\epsilon(|t_1|+\ldots+|t_\nu|)}T\left(v(t_1)_I\ldots v(t_\nu)_I O(t)_I\right)\mid\Phi_0\rangle,
\end{aligned}\tag{18.9}$$

with the abbreviation $S_\epsilon\equiv U_\epsilon(\infty,-\infty)$. To prove this identity, we first use the fact that the Gell-Mann–Low theorem can be proved also for the quantity

$$\mid\tilde{\xi}\rangle\equiv\lim_{\epsilon\to 0}\frac{U_\epsilon(0,+\infty)|\,\Phi_0\rangle}{\langle\Phi_0\mid U_\epsilon(0,+\infty)|\,\Phi_0\rangle}$$

i.e., for a state which develops backwards from $\mid\Phi_0\rangle$ at infinitely large positive times. If $\mid\Phi_0\rangle$ is non-degenerate, the state developed in this way can only differ from the one developed forward in time by an overall phase, which is in any case eliminated by the common normalization $\langle\Phi_0\mid\tilde{\xi}\rangle=1=\langle\Phi_0\mid\xi\rangle$.

If we now substitute the backward developed state $\langle\tilde{\xi}\mid$ for all bra-vectors $\langle\Psi_0\mid$, and the forward developed state $\mid\xi\rangle$ for all ket-vectors $\mid\Psi_0\rangle$ in equation (18.9), we obtain

$$\frac{\langle\Psi_0\mid O(t)_H|\,\Psi_0\rangle}{\langle\Psi_0|\,\Psi_0\rangle}=\lim_{\epsilon\to 0}\frac{\langle\Phi_0\mid U_\epsilon(\infty,0)O(t)_H U_\epsilon(0,-\infty)|\,\Phi_0\rangle}{\langle\Phi_0\mid U_\epsilon(\infty,0)U_\epsilon(0,-\infty)|\,\Phi_0\rangle}.$$

It should be emphasized that neither the numerator nor the denominator exists in the limit $\epsilon \to 0$; only for the ratio of them will the infinite phases cancel out simultaneously.

We use (*cf.* equation (14.16))

$$O(t)_H = U_\epsilon(0,t)O(t)_I U_\epsilon(t,0)$$

together with the property

$$U(t,t')U(t',t'') = U(t,t'')$$

to obtain

$$\frac{\langle \Psi_0 \mid O(t)_H \mid \Psi_0\rangle}{\langle \Psi_0 \mid \Psi_0\rangle} = \lim_{\epsilon\to 0} \frac{\langle \Phi_0 \mid U_\epsilon(\infty,t)O(t)_I U(t,-\infty) \mid \Phi_0\rangle}{\langle \Phi_0 \mid S_\epsilon \mid \Phi_0\rangle}.$$

It remains to be shown that

$$\begin{aligned}&\sum_{\nu=0}^{\infty} \frac{(-i)^\nu}{\nu!} \int_{-\infty}^{\infty} \mathrm{d}t_1 \ldots \int_{-\infty}^{\infty} \mathrm{d}t_\nu \, \mathrm{e}^{-\epsilon(|t_1|+\ldots+|t_\nu|)} T\left[v(t_1)_I \ldots v(t_\nu)_I O(t)_I\right] \\ &= \ U_\epsilon(\infty,t)O(t)_I U_\epsilon(t,-\infty).\end{aligned}$$

To show this, we split up the ν-dimensional integration in distinct pieces, the boundaries of which form the surfaces $t_i = t$. In each piece, there are a certain number of variables with $t_i > t$ and a number with $t_i < t$. The situation in two dimensions, for example, is depicted in figure 18.1. For each piece, we introduce the notations

for each t_i with $t_i > t$: $\tau_1 \ldots \tau_n$
and for each t_i with $t_i < t$: $\sigma_1 \ldots \sigma_{\nu-n}$.

The number n depends on the particular piece.

Within a single piece, it holds that

$$\begin{aligned}T\left[v(t_1)_I \ldots v(t_\nu)_I O(t)_I\right] &= T\left[v(\tau_1)_I \ldots v(\tau_n)_I\right] \\ &\quad \times O(t)_I T\left[v(\sigma_1)_I \ldots v(\sigma_{\nu-n})_I\right],\end{aligned}$$

and the contribution of this piece to the integral above is

$$\begin{aligned}&\int_t^{\infty} \mathrm{d}\tau_1 \ldots \int_t^{\infty} \mathrm{d}\tau_n \, \mathrm{e}^{-\epsilon(|\tau_1|+\ldots+|\tau_n|)} T\left[v(\tau_1)_I \ldots v(\tau_n)_I\right] O(t)_I \\ &\quad \times \int_{-\infty}^{t} \mathrm{d}\sigma_1 \ldots \int_{-\infty}^{t} \mathrm{d}\sigma_{\nu-n} \, \mathrm{e}^{-\epsilon(|\sigma_1|+\ldots+|\sigma_{\nu-n}|)} T\left[v(\sigma_1)_I \ldots v(\sigma_{\nu-n})_I\right].\end{aligned}$$

The entire integral is obtained by summing over the 2^ν pieces. It is not necessary to consider each piece individually since most of the integrals give

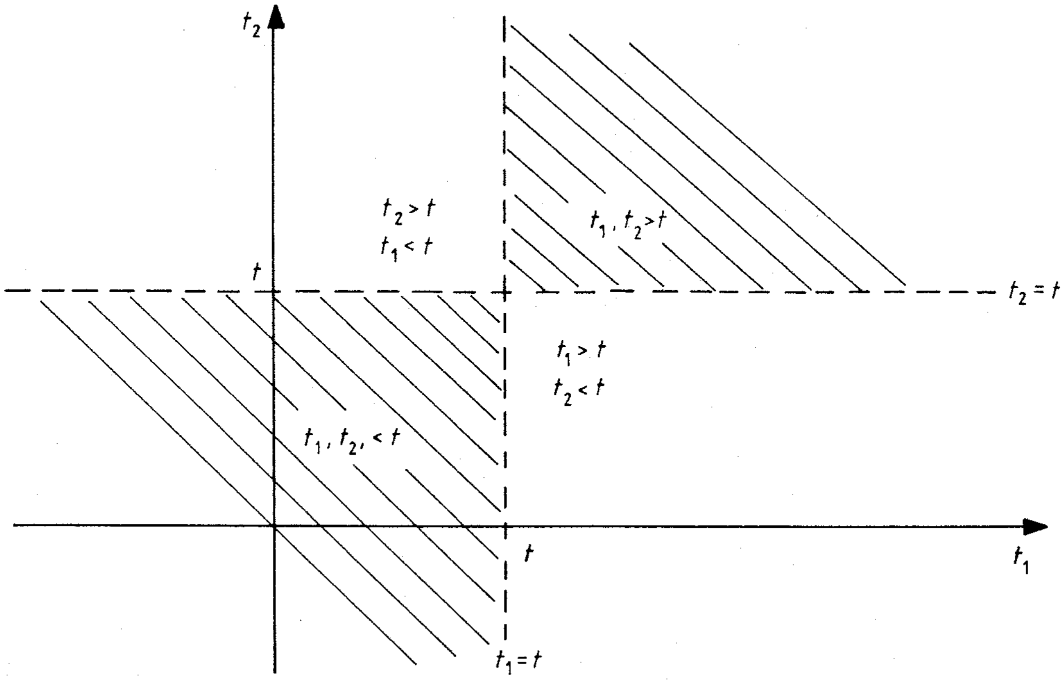


Figure 18.1 *Integration areas for* $\nu = 2$.

the same value: only the number n plays a role. For fixed n, which of the original t_i are transformed to τ and which are transformed to σ is completely irrelevant, since they are only dummy integration variables. Given ν and n, there are

$$\binom{\nu}{n} = \frac{\nu!}{n!(\nu - n)!}$$

possibilites to select n times t_i such that $t_i > t$. All corresponding pieces give the same contribution. Hence, it is necessary only to sum over all possible values of n from $n = 0$ to $n = \nu$:

$$\begin{aligned}
&\sum_{\text{pieces}} \int_t^\infty \mathrm{d}\tau_1 \ldots \int_t^\infty \mathrm{d}\tau_n \int_{-\infty}^t \mathrm{d}\sigma_1 \ldots \int_{-\infty}^t \mathrm{d}\sigma_{\nu-n} \cdots \\
&= \sum_{\nu=0}^\infty \frac{\nu!}{n!(\nu-n)!} \int_t^\infty \mathrm{d}\tau_1 \ldots \int_t^\infty \mathrm{d}\tau_n \int_{-\infty}^t \mathrm{d}\sigma_1 \ldots \int_{-\infty}^t \mathrm{d}\sigma_{\nu-n} \cdots \\
&= \sum_{n=0}^\infty \sum_{m=0}^\infty \delta_{\nu,m+n} \frac{\nu!}{n!m!} \int_t^\infty \mathrm{d}\tau_1 \ldots \int_t^\infty \mathrm{d}\tau_n \int_{-\infty}^t \mathrm{d}\sigma_1 \int_{-\infty}^t \mathrm{d}\sigma_m \ldots .
\end{aligned}$$

The desired result follows:

$$
\begin{aligned}
&\sum_{\nu=0}^{\infty}\frac{(-i)^\nu}{\nu!}\int_{-\infty}^{\infty}\mathrm{d}t_1\ldots\int_{-\infty}^{\infty}\mathrm{d}t_\nu\,\mathrm{e}^{-\epsilon(|t_1|+\ldots+|t_\nu|)}T\left[v(t_1)_I\ldots v(t_\nu)_I O(t)_I\right]\\
&= \sum_{n=0}^{\infty}\frac{(-i)^n}{n!}\int_t^{\infty}\mathrm{d}\tau_1\ldots\int_t^{\infty}\mathrm{d}\tau_n\,\mathrm{e}^{-\epsilon(|\tau_1|+\ldots+|\tau_n|)}T\left[v(\tau_1)_I\ldots v(\tau_n)_I\right]\\
&\quad\times O(t)_I\sum_{m=0}^{\infty}\frac{(-i)^m}{m!}\int_{-\infty}^{t}\mathrm{d}\sigma_1\ldots\int_{-\infty}^{t}\mathrm{d}\sigma_m\\
&\quad\times\mathrm{e}^{-\epsilon(|\sigma_1|+\ldots+|\sigma_m|)}T\left[v(\sigma_1)_I\ldots v(\sigma_m)_I\right]\\
&= U_\epsilon(\infty,t)O(t)_I U_\epsilon(t,-\infty),
\end{aligned}
$$

which concludes the proof of equation (18.9) Another interesting conclusion we can make is that

$$
\begin{aligned}
&\frac{\langle\Psi_0\mid T\left[O(t)_H O(t')_H\right]\mid\Psi_0\rangle}{\langle\Psi_0|\,\Psi_0\rangle}\\
&= \lim_{\epsilon\to 0}\frac{1}{\langle\Phi_0\mid S_\epsilon|\,\Phi_0\rangle}\langle\Phi_0\mid\sum_{\nu=0}^{\infty}\frac{(-i)^\nu}{\nu!}\int_{-\infty}^{\infty}\mathrm{d}t_1\ldots\int_{-\infty}^{\infty}\mathrm{d}t_\nu\,\mathrm{e}^{-\epsilon(|t_1|+\ldots+|t_\nu|)}\\
&\quad\times T\left[v(t_1)_I\ldots v(t_\nu)_I O(t)_I O(t')_I\right]\mid\Phi_0\rangle. \qquad (18.10)
\end{aligned}
$$

Just as in the preceding proof, for $t > t'$ we can write:

$$
\begin{aligned}
&\frac{\langle\Psi_0\mid T\left[O(t)_H O(t')_H\right]\mid\Psi_0\rangle}{\langle\Psi_0\,|\Psi_0\rangle}\\
&= \lim_{\epsilon\to 0}\frac{1}{\langle\Phi_0\mid S_\epsilon|\,\Phi_0\rangle}\langle\Phi_0\mid U_\epsilon(\infty,t)O(t)_I U_\epsilon(t,t')O(t')_I U_\epsilon(t',-\infty)|\,\Phi_0\rangle.
\end{aligned}
$$

The identity for the numerator can then be proved by spitting up the calculation of the ν-dimensional t-integrals in single pieces with boundary surfaces $t_i = t$ *and* $t_i = t'$ and then calculate their contributions by a similar summation.

With the identity equation (18.10) we finally obtain the following important representation of the single-particle Green's function:

$$
\begin{aligned}
&iG_{\alpha\beta}(\mathbf{r}t,\mathbf{r}'t')\\
&= \lim_{\epsilon\to 0}\left[\frac{1}{\langle\Phi_0\mid S_\epsilon|\,\Phi_0\rangle}\sum_{n=0}^{\infty}\frac{(-i)^n}{n!}\int_{-\infty}^{\infty}\mathrm{d}t_1\ldots\int_{-\infty}^{\infty}\mathrm{d}t_n\right.\\
&\quad\left.\times\mathrm{e}^{-\epsilon(|t_1|+\ldots+|t_n|)}\langle\Phi_0\mid T\left[v(t_1)_I\ldots v(t_n)_I\psi_\alpha(\mathbf{r}t)_I\psi_\beta^\dagger(\mathbf{r}'t')_I\right]\mid\Phi_0\rangle\right].
\end{aligned}
\qquad (18.11)
$$

This is the form of the Green's function that we will use in the diagrammatic analysis. Corresponding equations can be obtained for the momentum-Green's function or any other choice of representation.

Chapter 19

Particle and hole operators and Wick's theorem

Most of the work in the calculation of the energy shift and the Green's function according to equations (18.8) and (18.11) is the evaluation of the matrix elements relative to $\mid \Phi_0\rangle$ of time-ordered products of the potential in the interaction representation. If this potential is represented in second quantization, a time-ordered product of creation and annihilation operators in the interaction representation is obtained. Wick's theorem [14] provides a method to calculate the $\mid \Phi_0\rangle$-expectation value of such time-ordered products. In this chapter we will prove Wick's theorem.

We first define particle and hole operators. We assume that the eigenvalue problem given by

$$H_0 = \sum_{i=1}^{N} h(i)$$

is solved by the single-particle orbitals

$$h\varphi_\nu = \epsilon_\nu \varphi_\nu .$$

In the ground state, the orbitals with single-particle energies up to ϵ_F are occupied. Furthermore, let $c_i^\dagger$ and c_i denote the creation and annihilation operators of the single-particle orbital φ_i. We then define the following operators for particles and holes, respectively. For particles:

$$\left.\begin{array}{ll} \text{creation operator} & a_i^\dagger \equiv c_i^\dagger \\ \text{annihilation operator} & a_i \equiv c_i \end{array}\right\} \text{for } \epsilon_i > \epsilon_F \tag{19.1}$$

and for holes:

$$\left.\begin{array}{ll} \text{creation operator} & b_j^\dagger \equiv c_j \\ \text{annihilation operator} & b_j \equiv c_j^\dagger \end{array}\right\} \text{for } \epsilon \leq \epsilon_F . \tag{19.2}$$

Clearly, the annihilation of a real particle with energy less than ϵ_F corresponds to the creation of a hole with the same single-particle energy. We obtain in the interaction picture

$$\begin{aligned} a_j(t)_I &= a_j e^{-i\epsilon_j t} \\ a_j^\dagger(t)_I &= a_j^\dagger e^{+i\epsilon_j t} \\ b_j(t)_I &= b_j e^{+i\epsilon_j t} \\ b_j^\dagger(t)_I &= b_j^\dagger e^{-i\epsilon_j t}. \end{aligned}$$

Since $\{c_i^\dagger, c_k\} = \delta_{ik}$ we have furthermore

$$\{a_i^\dagger, a_k\} = \delta_{ik} \quad \text{and} \quad \{b_j^\dagger, b_\ell\} = \delta_{j\ell}. \tag{19.3}$$

Moreover, any possible particle operator anticommutes with any possible hole operator, since they act on different states. The operators defined in this way satisfy

$$a_i \mid \Phi_0\rangle = 0 \quad \text{and} \quad b_j \mid \Phi_0\rangle = 0 \tag{19.4}$$

i.e., the ground state of the H_0-problem contains neither particles nor holes. Thus, we will call $\mid \Phi_0\rangle$ the *vacuum state* (relative to the particle–hole representation).

We can now express the operator H_0 in terms of the particle and hole operators:

$$\begin{aligned} H_0 &= \sum_i \epsilon_i c_i^\dagger c_i = \sum_{\epsilon_i \le \epsilon_F} \epsilon_i c_i^\dagger c_i + \sum_{\epsilon_i > \epsilon_F} \epsilon_i c_i^\dagger c_i \\ &= \sum_{\epsilon_i \le \epsilon_F} \epsilon_i b_i b_i^\dagger + \sum_{\epsilon_i > \epsilon_F} \epsilon_i a_i^\dagger a_i \\ &= \sum_{\epsilon_i \le \epsilon_F} \epsilon_i - \sum_{\epsilon_i \le \epsilon_F} \epsilon_i b_i^\dagger b_i + \sum_{\epsilon_i > \epsilon_F} \epsilon_i a_i^\dagger a_i \\ &= W_0 - \sum_H \epsilon_H n_H + \sum_P \epsilon_P n_P \end{aligned} \tag{19.5}$$

where n_H and n_P arethe number operators for holes and particles, respectively. From this representation of H_0 we see that the energy of an arbitrary eigenstate of H_0 is obtained as the ground state energy plus the sum of the particle energies minus the sum of the hole energies.

Next, we express the field operators in terms of particle and hole operators.

$$\begin{aligned} \psi(x) &= \sum_{\epsilon_i \le \epsilon_F} \varphi_i(x) c_i + \sum_{\epsilon_i > \epsilon_F} \varphi_i(x) c_i \\ &= \sum_{\epsilon_i \le \epsilon_F} \varphi_i(x) b_i^\dagger + \sum_{\epsilon_i > \epsilon_F} \varphi_i(x) a_i \equiv \psi_+(x) + \psi_-(x). \end{aligned}$$

We can apparently separate $\psi(x)$ into a hole-creation part $\psi_+(x)$ and a particle-annihilation part $\psi_-(x)$. Similarly, we can separate $\psi^\dagger(x)$ into a particle-creation part and a hole-annihilation part:

$$\begin{aligned}
\psi^\dagger(x) &= \sum_{\epsilon_i \leq \epsilon_F} \varphi_i^*(x) c_i^\dagger + \sum_{\epsilon_i > \epsilon_F} \varphi_i^*(x) c_i^\dagger \\
&= \sum_{\epsilon_i \leq \epsilon_F} \varphi_i^*(x) b_i + \sum_{\epsilon_i > \epsilon_F} \varphi_i^*(x) a_i^\dagger \equiv \left(\psi^\dagger\right)_-(x) + \left(\psi^\dagger\right)_+(x).
\end{aligned}$$

The minus-index always denotes the annihilation part (for both particles and holes), and the plus-index denotes the creation part. From equation (19.4), we have the important equation

$$\psi_- |\Phi_0\rangle = 0 = \left(\psi^\dagger\right)_- |\Phi_0\rangle. \qquad (19.6)$$

The separation of creation and annihilation parts is invariant under transformations to other pictures. For example, we have

$$\begin{aligned}
\psi(xt)_- &= \psi_+(xt)_I + \psi_-(xt)_I \\
\text{with} \quad \psi_+(xt)_I &= \sum_{\epsilon_i \leq \epsilon_F} \varphi_i(x) b_i^\dagger(t)_I.
\end{aligned}$$

The *normal order* N of a product of particle and hole operators is defined by rearranging the product in such a way that all annihilation operators are to the right, multiplied with the sign of the permutations necessary to achieve this. In other words, the normal-ordered product is obtained by bringing all annihilation operators to the right, and in doing so, treating all operators as if they anticommute. For example

$$\begin{aligned}
& N[c_i(t_1) c_j(t_2) c_k^\dagger(t_3)] \\
&= N[a_i(t_1) b_j^\dagger(t_2) a_k^\dagger(t_3)] \\
&= (-1)^2 b_j^\dagger(t_2) a_k^\dagger(t_3) a_i(t_1) \\
&= +c_j(t_2) c_k^\dagger(t_3) c_i(t_1),
\end{aligned}$$

for $\epsilon_i, \epsilon_k > \epsilon_F$, $\epsilon_j < \epsilon_F$.

The time dependence of the operators in the interaction picture does not matter for the normal order. It is very important to recognize that the definition of a normal-ordered product is unique. Indeed, one could commute operators within the product of creation operators or within the product of annihilation operators and, for example, write

$$(-1)^3 a_k^\dagger(t_3) b_j^\dagger(t_2) a_i(t_1)$$

for the example above. However, all expressions obtained in this way are identical, since the creation operators anticommute (and similarly, the annihilation operators anticommute).

We now generalize our definition to include linear combinations

$$N(\alpha A+\beta B)\equiv \alpha N(A)+\beta N(B)$$

where A and B are products of particle and hole operators and α, β are complex numbers. It follows that

$$N\left[A(B+C)\right]=N(AB+AC)=N(AB)+N(AC)$$

or, in general

$$N\left(\sum_i \alpha_i A_i \sum_j \beta_j B_j\right)=\sum_{ij}\alpha_i\beta_j N(A_iB_j).$$

As an example, we calculate

$$\begin{aligned}
N\left[\psi^\dagger(x)\psi(y)\right] &= N\left\{\left[(\psi^\dagger)_+(x)+(\psi^\dagger)_-(y)\right]\left[\psi_+(y)+\psi_-(y)\right]\right\}\\
&= N\left[\left(\psi^\dagger\right)_+(x)\psi_+(y)\right]+N\left[\left(\psi^\dagger\right)_+(x)\psi_-(y)\right]\\
&\quad +N\left[(\psi^\dagger)_-(x)\psi_+(y)\right]+N\left[(\psi^\dagger)_-(x)\psi_-(y)\right]\\
&= \left(\psi^\dagger\right)_+(x)\psi_+(y)+\left(\psi^\dagger\right)_+(x)\psi_-(y)\\
&\quad -\psi_+(y)\left(\psi^\dagger\right)_-(x)+\left(\psi^\dagger\right)_-(x)\psi_-(y).
\end{aligned}$$

In the last line, we have used the previous representation of the field operators in terms of particle and hole operators; the third term, for example, is

$$\begin{aligned}
N\left[\left(\psi^\dagger\right)_-(x)\psi_+(y)\right] &= N\left[\sum_{\epsilon_i\le\epsilon_F}\varphi^*(x)b_i\sum_{\epsilon_j\le\epsilon_F}\varphi_j(y)b_j^\dagger\right]\\
&= \sum_{ij}\varphi_i^*(x)\varphi_j(y)\underbrace{N\left(b_ib_j^\dagger\right)}_{-b_j^\dagger b_i}\\
&= -\psi_+(y)\left(\psi^\dagger\right)_-(x).
\end{aligned}$$

Next, we define the so-called *pairing* of two arbitrary particle or hole operators A and B as

$$\underset{\sqcup}{AB}\equiv AB-N(AB). \tag{19.7}$$

From the rule we established earlier for the normal order of linear combinations of operators we readily obtain the generalization of the pairing to linear combinations:

$$\begin{aligned}
&\underbracket{\left(\sum \alpha_i A_i\right)\left(\sum \beta_j B_j\right)} \\
&\quad = \left(\sum \alpha_i A_i\right)\left(\sum \beta_j B_j\right) - N\left(\sum \alpha_i A_i \sum \beta_j B_j\right) \\
&\quad = \sum \alpha_i \beta_j A_i B_j - \sum \alpha_i \beta_j N\left(A_i B_j\right) \\
&\quad = \sum \alpha_i \beta_j \left(A_i B_j - N\left(A_i B_j\right)\right) \\
&\quad = \sum \alpha_i \beta_j \, \underbracket{A_i B_j} \, .
\end{aligned}$$

It should be emphasized, that the pairing is *not* defined for the case when both A and B themselves are *products* of particle and hole operators.

Let us consider some examples:

$$\begin{aligned}
\underbracket{a_i(t)a_j^\dagger(t')} &= a_i(t)a_j^\dagger(t') - N\left[a_i(t)a_j^\dagger(t')\right] \\
&= a_i(t)a_j^\dagger(t') + a_j^\dagger(t')a_i(t) \\
&= e^{i(\epsilon_j t' - \epsilon_i t)}\left(a_i a_j^\dagger + a_j^\dagger a_i\right) \\
&= e^{i\epsilon_j(t'-t)}\delta_{ij},
\end{aligned}$$

and, analogously

$$\underbracket{b_i(t)b_j^\dagger(t')} = e^{i\epsilon_j(t-t')}\delta_{ij}.$$

For all other possible combinations of two particle and hole operators, the pairing vanishes, since the pairing always vanishes for two anticommuting operators:

$$\{A, B\} = 0 \;\Rightarrow\; \underbracket{AB} = 0.$$

Proof:

$$\underbracket{AB} = AB - N(AB) = AB - \left\{\begin{array}{c} AB \\ -BA \end{array}\right\} = 0.$$

The statement holds also for linear combinations $A = \sum_i \alpha_i A_i$, $B = \sum_j \beta_j B_j$, if all components anticommute, (*i.e.*, $\{A_i, B_j\} = 0$):

$$\underbracket{\left(\sum_i \alpha_i A_i\right)\left(\sum_j \beta_j B_j\right)} = \sum_{ij} \alpha_i \beta_j \, \underbracket{A_i B_j} = 0.$$

Most pairings are also zero. However, if they do not vanish, the result is always a c-number. At this point we can begin to see the purpose of the definition: with it, we can very simply calculate the vacuum expectation value of two linear combinations A, B of particle and hole operators:

$$\langle \Phi_0 \mid AB \mid \Phi_0 \rangle = \langle \Phi_0 \mid N(AB) + \underbrace{AB} \mid \Phi_0 \rangle .$$

Since the vacuum expectation value of a normal ordered product always vanishes, this expression is

$$\langle \Phi_0 \mid \underbrace{AB} \mid \Phi_0 \rangle = \underbrace{AB} .$$

Thus, in the end we only have to calculate the pairings to determine the vacuum expectation value. We will now calculate another pairing as an exercise:

$$\begin{aligned}
\underbrace{\left(\psi^\dagger\right)_-(xt)\psi_+(yt')} &= \underbrace{\left[\sum_{\epsilon_i \leq \epsilon_F} \varphi_i^*(x) b_i(t)\right]\left[\sum_{\epsilon_j \leq \epsilon_F} \varphi_j(y) b_j^\dagger(t')\right]} \\
&= \sum_{\epsilon_i, \epsilon_j \leq \epsilon_F} \varphi_i^*(x)\varphi_j(y)\, \underbrace{b_i(t) b_j^\dagger(t')} \\
&= \sum_{\epsilon_j \leq \epsilon_F} \varphi_j^*(x)\varphi_j(y) \mathrm{e}^{i\epsilon_j(t-t')}
\end{aligned}$$

and, analogously

$$\underbrace{\psi_-(xt)\left(\psi^\dagger\right)_+(yt')} = \sum_{\epsilon_j > \epsilon_F} \varphi_j(x)\varphi_j^*(y) \mathrm{e}^{i\epsilon_j(t'-t)} .$$

All other 14 pairings which can be formed from the operators $\psi_\pm$ and $\left(\psi^\dagger\right)_\pm$ vanish, since the operators either anticommute or are already normal-ordered:

$$
\begin{aligned}
0 &= \underbracket{\psi_+\psi_+} & \qquad 0 &= \underbracket{\psi_-\psi_+} \\
&= \underbracket{\left(\psi^\dagger\right)_+\left(\psi^\dagger\right)_+} & &= \underbracket{\left(\psi^\dagger\right)_-\left(\psi^\dagger\right)_+} \\
&= \underbracket{\psi_-\psi_-} & &= \underbracket{\psi_+\psi_-} \\
&= \underbracket{\left(\psi^\dagger\right)_-\left(\psi^\dagger\right)_-} & &= \underbracket{\left(\psi^\dagger\right)_+\left(\psi^\dagger\right)_-} \\
&= \underbracket{\left(\psi^\dagger\right)_+\psi_+} & &= \underbracket{\psi_+\left(\psi^\dagger\right)_+} \\
&= \underbracket{\left(\psi^\dagger\right)_-\psi_-} & &= \underbracket{\psi_-\left(\psi^\dagger\right)_-} \\
&= \underbracket{\psi_+\left(\psi^\dagger\right)_-} & &= \underbracket{\left(\psi^\dagger\right)_+\psi_-}\,.
\end{aligned}
$$

From this we obtain the pairings for the field operator themselves:*

$$
\begin{aligned}
\underbracket{\psi(xt)\psi^\dagger(yt')} &= \underbracket{[\psi_+(xt)+\psi_-(xt)]\left[\left(\psi^\dagger\right)_+(yt')+\left(\psi^\dagger\right)_-(yt')\right]} \\
&= \underbrace{\underbracket{\psi_+(xt)\left(\psi^\dagger\right)_+(yt')}}_{=0} + \underbrace{\underbracket{\psi_+(xt)\left(\psi^\dagger\right)_-(yt')}}_{=0} \\
&\quad + \underbracket{\psi_-(xt)\left(\psi^\dagger\right)_+(yt')} + \underbrace{\underbracket{\psi_-(xt)\left(\psi^\dagger\right)_-(yt')}}_{=0} \\
&= \sum_{\epsilon>\epsilon_F}\varphi_j(x)\varphi_j^*(y)\mathrm{e}^{i\epsilon_j(t'-t)},
\end{aligned}
$$

and, analogously,

$$
\begin{aligned}
\underbracket{\psi^\dagger(xt)\psi(yt')} &= \sum_{\epsilon_j\leq\epsilon_F}\varphi_j^*(x)\varphi_j(y)\mathrm{e}^{i\epsilon_j(t-t')} \\
\underbracket{\psi^\dagger(xt)\psi^\dagger(yt')} &= 0 = \underbracket{\psi(xt)\psi(yt')}.
\end{aligned}
$$

Finally, we also define the normal order products of operators which contain pairings:

$$
N(A^{\bullet}B\,C^{\bullet\bullet}D^{\bullet}E\ldots X\,Y^{\bullet\bullet}Z) \equiv (-)^q\,\underbracket{AD}\;\underbracket{CY}\;N(BE\ldots XZ).
$$

Here q is the number of commutations necessary to bring the paired operators to the left of the product, *i.e.*, in this example the number of pairwise commutations needed to get from $ABCD\ldots XYZ$ to $ADCYBE\ldots XZ$.

Wick's theorem for normal products states that

$$\begin{aligned}
A_1A_2\ldots A_n \quad = \quad & N(A_1\ldots A_n) \\
& +N(\underbracket{A_1A_2}\,A_3\ldots A_n)+N(\underbracket{A_1A_2A_3}\ldots) \\
& +\ldots \text{ all other terms with one pairing} \\
& +N(\underbracket{A_1A_2}\,\underbracket{\ldots}\,A_n) \\
& +\ldots \text{ all other terms with two pairings} \\
& + \\
& \vdots \\
& + \text{ all completely paired terms} \\
& \quad \text{(they appear only for even } n).
\end{aligned}$$

For a proof, we first show the following lemma:

$$N(A_1A_2\ldots A_n)B=\sum_{r=1}^{n}N(A_1A_2\ldots \underbracket{A_r\ldots A_nB})+N(A_1A_2\ldots A_nB).$$

In the case that B is an annihilation operator, all pairings $\underbracket{A_rB}$ vanish, and the lemma is trivially satisfied. If B is a creation operator, all pairings $\underbracket{A_rB}$ where A_r also is a creation operator vanish. Hence, it suffices to prove the lemma for the case where all A_i are annihilation operators. All cases with an additional creation operator A_j can then readily be constructed by multiplying the equation without the creation operator A_j on the left by A_j. The normal order is then satisfied and additional pairings do not arise.

Thus, for annihilation operators $A_1\ldots A_n$ it remains to be shown that

$$A_1\ldots A_nB=\sum_{r=1}^{n}(1)^{r+n}\,\underbracket{A_rB}\;A_1\ldots \cancel{A}_r\ldots A_n+(-1)^nBA_1\ldots A_n.$$

(The slashed operator $\cancel{A}_r$ means that this operator is omitted.) The prefactor $(-1)^{r+n}$ comes from $(r-1)$ commutations of A_r and $(n-1)$ commutations of B. We prove the statement by induction. For $n=1$, we have from the definition of the pairing

$$\underbracket{A_1B}=A_1B-BA_1.$$

We assume that the statement is true for n. By multiplication from the left by an annihilation operator A_0, we have

$$\begin{aligned} & A_0A_1\dots A_nB \\ = \; & \sum_{r=1}^{n}(-1)^{r+n}\,\underbrace{A_rB}\,A_0A_1\dots \not{A}_r\dots A_n+(-1)^nA_0BA_1\dots A_n \\ = \; & \sum_{r=1}^{n}(-1)^{r+n}\,\underbrace{A_rB}\,A_0A_1\dots A_r\dots A_n+(-1)^n\,\underbrace{A_0B}\,A_1\dots A_n \\ & +(-1)^{n+1}BA_0A_1\dots A_n, \end{aligned}$$

where we have used $A_0B=-BA_0+\underbrace{A_0B}$. This is the statement for $(n+1)$ and the proof of the lemma is complete. With the help of this lemma we will now prove Wick's theorem in a similar way by induction. For $n=1,2$ the statement is trivially satisfied by the definition of the pairing. Assume that the statement is true for n. By multiplying from the right by an operator A_{n+1} we obtain

$$\begin{aligned} A_1\dots A_nA_{n+1} \; = \; & N(A_1\dots A_n)A_{n+1} \\ & +N(\underbrace{A_1A_2}\dots)A_{n+1}+\dots \end{aligned}$$

By the lemma, we obtain for the first term

$$N(A_1\dots A_n)A_{n+1}=\underline{N(A_1\dots A_nA_{n+1})}+\underbrace{\sum_r N(A_1\dots \underbrace{A_r\dots A_nA_{n+1}})}$$

and, for the second term

$$\begin{aligned} & \sum_{1\le x<y\le n} N(A_1\dots \underbrace{A_x\dots A_y}\dots A_n)A_{n+1} \\ = \; & \sum_{1\le x<y\le n}(\pm)\,\underbrace{A_xA_y}\,N(A_1\dots \not{A}_x\dots \not{A}_y\dots A_n)A_{n+1} \\ = \; & \sum_{1\le x<y\le n}(\pm)\,\underbrace{A_xA_y}\Big[N(A_1\dots \not{A}_x\dots \not{A}_y\dots A_nA_{n+1}) \\ & +\sum_{r\ne x,y}N(A_1\dots \not{A}_x\dots \underbrace{A_r\dots \not{A}_y\dots A_nA_{(n+1)}})\Big] \\ = \; & \underbrace{\sum_{1\le x<y\le n} N(A_1\dots \underbrace{A_x\dots A_y}\dots A_nA_{N+1})} \end{aligned}$$

$$+\sum_{1\le x<y\le n}\sum_{r\neq x,y} N(A_1\dots \underbracket{A_x\dots \underbracket{A_r\dots A_y\dots A_n A_{(n+1)}}}.$$

The underlined expression is the first term of Wick's theorem for $(n+1)$. The two expression marked by underbraces yield all terms with one pairing, and so on. Repeated application of the lemma will eventually lead to all terms for Wick's theorem for $(n+1)$.

Due to the linearity of normal-ordered products (and of the pairings), Wick's theorem also holds for linear combinations of particle and hole operators, and consequently also for the field operators themselves.

We have now come to the last crucial step: the calculation of vacuum expectation values of time-ordered products. For two linear combinations

$$A(t)=\sum_i \alpha_i A_i(t), \quad B(t')=\textstyle\sum_j \beta_j B_j(t')$$

of particle and hole operators A_i, B_j, we define the so-called *contraction* by

$$\overbracket{A(t)B(t')}\equiv T\left(A(t)B(t')\right)-N\left(A(t)B(t')\right). \tag{19.8}$$

From the properties of normal-ordered and time-ordered products it follows that

$$\begin{aligned}-\overbracket{A(t)B(t')} &= -T(A(t)B(t'))+N(A(t)B(t'))\\ &= T(B(t')A(t))-N(B(t')A(t))\\ &= \overbracket{B(t')A(t)}.\end{aligned} \tag{19.9}$$

With the help of the definition of time-ordered products we can readily calculate the contraction $\overbracket{A(t)B(t')}$:

$$T(A(t)B(t'))=\begin{cases} A(t)B(t') & \text{if } t>t' \\ -B(t')A(t) & \text{if } t'>t\end{cases}$$

$$\begin{aligned} A(t)B(t') &= N(A(t)B(t'))+\underbracket{A(t)B(t')}\\ -B(t')A(t) &= -N(B(t')A(t))-\underbracket{B(t')A(t)}\\ &= N(A(t)B(t'))-\underbracket{B(t')A(t)}.\end{aligned}$$

Hence

$$\begin{aligned}\wick{\c A(t) \c B(t')} &= T(A(t)B(t')) - N(A(t)B(t')) \\ &= \begin{cases} \underbracket{A(t)B(t')} & \text{if } t > t' \\ -\underbracket{B(t')A(t)} & \text{if } t' > t. \end{cases}\end{aligned}$$

Thus, contractions correspond to two different pairings, depending on the time-order. In particular, contractions are always c-numbers, so that

$$\langle \Phi_0 \mid T(A(t)B(t')) \mid \Phi_0 \rangle = \wick{\c A(t) \c B(t')}.$$

From the corresponding property of pairings, it follows that

$$N(\wick{\c1 A \c2 B C \c1 D E \dots X \c2 Y Z}) = (-1)^q \wick{\c A \c D}\ \wick{\c B \c Y}\ N(CE\dots XZ).$$

With this result, we can now state *Wick's theorem for time-ordered products*:

$$\begin{aligned} T(A_1A_2\dots A_n) &= N(A_1A_2\dots A_n) \\ &\quad + N(\wick{\c A_1 \c A_2} \dots A_n) + \\ &\quad + \dots \text{ all other terms with one contraction} \\ &\quad + N(\wick{\c1 A_1 \c1 A_2 \c2 . \c2 . . } A_n) + \dots \\ &\quad + \dots \text{ all other terms with two contractions} \\ &\quad + \\ &\quad \vdots \\ &\quad + \text{ all completely contracted terms} \\ &\quad\ \ \text{(they appear only for even } n) \end{aligned}$$

The proof follows directly from the theorem for usual products:

$$\begin{aligned} & T(A_1A_2\dots A_n) \\ &\quad = \operatorname{sgn}(P) A_{P(1)}A_{P(2)}\cdots A_{P(n)} \\ &\quad = \operatorname{sgn}(P)\left[N\left(A_{P(1)}A_{P(2)}\cdots\right) + \sum N\left(\sqcup\right) + \sum N\left(\sqcup\ \sqcup\right) + \dots\right] \end{aligned}$$

where $t_{P(1)} > t_{P(2)} > \dots$ and we have indicated sums over all terms with one pairing, two pairings and so on. Since the times are ordered, the pairings are precisely equal to the contractions:

$$
\begin{aligned}
&T(A_1A_2\dots A_n)\\
&\quad= \operatorname{sgn}(P)\left[N\left(A_{(p1)}A_{P(2)}\cdots\right)+\sum N\left(\sqcap\right)+\sum N\left(\sqcap\ \sqcap\right)+\dots\right]\\
&\quad= N\left(A_1A_2\dots A_n\right)+\sum_{xy}N\left(A_1A_2\dots \overbracket{A_x\dots A_y}\dots A_n\right)+\dots
\end{aligned}
$$

and the proof is complete. We conclude this chapter by calculating a few additional contractions. First, we consider the creation and annihilation operators of the H_0-problem:

$$
\begin{aligned}
&\overbracket{c_j(t)c_k^\dagger}(t')\\
&= \begin{cases}
\text{for } \epsilon_j,\epsilon_k > \epsilon_F: & \overbracket{a_j(t)a_k^\dagger} = \begin{cases} \underbracket{a_j(t)a_k^\dagger}(t') & \text{for } t>t' \\ -\underbracket{a_k^\dagger(t')a_j}(t)=0 & \text{for } t'>t \end{cases}\\
\text{for } \epsilon_j,\epsilon_k \le \epsilon_F: & \overbracket{b_j^\dagger(t)b_k}(t') = \begin{cases} \underbracket{b_j^\dagger(t)b_k}(t) = 0 & \text{for } t>t' \\ -\underbracket{b_k(t')b_j^\dagger}(t) & \text{for } t'>t \end{cases}\\
\text{otherwise}: & 0
\end{cases}\\
&= \begin{cases}
\delta_{jk}e^{-i\epsilon_j(t-t')} & \epsilon_j>\epsilon_F,\ t>t'\\
-\delta_{jk}e^{-i\epsilon_j(t-t')} & \epsilon_j\le\epsilon_F,\ t'>t\\
0 & \text{otherwise}
\end{cases}\\
&= \delta_{jk}e^{-i\epsilon_j(t-t')}\left[\theta(t-t')\theta(\epsilon_j-\epsilon_F)-\theta(t'-t)\theta(\epsilon_F-\epsilon_j)\right].
\end{aligned}
\tag{19.10}
$$

This expression is reminiscent of the momentum Green's function for translationally invariant systems discussed earlier (*cf.* equation (15.23):

$$
\begin{aligned}
&iG^{(0)}_{\alpha\beta}(\mathbf{k}t,\mathbf{k}'t')\\
&\quad= \delta_{\alpha\beta}\delta_{\mathbf{k}\mathbf{k}'}e^{-i\epsilon_k(t-t')}\left[\theta(t-t')\theta(k-k_F)-\theta(t'-t)\theta(k_F-k)\right].
\end{aligned}
$$

In fact, the contraction $\overbracket{c_j(t)c_k^\dagger}(t')$ is in general the Green's function for the free H_0-propagator:

$$
iG^{(0)}(jt,kt') = \langle\Phi_0\mid T\left[c_j(t)_Hc_k^\dagger(t')_H\right]\mid\Phi_0\rangle
$$

so for $H = H_0$ we have

$$iG^{(0)}(jt, kt') = \langle\Phi_0 \mid T\left[c_j(t)_I c_k^\dagger(t')_I\right] \mid \Phi_0\rangle = \overbracket{c_j(t)_I c_k^\dagger(t')_I}. \tag{19.11}$$

For the remaining contractions that can be formed from the H_0 creation and annihilation operators, we have

$$\overbracket{c_k^\dagger(t')c_j(t)} = -\overbracket{c_j(t)c_k^\dagger(t')}$$

and

$$\overbracket{c_j(t)c_k(t')} = 0 = \overbracket{c_j^\dagger(t)c_k^\dagger(t')}.$$

from the general proof above. The last equations follow directly from the earlier calculated pairings.

In an analogous manner, we obtain for the field operators:

$$\begin{aligned}\overbracket{\psi(xt)\psi^\dagger(yt')} &= -\overbracket{\psi^\dagger(yt')\psi(xt)} \\ &= \langle\Phi_0 \mid T\left(\psi(xt)\psi^\dagger(yt')\right) \mid \Phi_0\rangle \\ &= iG^{(0)}(xt, yt')\end{aligned} \tag{19.12}$$

and

$$\overbracket{\psi(xt)\psi(yt')} = 0 = \overbracket{\psi^\dagger(xt)\psi^\dagger(yt')}.$$

Thus, all contractions that can be formed from field operators or from the creation and annihilation operators of the H_0 problem either vanish or correspond to free H_0-propagators.

Chapter 20

Feynman diagrams

We have now arrived at the diagrammatic calculation of the energy shift ΔE and the single-particle Green's function. By using the procedure of 'adiabatic turning-on', we derived the following perturbation series in the coupling constant g (*cf.* equations (18.1), (18.8) and (18.11)) for the energy shift and the Green's function:

$$\begin{aligned}\Delta E &= \lim_{\epsilon\to 0} i\frac{\partial}{\partial t}\ln\langle\Phi_0 \mid U_\epsilon(t,-\infty)\mid\Phi_0\rangle\Big|_{t=0}\\ &= \lim_{\epsilon\to 0} i\frac{\partial}{\partial t}\ln\Big\{\sum_{n=0}^{\infty}\frac{(-i)^n}{n!}\int_{-\infty}^{t}\mathrm{d}t_1\ldots\int_{-\infty}^{t}\mathrm{d}t_n\,\mathrm{e}^{-\epsilon(|t_1|+\ldots+|t_n|)}\\ &\quad\times\langle\Phi_0\mid T\left[v(t_1)_I\ldots v(t_n)_I\right]\mid\Phi_0\rangle\Big\}\Big|_{t=0}\end{aligned}$$

and

$$\begin{aligned}&iG_{\alpha\beta}(\mathbf{r}t,\mathbf{r}'t')\\ &= \lim_{\epsilon\to 0}\frac{1}{\langle\Phi_0\mid U_\epsilon(\infty,-\infty)\mid\Phi_0\rangle}\sum_{n=0}^{\infty}\frac{(-i)^n}{n!}\int_{-\infty}^{\infty}\mathrm{d}t_1\ldots\int_{-\infty}^{\infty}\mathrm{d}t_n\\ &\quad\times\mathrm{e}^{-\epsilon(|t_1|+\ldots+|t_n|)}\langle\Phi_0\mid T\left[v(t_1)_I\ldots v(t_n)_I\psi_\alpha(\mathbf{r}t)_I\psi^\dagger_\beta(\mathbf{r}'t')_I\right]\mid\Phi_0\rangle.\end{aligned}$$

If we now use the second-quantized representation of the potential, either through the H_0-creation and annihilation operators

$$v(t)_I = \frac{1}{2}\sum_{ijk\ell}\langle ij|v|k\ell\rangle c^\dagger_i(t)_I c^\dagger_j(t)_I c_\ell(t)_I c_k(t)_I$$

or through the field operators

$$v(t)_I = \frac{1}{2}\int\mathrm{d}x\int\mathrm{d}x'\,v(x,x')\psi^\dagger(xt)_I\psi^\dagger(x't)_I\psi(x't)_I\psi(xt)_I$$

we will obtain terms of the form

$$\begin{aligned}&\langle ij \mid v \mid k\ell\rangle\langle i'j' \mid v \mid k'\ell'\rangle\ldots\\&\qquad\times\langle\Phi_0 \mid T\left[c_i^\dagger(t_1)c_j^\dagger(t_1)c_\ell(t_1)c_k(t_1)c_{i'}^\dagger(t_2)c_{j'}^\dagger(t_2)c_{\ell'}(t_2)c_{k'}(t_2)\ldots\right] \mid \Phi_0\rangle\end{aligned}$$

and

$$\begin{aligned}&v(x_1x_1')v(x_1x_2')\ldots\\&\qquad\times\langle\Phi_0 \mid T\Big[\psi^\dagger(x_1t_1)\psi^\dagger(x_1't_1)\psi(x_1't_1)\psi(x_1t_1)\\&\qquad\times\psi^\dagger(x_2t_2)\psi^\dagger(x_2't_2)\psi(x_2't_2)\psi(x_2t_2)\ldots\Big] \mid \Phi_0\rangle\end{aligned}$$

respectively. Apart from the matrix elements $\langle ij \mid v \mid k\ell\rangle$ in the H_0-representation, or $v(x,x')$ in the space–spin representation, which we as usual assume known, we only have to calculate vacuum expectation values of time-ordered products of creation and annihilation operators. According to Wick's theorem, the result is the sum over all completely contracted combinations of these creation and annihilation operators. Depending on each separate contraction, the terms either identically vanish or consist of a product of free propagators $G^{(0)}$. Hence, all that appears in the perturbation expansion are matrix elements of the potential and free propagators $G^{(0)}$. The general form of the nth order term in the perturbation series is then

$$\begin{aligned}&\frac{(-i)^n}{n!2^n}\times\left\{\begin{array}{l}\sum_{ijk\ell}\cdots\\ \text{or}\\ \int \mathrm{d}x_1\int\mathrm{d}x_1'\ldots\end{array}\right\}\int\mathrm{d}^n t\,\mathrm{e}^{-\epsilon(|t_1|\ldots)}\\&\qquad\times\sum(\pm)\underbrace{\langle v\rangle\ldots\langle v\rangle}_{n\text{ factors}}\;\underbrace{(iG^{(0)})\ldots(iG^{(0)})}_{\substack{2n\text{ factors for }\Delta E\\(2n+1)\text{ factors for }G}}.\end{aligned}$$

The product of the matrix elements of the potential is the same in all terms of nth order; hence, we only have to find all possible products of free propagators with the corresponding arguments. A diagrammatic method for the investigation of the terms that arise uses the famous Feynman diagrams. In this method, each occurring term is assigned a diagrammatic representation through a unique translation recipe. The translation recipe is usually summarized in a number of rules, the so-called Feynman rules:

(1) We *imagine* a time-axis with time increasing from below to above.

(2) The Green's function $G^{(0)}(\lambda t,\lambda' t')$, which in any representation λ describe the 'free' propagation, *i.e.*, the H_0-propagation of particles (for $t > t'$), and holes (for $t < t'$), respectively, from state λ to state λ',

is represented by a continuous line from (λt) to $(\lambda' t')$. According to the propagation from λ' to λ, we draw an arrow, which points from the second to the first argument, on the line. The endpoints of the line must be ordered according to the imagined time-axis (see figure 20.1). The length, curvature or tilt of the lines do not matter; the only important thing is the order of the endpoints with respect to the imagined time-axis. Thus, a line with the arrow pointing up describes the propagation of a particle, and a line with the arrow pointing down describes the propagation of a hole. We will later discuss how to calculate and interpret the propagator for $t = t'$. Furthermore, it should be remarked that we cannot use these rules to represent the four-dimensional Fourier transform $G(\mathbf{k}, \omega)$, since this one does not contain any time argument. We will treat the diagrammatic representation of this Green's function in Chapter 24.

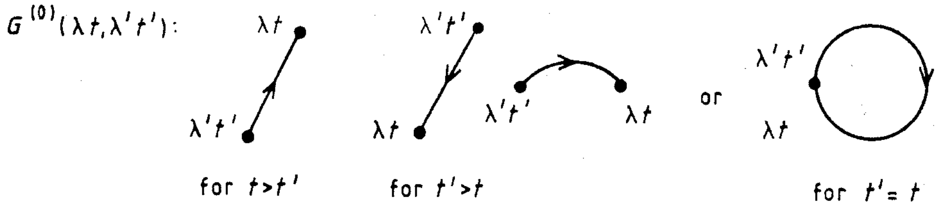


Figure 20.1 *The propagator is represented by a line, with the direction of propagation indicated by arrows.*

The simplest example that we know is the spatial Green's function $G^{(0)}(\mathbf{r}t, \mathbf{r}'t')$, or, with spin-indices labeled, $G_{\alpha\beta}(\mathbf{r}t, \mathbf{r}'t') = \delta_{\alpha\beta} G^{(0)}(\mathbf{r}t, \mathbf{r}'t')$. These Green's functions are depicted diagrammatically in figure 20.2. Another example is the momentum Green's function. This one is diago-

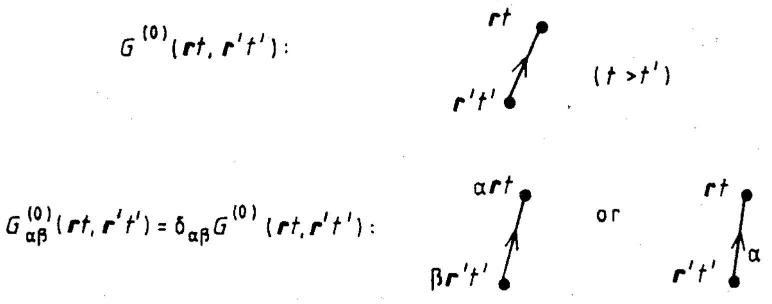


Figure 20.2 *Diagrammatic representations of the Green's functions* $G^{(0)}(\mathbf{r}t, \mathbf{r}'t')$ *and* $G_{\alpha\beta}(\mathbf{r}t, \mathbf{r}'t')$.

nal for $H_0 = \sum_{\mathbf{k},\sigma} k^2/(2m)c^\dagger_{\mathbf{k},\sigma}c_{\mathbf{k},\sigma}$: $G_{\alpha\beta}(\mathbf{k}t, \mathbf{k}'t') = \delta_{\alpha\beta}\delta_{\mathbf{k}\mathbf{k}'}G^{(0)}(\mathbf{k}, t - t')$ (see figure 20.3).

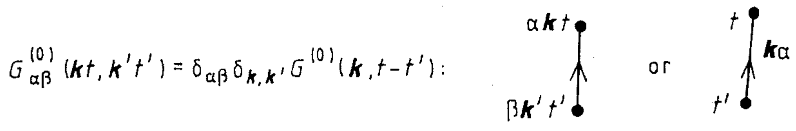


Figure 20.3 *Diagrammatic representation of the momentum Green's function* $G^{(0)}_{\alpha\beta}(\mathbf{k}t, \mathbf{k}'t') = \delta_{\alpha\beta}\delta_{\mathbf{k},\mathbf{k}'}G^{(0)}(\mathbf{k}, t - t')$.

(3) The matrix elements of the interaction are represented by a wiggly line with the endpoints labeled according to figure 20.4. The point

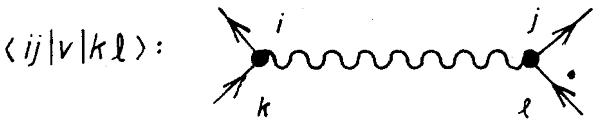


Figure 20.4 *Diagrammatic representation of the interaction matrix element* $\langle ij \mid v \mid j\ell\rangle$. *The connection points between the interaction line and the propagator are called* internal vertices.

where the interaction lines are connected to propagators are called *internal vertices.* They are start or endpoints for each $G^{(0)}$-line which is the result of a contraction of four operators belonging to this matrix element:

$$\langle ij \mid v \mid k\ell\rangle c_i^\dagger(t)c_j^\dagger(t)c_\ell(t)c_k(t). \tag{20.1}$$

The direction of the arrow on the particle lines relative to the imagined time-axis is not fixed. For example, the lines of the $G^{(0)}$-propagator in the matrix element equation (20.1) can be represented as either of the diagrams in figure 20.5. The crucial point is that at each internal vertex, there is one line with the arrow pointing toward the interaction line, and one line with the arrow pointing away. The indices of the two arrows that point away correspond to the creation operators $c_i^\dagger$ and $c_j^\dagger$; the indices of the arrows that point in to the vertex correspond to the annihilation operators c_k and c_ℓ.

Within the framework of the non-relativistic theory, which we are considering here, the Coulomb interaction between electrons is instantaneous; hence, the interaction lines run horizontally. (Other interactions, such as

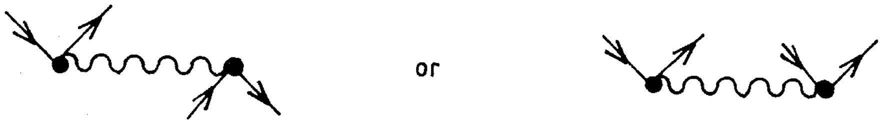


Figure 20.5 *Possible diagrammatic representations of the propagator lines belonging to the matrix element in equation (20.1).*

electron–phonon interactions, are retarded even in non-relativistic theories. Hence, interaction lines for such interactions begin and end at different times.) This means that the left and right endpoints of these (as later starting points or endpoints of the Green's function lines) belong to the same time-point of the imagined vertical time axis. This time-point is common for all four operators which are connected by this matrix element. In relativistic theories, in which the Coulomb interaction has a finite velocity of propagation, the requirement that the interaction lines are horizontal will be dropped (see Chapter 24).

A potential which is local in the space-representation and diagonal with respect to spin-coordinates, *i.e.*, $v(x, x') = v(\mathbf{r}s, \mathbf{r}s')$, will be represented as shown in figure 20.6. If the potential is local in space, but non-diagonal in the spin coordinates, the diagrammatical representation is as depicted in figure 20.7. For the translationally invariant interaction discussed in Chapter 5, the momentum representation is particularly simple:

Figure 20.6 *For potentials which are local in space, only one index is needed at each internal vertex.*

$$V = \frac{1}{2\Omega} \sum_{\mathbf{q}} \sum_{\substack{\mathbf{k}\sigma \\ \mathbf{k}'\sigma'}} v_{\mathbf{q}} a^{\dagger}_{(\mathbf{k}+\mathbf{q})\sigma} a^{\dagger}_{(\mathbf{k}'-\mathbf{q})\sigma'} a_{\mathbf{k}'\sigma'} a_{\mathbf{k}\sigma} .$$

In this case, the matrix element depends only on one index, $\mathbf{q}$. The creation and annihilation operators that belong to the incoming and outgoing particle

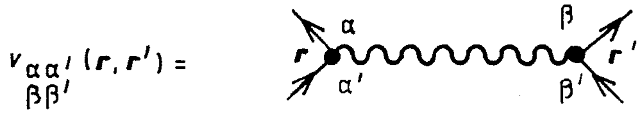


Figure 20.7 *The representation of a potential which is local in space, but non-diagonal in spin.*

lines at a vertex tell us how to label these lines (see figure 20.8). Apparently, conservation of momentum holds at the internal vertices. Thus, the matrix elements of the interaction can be interpreted as a propagator for a particle with momentum $\mathbf{q}$.

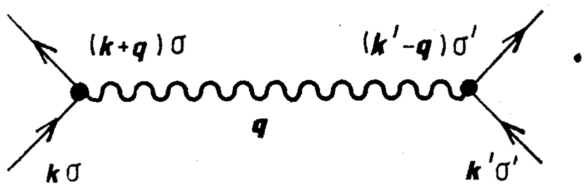


Figure 20.8 *Interaction line for a translationally invariant potential in momentum representation.*

With the three above rules, we will now draw a few Feynman diagrams. We begin with the representation of the so-called ***vacuum amplitude*** $\langle\Phi_0 \mid U_\epsilon \mid \Phi_0\rangle$, which is necessary for the calculation of the energy shift ΔE, and which also appears in the denominator of the single-particle Green's function. The quantity has acquired this name, since it is the probability amplitude for the transition from the vacuum state $\mid \Phi_0\rangle$ back to $\mid \Phi_0\rangle$. In the vacuum amplitude, all the contractions that appear have indices which are also found on the interaction matrix elements, *i.e.*, all $G^{(0)}$-lines begin and end on the endpoints of interaction lines. In first order, *i.e.*, one interaction line, there are only two different diagrams. We draw them in figure 20.9 for the case of a potential which is local in space, but non-diagonal in spin-indices. In contrast to the vacuum amplitude, all $G^{(0)}$-lines in the diagrammatical representation of the numerator of the single-particle Green's function do not start and end on endpoints of interaction lines. Furthermore, the two operators $\psi_\alpha(\mathbf{r},t)$ and $\psi^\dagger_\beta(\mathbf{r}'t')$, which correspond to the arguments of the exact Green's function, define two additional endpoints. In first order, we obtain the six diagrams shown in figure 20.10. Since only the starting

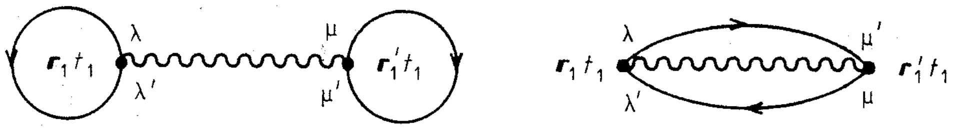


Figure 20.9 *The two first-order vacuum amplitude diagrams.*

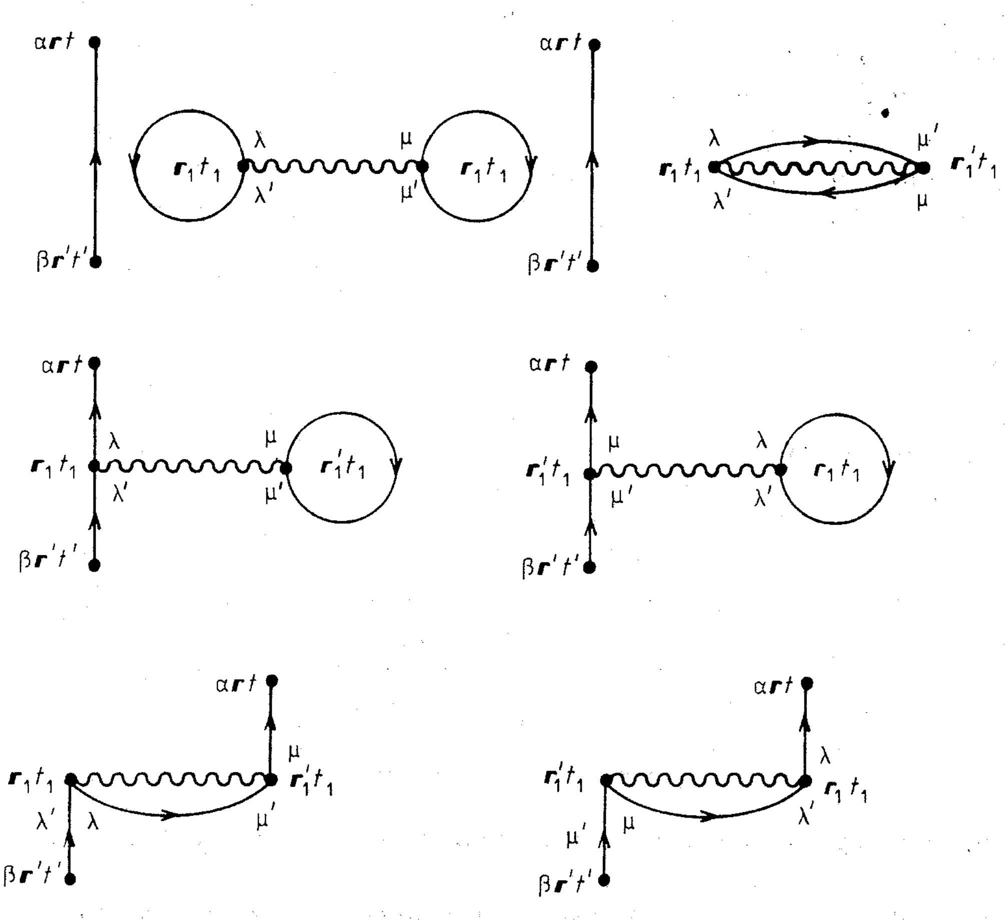


Figure 20.10 *The six possible first-order diagrams in the numerator of the Green's function.*

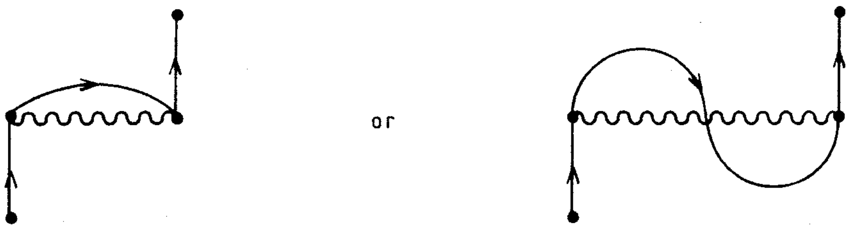


Figure 20.11 *The last of the diagrams in figure 20.10 can, for example, be drawn in either of these two ways.*

point and endpoint are important for the $G^{(0)}$-line, the last two diagrams can for example be drawn as shown in figure 20.11. All Green's functions diagrams drawn here are for particle propagation ($t > t'$). The corresponding diagrams for hole-propagation are obtained by exchanging the indices and by changing the direction of all arrows.

In all depicted diagrams for the vacuum amplitude, $G^{(0)}$-functions with two equal time-arguments appear. To determine these particular ones, we once again return to the original formula for the first-order vacuum amplitude:

$$\langle\Phi_0 \mid U_\epsilon^{(1)} \mid \Phi_0\rangle = -i\frac{1}{2}\int \mathrm{d}t_1\, \mathrm{e}^{-\epsilon|t_1|} \sum_{\substack{\lambda\mu\\ \lambda'\mu'}} \int \mathrm{d}^3r_1 \int \mathrm{d}^3r_1'\, v_{\substack{\lambda\lambda'\\ \mu\mu'}}(\mathbf{r}_1,\mathbf{r}_1')M$$

where we use Wick's theorem for normal products to calculate the matrix element M:

$$\begin{aligned} M &= \langle\Phi_0 \mid \psi^\dagger_\lambda(\mathbf{r}_1t_1)\psi^\dagger_\mu(\mathbf{r}_1't_1)\psi_{\mu'}(\mathbf{r}_1't_1)\psi_{\lambda'}(\mathbf{r}_1t_1) \mid \Phi_0\rangle \\ &= \underbrace{\psi^\dagger_\lambda(\mathbf{r}_1t_1)\psi_{\lambda'}(\mathbf{r}_1t_1)}\,\underbrace{\psi^\dagger_\mu(\mathbf{r}_1't_1)\psi_{\mu'}(\mathbf{r}_1't_1)} \\ &\quad -\underbrace{\psi^\dagger_\lambda(\mathbf{r}_1t_1)\psi_{\mu'}(\mathbf{r}_1't_1)}\,\underbrace{\psi^\dagger_\mu(\mathbf{r}_1't_1)\psi_{\lambda'}(\mathbf{r}_1t_1)}. \end{aligned}$$

Only pairings of the form $\underbrace{\psi^\dagger\psi}$ appear, since the sequence of creation and annihilation operators is already determined by the representation of the potential $v(t)_I$ in second quantization. Furthermore, we have

$$\begin{aligned} \underbrace{\psi^\dagger(xt)\psi(yt)} &= \lim_{\tilde{t}\to t+}\langle\Phi_0 \mid T\left[\psi(yt)\psi^\dagger(x\tilde{t})\right] \mid \Phi_0\rangle \\ &= -iG^{(0)}(yt,xt^+). \end{aligned}$$

Since the Green's functions with equal time-arguments, also in higher order, *always* arise from pairings *within* a $v(t)_I$, we can formulate the fourth Feynman rule:

(4) Green's functions with equal time-arguments of the form shown in figure 20.12 shall be interpreted as $G^{(0)}(\lambda t, \lambda' t^+)$.

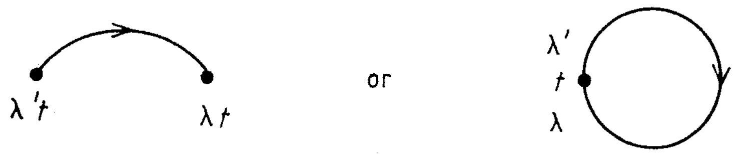


Figure 20.12 *Equal-time Green's functions.*

In all, we obtain for the first order vacuum amplitude:

$$\begin{aligned}
&\langle \Phi_0 \mid U_\epsilon^{(1)} \mid \Phi_0 \rangle \\
&= \frac{i}{2} \int \mathrm{d}t_1 \, \mathrm{e}^{-\epsilon |t_1|} \sum_{\substack{\lambda\mu \\ \lambda'\mu'}} \int \mathrm{d}^3 r_1 \int \mathrm{d}^3 r_1' \, v_{\substack{\lambda\lambda' \\ \mu\mu'}}(\mathbf{r}_1, \mathbf{r}_1') G^{(0)}_{\lambda\lambda'}(\mathbf{r}_1 t_1, \mathbf{r}_1 t_1^+) \\
&\times G^{(0)}_{\mu\mu'}(\mathbf{r}_1' t_1, \mathbf{r}_1' t_1^+) \\
&- \frac{i}{2} \int \mathrm{d}t_1 \, \mathrm{e}^{-\epsilon |t_1|} \sum_{\substack{\lambda\mu \\ \lambda'\mu'}} \int \mathrm{d}^3 r_1 \int \mathrm{d}^3 r_1' \, v_{\substack{\lambda\lambda' \\ \mu\mu'}}(\mathbf{r}_1, \mathbf{r}_1') G^{(0)}_{\mu'\lambda}(\mathbf{r}_1' t_1, \mathbf{r}_1 t_1^+) \\
&\times G^{(0)}_{\lambda'\mu}(\mathbf{r}_1 t_1, \mathbf{r}_1' t_1^+).
\end{aligned}$$

The two expressions clearly correspond to the two diagrams depicted in figure 20.9. At this point, it is clear that to evaluate the diagrams, we need the following additional rule:

(5) All indices and coordinates attached to an internal vertex should be summed and integrated over, respectively. The adiabatic switching factor $\mathrm{e}^{-\epsilon|t|}$ shall be added to the time-integrations.

We must now determine the overall sign and the prefactor. The rule which determines the sign is known as the 'loop theorem':

(6) The sign of a term of arbitrary order is $(-1)^\ell$, where ℓ is the number of closed loops formed by $G^{(0)}$-lines.

For example, the third-order term in figure 20.13 has three loops which result in a negative sign.

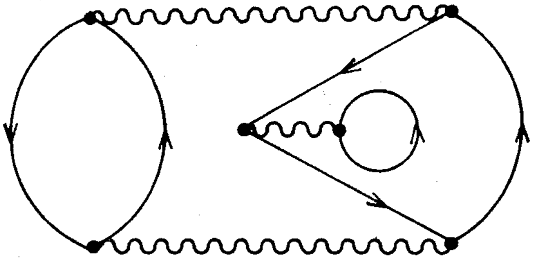


Figure 20.13 *A third-order diagram with three loops.*

To prove this theorem, we consider an arbitrary fully contracted term which contributes to the vacuum amplitude:

$$\overbrace{\underbrace{c_k^\dagger \underbrace{c_\ell^\dagger c_m}_{} c_n}_{} \underbrace{c_p^\dagger \underbrace{c_q^\dagger c_r}_{} c_s}_{} \ldots \underbrace{c_t^\dagger \underbrace{c_u^\dagger c_v}_{} c_w}_{}}^{} .$$

Such a term consists of distinct groups of four operators of the form $c^\dagger c^\dagger cc$. We can say with certainty that if the first and last operator in such a four-group belong to the same loop, then they belong to the same internal vertex and are consequently connected diagrammatically (see Fig 20.14). The same holds for the two middle operators of each four-group. To indicate this fact, we have connected the corresponding operators in the expression above with vertex 'bows'. By rearranging, we obtain

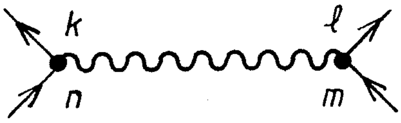
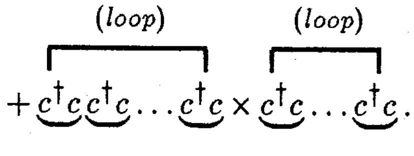


Figure 20.14 *If, for example, the indices k and n belong to the same loop, they must be connected diagrammatically.*

$$+\overbrace{\underbrace{c_k^\dagger c_n}_{} \underbrace{c_\ell^\dagger c_m}_{} \underbrace{c_p^\dagger c_s}_{} \underbrace{c_q^\dagger c_r}_{} \ldots \underbrace{c_t^\dagger c_w}_{} \underbrace{c_u^\dagger c_v}_{}}^{} .$$

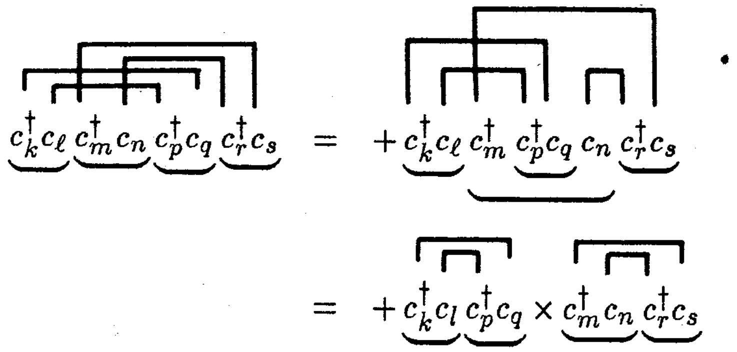
The sign of this expression is obtained from the fact that in this rearrangement, *two* operators per four-group have been commuted.

A single loop apparently consists of a group of operators which are connected by a closed chain of alternating contraction brackets and vertex bows within a contraction. We now separate the general term above in single factors, each of which corresponds to a single loop:



$$+\underbrace{c^\dagger c}\underbrace{c^\dagger c}\dots\underbrace{c^\dagger c}\times\underbrace{c^\dagger c}\dots\underbrace{c^\dagger c}.$$

By this rearrangement we also obtain the overall sign of the expression, since by factorizing a particular loop we can determine if each pair $c^\dagger c$ belongs to the loop or not. By rearranging, each pair is thus shifted as a unit, which gives the sign. For example



$$\underbrace{c_k^\dagger c_\ell}\underbrace{c_m^\dagger c_n}\underbrace{c_p^\dagger c_q}\underbrace{c_r^\dagger c_s} = +\underbrace{c_k^\dagger c_\ell}\,\underbrace{c_m^\dagger\,\underbrace{c_p^\dagger c_q}\,c_n}\,\underbrace{c_r^\dagger c_s}\,.$$

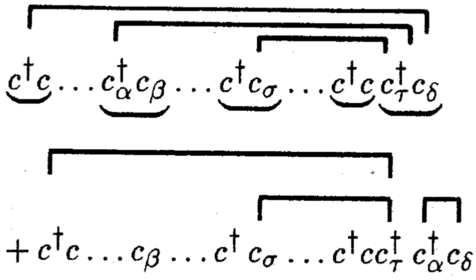
$$= +\underbrace{c_k^\dagger c_l}\underbrace{c_p^\dagger c_q}\times\underbrace{c_m^\dagger c_n}\underbrace{c_r^\dagger c_s}$$

It then only remains to show that each loop-factor can be written in the form

$$-\overbrace{cc^\dagger}\,\overbrace{cc^\dagger}\,\overbrace{cc^\dagger}\dots\overbrace{cc^\dagger}. \tag{20.2}$$

Since $\overbrace{cc^\dagger} = iG^{(0)}$, the contribution from the complete expression is then $(-)^\ell\left(iG^{(0)}\right)\left(iG^{(0)}\right)\dots$, where ℓ is the total number of loops, as we stated.

To show equation (20.2), we must factor out the single contractions:



$$\underbrace{c^\dagger c}\dots\underbrace{c_\alpha^\dagger c_\beta}\dots\underbrace{c^\dagger c_\sigma}\dots\underbrace{c^\dagger c}\underbrace{c_\tau^\dagger c_\delta}$$

$$= +c^\dagger c\dots c_\beta\dots c^\dagger c_\sigma\dots c^\dagger c c_\tau^\dagger\, c_\alpha^\dagger c_\delta$$

$$= \; -\overbrace{c^\dagger c\ldots c_\beta\ldots c^\dagger\,\overbrace{c_\sigma\ldots c^\dagger c c_\tau^\dagger}}\,\overbrace{c_\delta c_\alpha^\dagger}\,. \tag{20.3}$$

If the remaining term to the left only contains the contraction $\overbrace{c_\sigma c_\tau^\dagger}$ (which is the case if $c_\sigma = c_\beta$), we have precisely equation (20.2). If there are other contractions, we bring c_β to the right, with the result

$$+\overbrace{c^\dagger c\ldots c^\dagger\,\overbrace{c_\sigma\ldots c^\dagger c c_\tau^\dagger}\,c_\beta}\,\overbrace{c_\delta c_\alpha^\dagger}\,. \tag{20.4}$$

As far as the left factor is concerned, we are now at the beginning of the expressions equation (20.3) or equation (20.4), and can factor out the contraction that belongs to c_β, as shown in equation (20.3)–(20.3), and so on. In this way, we go from vertex to vertex in a closed chain, so long as we come back to the starting point: this is done in the last step in equation (20.3), where the the contraction $\overbrace{c_\delta c_\alpha^\dagger}$ is moved through in the remaining term on the left, which closes the circle, and the proof of the loop theorem for the vacuum amplitude is complete.

We now consider a completely contracted contribution to the numerator of the single-particle Green's function:

$$\overbrace{c^\dagger c^\dagger c c c^\dagger c^\dagger c c\ldots c^\dagger c^\dagger c c c_x c_y^\dagger}\,.$$

Apart from the groups of four operators, this term also contains two additional operators, which represent the external fixed points x and y. A $G^{(0)}$-line either belongs to a loop, or it is a part of the continuous chain which connects the two external points x and y. Therefore, if we factorize the loops as we did with the vacuum amplitude, we also obtain a contribution from the continuous line:

$$\overbrace{\underbrace{c^\dagger c}\ldots\underbrace{c^\dagger c}}^{\textit{loop}}\,\overbrace{\underbrace{c^\dagger c}\ldots\underbrace{c^\dagger c}}^{\textit{loop}}\ldots\overbrace{\underbrace{c^\dagger c}\ldots\underbrace{c^\dagger c}\,c_x c_y^\dagger}^{\textit{line}}\,.$$

Each loop gives a factor of (-1), as above. Hence, it remains to be shown that the part coming from the line does not contribute a minus sign. To do so, we factor out the single contractions:

$$\begin{aligned} \overbrace{c^\dagger c\ldots c^\dagger_\alpha\,\overbrace{c_\beta\ldots c^\dagger c c_x c^\dagger_y}} &= -\overbrace{c^\dagger c\ldots c^\dagger_\alpha\ldots c^\dagger c c_x}\,\overbrace{c_\beta c^\dagger_y} \\ &= -\overbrace{c^\dagger c\ldots c^\dagger c c^\dagger_\alpha c_x}\,\overbrace{c_\beta c^\dagger_y}\,. \end{aligned}$$

The first one of these two factors gives rise to a minus sign, just as a loop, so the term will have an overall positive sign:

$$+\overbrace{c c^\dagger}\,\overbrace{c c^\dagger}\ldots\overbrace{c c^\dagger}\,.$$

It now only remains to determine the prefactors of the translation recipe. First, each term of nth order has a prefactor $(-i)^n/(n!2^n)$. In the vacuum amplitude we have furthermore $(2n)$ contractions of the form $iG^{(0)}$. Thus, we obtain in all a prefactor $(i)^{2n}(-i)^n/(n!2^n) = (i)^n/(n!2^n)$. In the numerator of the Green's function we have in the nth order $(2n+1)$ contractions of the form $iG^{(0)}$. Finally, since the expansion for the Green's function really is an expansion for iG, the diagrams for the Green's function acquire an additional factor $(-i)$. Thus, the prefactor is in all $(-i)(i)^{2n+1}(-i)^n/(n!2^n) = (i)^n/(n!2^n)$. The recipe is then complete with the following additional rule:

(7) The prefactor of each term of nth order is

$$\left[\frac{(i)^n}{n!2^n}\right].$$

This holds both for the vacuum amplitude and the numerator of the single-particle Green's function.

As an exercise, we will now show all second-order diagrams which contribute to the vacuum amplitude. To construct these diagrams, we first draw the two interaction lines at the times t_1 and t_2 and find all ways to connect them with $G^{(0)}$-lines. We obtain the diagrams shown in figure 20.15. The question arises as to how many distinct diagrams there are of a certain order. The answer is quite simple: assume that we have drawn the n interaction lines of the vacuum amplitude. We then have to place the $2n$ arrows at the vertices of the diagram. There are $2n$ possible ways of placing the first arrow. On the other hand, there are only $(2n-1)$ possible ways of placing the second arrow, corresponding to $(2n-1)$ contractions, and so on. This gives $(2n)!$ different diagrams for the vacuum amplitude. For the numerator of the Green's function, there are the additional two external points. Correspondingly, there are $(2n+1)!$ different diagrams for particle propagation $(t > t')$ and hole-propagation $(t < t')$. Moreover, the contributions from visually different diagrams which give the same contributions to

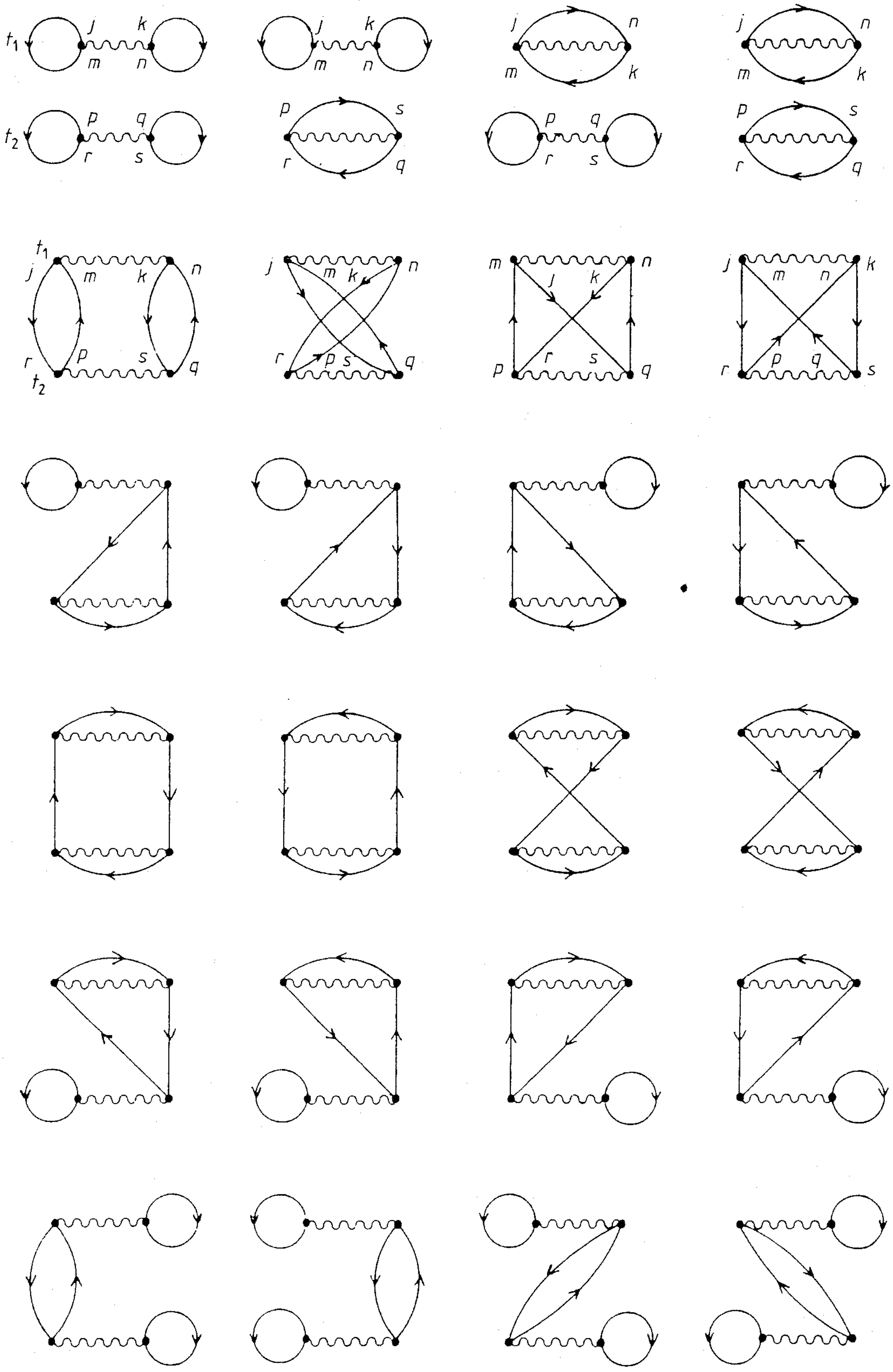


Figure 20.15 *All possible second-order vacuum amplitude diagrams.*

the perturbation expansion are included in the prefactors. This is clear for the first two and the last two diagrams of the second row in figure 20.15. These diagrams can be obtained from one another by permuting the internal vertices on a single interaction line. Their contributions are identical, since we sum over all indices. We will discuss this kind of 'degeneracy' in detail in the next chapter.

We will now translate two examples of the Feynman diagrams depicted above to mathematical language by using the Feynman rules. The first example is the diagram shown in figure 20.16. According to the rules, this

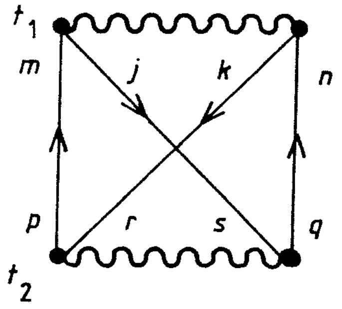


Figure 20.16 *Second-order vacuum amplitude diagram.*

diagram gives a contribution

$$(-)^1 \frac{i^2}{2!2^2} \sum_{pqrs} \sum_{jkmn} \int \mathrm{d}t_1 \int \mathrm{d}t_2 \, \mathrm{e}^{-\epsilon(|t_1|+|t_2|)}$$
$$\times \langle pq \mid v \mid rs \rangle \langle jk \mid v \mid mn \rangle G^{(0)}(mt_1, pt_2) G^{(0)}(st_2, jt_1)$$
$$G^{(0)}(nt_1, qt_2) G^{(0)}(rt_2, kt_1).$$

Since, up to this point, we have assumed that $t_1 > t_2$, the expression we obtain is strictly only valid in the domain of integration where $t_1 > t_2$. We obtain a family of equivalent diagrams if we assume that $t_2 > t_1$. We will further consider this kind of degeneracy in the next chapter by performing the time integrations.

As a second example, we translate the two disconnected diagrams shown in figure 20.17 by using the Feynman rules.

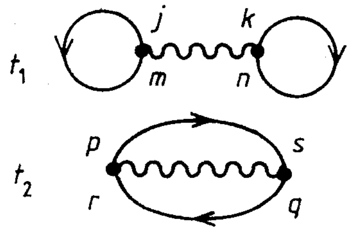


Figure 20.17 *These two disconnected first-order diagrams are included in the set of all second-order vacuum amplitude diagrams.*

$$
\begin{aligned}
&(-i)^3\frac{(-)^2}{2!2^2}\sum_{jkmn}\sum_{pqrs}\int \mathrm{d}t_1\int \mathrm{d}t_2\, \mathrm{e}^{-\epsilon(|t_1|+|t_2|)}\\
&\quad\times\langle jk\mid v\mid mn\rangle\langle pq\mid v\mid rs\rangle G^{(0)}(mt_1,jt_1^+)G^{(0)}(nt_1,kt_1^+)\\
&\quad G^{(0)}(st_2,pt_2^+)G^{(0)}(rt_2,qt_2^+) \qquad .\\
&= \frac{1}{8}\left[\sum_{jkmn}\int \mathrm{d}t_1\, \mathrm{e}^{-\epsilon|t_1|}\langle jk\mid v\mid mn\rangle G^{(0)}(mt_1,jt_1^+)G^{(0)}(nt_1,kt_1^+)\right]\\
&\quad\times\left[\sum_{pqrs}\int \mathrm{d}t_2\, \mathrm{e}^{-\epsilon|t_2|}\langle pq\mid v\mid rs\rangle G^{(0)}(st_2,pt_2^+)G^{(0)}(rt_2,qt_2^+)\right] .
\end{aligned}
$$

This example illustrates a very important fact: the contribution from a disconnected diagram is factorized into parts which belong to connected diagrams of lower order.

If the interaction conserves momentum, most of the depicted diagrams vanish. For example, in the diagram shown in figure 20.18, we must have $\mathbf{q} = 0$. Hence, both the vertical and diagonal $G^{(0)}$-lines have momentum $\mathbf{k}$, which cannot happen, since the vertical one is a particle line ($k > k_F$) and the diagonal one a hole-line ($k < k_F$). Consequently, this diagram must vanish. This may be shown explicitly by using the occurring δ-functions.

We have learnt that both in the vacuum amplitude and the numerator of the single-particle Green's function, there are connected and disconnected diagrams. In the next chapter, we will show that we only need to consider the connected diagrams: in the case of the Green's function, the disconnected diagrams are canceled by the denominator; in the vacuum amplitude, the disconnected diagrams can be summed analytically. At that point, we will make a discourse to calculate the correlation energy of a dense electron gas (Chapter 22). After that, we will continue the calculation of the single-particle Green's function.

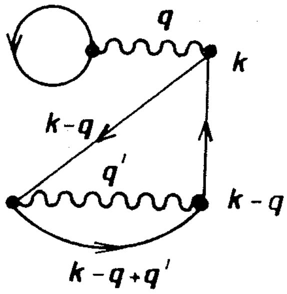


Figure 20.18 *A second-order diagram in momentum representation.*

Chapter 21

Diagrammatic calculation of the vacuum amplitude

In this chapter, we will sum all disconnected diagrams which contribute to the perturbation expansion of the vacuum amplitude. The goal is to show that only connected diagrams appear in the remaining expression of the vacuum amplitude. The final result of this summation is the so-called Linked-Cluster Theorem by Goldstone [15], which states that

$$\langle \Phi_0 \mid U \mid \Phi_0 \rangle = \exp\left[\langle \Phi_0 \mid U \mid \Phi_0 \rangle_L \right]. \tag{21.1}$$

The notation $\langle \Phi_0 \mid U \mid \Phi_0 \rangle_L$ means that only connected diagrams are included in the sum. For example, the expansion for the case of interactions which conserve momentum is shown in figure 21.1. According to the linked-cluster theorem, only the connected diagrams shown in figure 21.2 contribute. As a corollary of Goldstone's theorem, we obtain a very simple

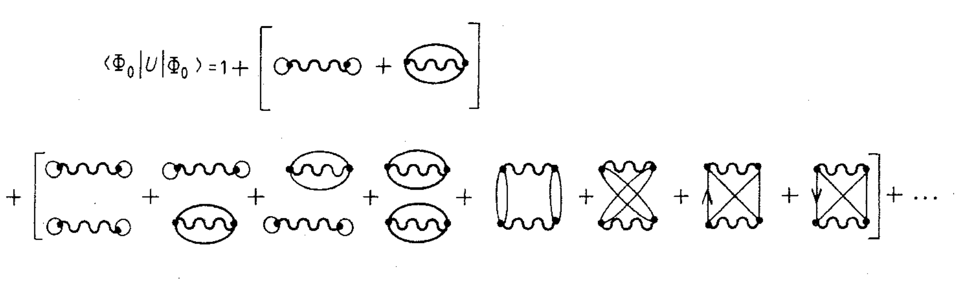


Figure 21.1 *Diagrams for the perturbation expansion of the vacuum amplitude for momentum conserving interactions.*

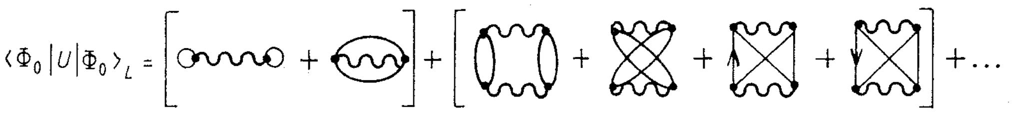


Figure 21.2 *The connected diagrams for the vacuum amplitude in figure 21.1.*

formula for the energy shift:

$$\begin{aligned} \Delta E &= \lim_{\epsilon\to 0} i\frac{\partial}{\partial t}\ln\langle\Phi_0 \mid U_\epsilon(t,-\infty) \mid \Phi_0\rangle\Big|_{t=0} \\ &= \lim_{\epsilon\to 0} i\frac{\partial}{\partial t}\langle\Phi_0 \mid U_\epsilon(t,-\infty) \mid \Phi_0\rangle_L\Big|_{t=0} . \end{aligned} \tag{21.2}$$

To prove the theorem, we first consider two arbitrary diagrams, $\gamma^{(n)}$ and $\tilde{\gamma}^{(\tilde{n})}$, of order n and $\tilde{n}$. These diagrams may be connected or disconnected. In the expansion of the vacuum amplitude, there will also be a disconnected diagram $\Gamma^{(n+\tilde{n})}$ of order $(n+\tilde{n})$, which is constructed from the first two diagrams:

$$\Gamma^{(n+\tilde{n})} \propto \left(\gamma^{(n)} \times \tilde{\gamma}^{(\tilde{n})}\right).$$

From the fact discussed earlier, that disconnected diagrams may be factorized into contributions from their sub-diagrams, and from Feynman rule (7) for the prefactors, we obtain the following important equation:

$$\Gamma^{(n+\tilde{n})} = \frac{n!\tilde{n}!}{(n+\tilde{n})!}\left(\gamma^{(n)} \times \tilde{\gamma}^{(\tilde{n})}\right). \tag{21.3}$$

With the help of this equation, we can factorize an arbitrary disconnected diagram which contributes to $\langle\Phi_0 \mid U \mid \Phi_0\rangle$ in a product of connected diagrams with given prefactors. There are in general also many other diagrams, which give *the same* contribution to the perturbation expansion. These are the diagrams which consist of the same sub-diagrams and which all can be factorized into the same product, equation (21.3). As an example, we consider all diagrams of fifth order, which can be constructed from the three first-order sub-diagrams shown in figure 21.3. All such fifth-order diagrams are shown in figure 21.4. These diagrams are obtained from one another by permuting two single interaction lines, *i.e.,* the indices of the interaction lines are interchanged. However, it is clear that all 5! possible permutations of the interaction lines will not lead to distinct diagrams. For example, permuting the interaction lines within a particular connected sub-diagram will

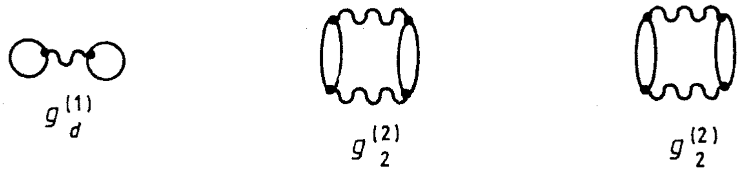


Figure 21.3 *Three connected diagrams. The first one,* $g_d^{(1)}$, *is distinct from the other two ones, which are the same diagram* $g_2^{(2)}$.

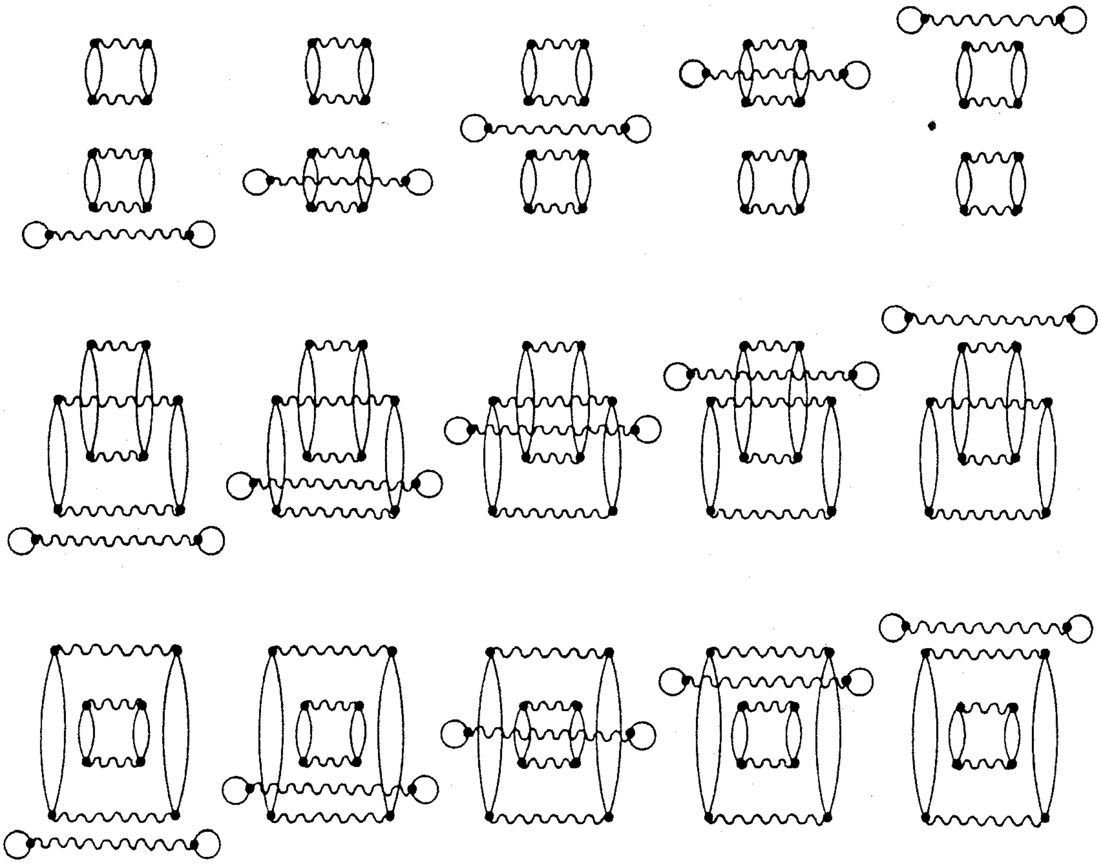


Figure 21.4 *All fifth-order diagrams that can be constructed from the diagrams in figure 21.3.*

not lead to a new diagram. If we want to calculate the number of distinct diagrams which can be constructed from the three sub-diagrams, we must divide 5! by the number of permutations of the sub-diagrams, which is two times 2!. Furthermore, we note that permuting identical sub-diagrams does not lead to distinct diagrams. Since in this example we have two identical sub-diagrams, we must also divide by another factor of 2!. This leaves 5!/(2!2!2!) = 15 distinct diagrams, which is in agreement with figure 21.4. The contribution of all diagrams in figure 21.3 to the perturbation expansion is obtained by applying equation (21.3) twice:

$$\frac{5!}{2!2!2!}\frac{2!2!1!}{(2+2+1)!}\times\left(g_2^{(2)}\right)^2\times g_d^{(1)}=\frac{1}{2!}\left(g_2^{(2)}\right)^2\times g_d^{(1)}.$$

After this example, we will now prove the theorem. We start by enumerating all *connected* diagrams of the perturbation series and denoting them by

$$g_1^{(n_1)}, g_2^{(n_2)}, g_3^{(n_3)} \ldots$$

where the superscript denotes the order. An *arbitrary* diagram of the perturbation series can be constructed by k_1 diagrams $g_1^{(n_1)}$, k_2 diagrams $g_2^{(n_2)}$, k_3 diagrams $g_3^{(n_3)}$, and so on. By repeated use of equation (21.3), we obtain the following contribution from this diagram:

$$
\begin{array}{ll}
k_1 & \left\{ \begin{array}{l} g_1^{(n_1)} \\ g_1^{(n_1)} \\ \vdots \\ g_1^{(n_1)} \end{array} \right. \\
 & \\
k_2 & \left\{ \begin{array}{l} g_2^{(n_2)} \\ g_2^{(n_2)} \\ \vdots \\ g_2^{(n_2)} \end{array} \right. \\
 & \\
k_3 & \left\{ \begin{array}{l} g_3^{(n_3)} \\ \vdots \end{array} \right.
\end{array}
= \frac{(n_1!)^{k_1}(n_2!)^{k_2}\ldots}{(k_1n_1+k_2n_2+\ldots)!}(g_1)^{k_1}(g_2)^{k_2}\ldots \tag{21.4}
$$

As we have seen, there is in general a whole series of different diagrams, which all give the same contribution to the perturbation expansion. All these degenerate diagrams can be obtained by suitable permutations of interaction lines. If we want to determine the number of these different diagrams, we must divide the number $(k_1n_1+k_2n_2+\ldots)!$ of *all* permutations by the number of permutations which lead to degenerate diagrams. First of all, identical diagrams are obtained if interaction lines *within* connected sub-diagrams are permuted. In each sub-diagram $g_i^{(n_i)}$, there are $(n_i!)$ such permutations possible, so in total we must divide by $(n_1!)^{k_1} \ldots (n_i!)^{k_i} \ldots$. Secondly, we also obtain identical diagrams when entire identical sub-diagrams are permuted with one another. In each class $g_i^{(n_i)}$ of sub-diagrams, there are $(k_i!)$ such permutations, so that we must divide by another factor of $(k_1!k_2! \ldots k_i! \ldots)$. In all, we obtain

$$\frac{(k_1 n_1 + \ldots + k_i n_i + \ldots)!}{(n_1!)^{k_1} \ldots (n_i!)^{k_i} \ldots (k_1!) \ldots (k_i!) \ldots}$$

different diagrams, which contain $k_1 \times g_1$, $k_2 \times g_2, \ldots$, and which all give the same contribution , equation (21.4), to the perturbation expansion. If we sum over all these contributions, we obtain

$$\sum_{\substack{\text{all distinct diagrams which contain} \\ k_1 \times g_1, k_2 \times g_2, \ldots}} = \frac{1}{k_1! \ldots k_i! \ldots} (g_1)^{k_1} \ldots (g_i)^{k_i} \ldots .$$

All diagrams of the vacuum amplitude are then obtained by summing over all $k_1, k_2, \ldots$ from zero to infinity:

$$\begin{aligned} \langle \Phi_0 \mid U \mid \Phi_0 \rangle &= \sum_{k_1=0}^{\infty} \cdots \sum_{k_i=0}^{\infty} \cdots \frac{1}{k_1! \ldots k_i! \ldots} (g_1)^{k_1} \ldots (g_i)^{k_i} \\ &= \exp\left[g_1 + g_2 + \ldots + g_i + \ldots\right] = \exp\left[\langle \Phi_0 \mid U \mid \Phi_0 \rangle_L\right]. \end{aligned}$$

This concludes the proof of the linked-cluster theorem.

We also need to examine the connected diagrams. In these, too, we can factor out degenerate ones, just as we have seen earlier. For example, two of the diagrams shown in figure 21.5 leave identical contributions, since they can be obtained from one another by interchanging the internal vertices of an interaction line. Since the matrix elements always satisfy the symmetry relation

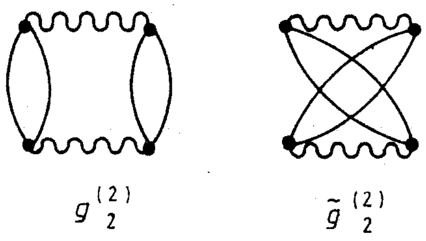


Figure 21.5 *Two connected diagrams, $g_2^{(2)}$ and $\tilde{g}_2^{(2)}$, of second order. The diagrams give identical contributions to the vacuum amplitude.*

$$\langle jk \mid v \mid mn \rangle = \langle kj \mid v \mid nm \rangle$$

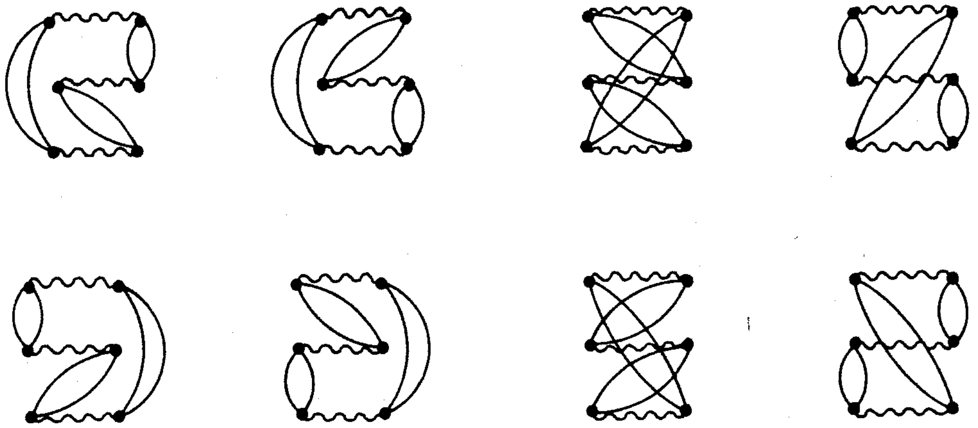


Figure 21.6 *Third-order ring-diagrams. The ones depicted here are asymmetric under reflection in a vertical line through the middle of the diagrams.*

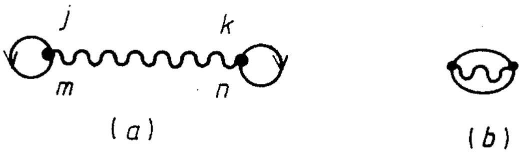
2^{n-1} topologically equivalent diags

and since all indices will be summed over, the contributions are identical. Such diagrams are usually called ***topologically equivalent.*** At this point, the question arises of how many topologically equivalent diagrams there are to a certain diagram of order n. The answer is simple. If we fix the lowest interaction line, there are two permutations possible for each of the remaining $(n-1)$ interaction lines, so there are in total 2^{n-1} different topologically equivalent diagrams. If the diagrams are symmetric under reflection in a vertical line through the middle of the diagram, we do not obtain any new diagrams by interchanging the vertices of the lowest interaction line. In this case the family then contains 2^{n-1} topologically equivalent diagrams. If the diagrams are asymmetric under reflection in such a line, we obtain twice as many, *i.e.*, 2^n different diagrams in a family of topologically equivalent ones. The so-called ring-diagrams of third order shown in figure 21.6 are examples of asymmetric diagrams.

All diagrams that we have considered so far correspond to a fixed order of the times $t_1, t_2, \ldots, t_n$, as we have mentioned, with which the individual interaction lines are labeled. For each of the $(n!)$ other orders of the time arguments, we obtain a diagram which looks identical and which differs from the first only with respect to the order of the times. This form of degeneracy can be taken into consideration quite simply: if we consider the equation proven in Chapter 14

$$\begin{aligned}
&\langle\Phi_0 \mid U^{(n)}(t,-\infty) \mid \Phi_0\rangle \\
&= \frac{(-i)^n}{n!}\int_{-\infty}^{t} \mathrm{d}t_1 \ldots \int_{-\infty}^{t} \mathrm{d}t_n \langle\Phi_0 \mid T\left[v(t_1)_I \ldots v(t_n)_I\right] \mid \Phi_0\rangle \\
&= (-i)^n \int_{-\infty}^{t} \mathrm{d}t_1 \int_{-\infty}^{t_1} \mathrm{d}t_2 \ldots \int_{-\infty}^{t_{n-1}} \mathrm{d}t_n \langle\Phi_0 \mid T\left[v(t_1)_I \ldots v(t_n)_I\right] \mid \Phi_0\rangle,
\end{aligned}$$

it is sufficient to consider the family of diagrams with $t_1 > t_2 > \ldots > t_n$. The only thing that we have to do now, is to explicitly perform the time-integration. We first investigate an example of low order, the first-order connected diagram $g_d^{(1)}$ of figure 21.7 (*a*):



(a) (b)

Figure 21.7 *The first-order connected diagrams* (a) $g_d^{(1)}$ *and* (b) $g_x^{(1)}$.

$$\begin{aligned}
g_d^{(1)} &= (-)^2\frac{i}{2}\sum_{jkmn}\int_{-\infty}^{t} \mathrm{d}t_1\, \mathrm{e}^{-\epsilon|t_1|}\langle jk \mid v \mid mn\rangle \\
&\quad \times G^{(0)}(mt_1, jt_1^+)G^{(0)}(nt_1, kt^+).
\end{aligned}$$

If we insert the free Green's functions (*cf.* equations (19.10) and (19.11))

$$iG^{(0)}(jt,kt') = \delta_{jk}\mathrm{e}^{-i\epsilon_j(t-t')}\left[(\theta(t-t')\theta(\epsilon_j-\epsilon_F) - \theta(t'-t)\theta(\epsilon_F-\epsilon_j)\right]$$

and use $t_1 \le t \le 0$, the diagram is

$$\begin{aligned}
&\frac{i}{2}\sum_{jkmn}\int_{-\infty}^{t} \mathrm{d}t_1\, \mathrm{e}^{\epsilon t_1}\langle jk \mid v \mid mn\rangle \left[-(-i)\delta_{mj}\theta(\epsilon_F-\epsilon_j)\right]\left[-(-i)\delta_{nk}\theta(\epsilon_F-\epsilon_j)\right] \\
&\quad = -\frac{i}{2}\sum_{\substack{j:\epsilon_j<\epsilon_F \\ k:\epsilon_k>\epsilon_F}} \langle jk \mid v \mid jk\rangle \int_{-\infty}^{t} \mathrm{d}t_1\, \mathrm{e}^{\epsilon t_1}.
\end{aligned}$$

This expression gives the direct term of the energy shift:

$$(\Delta E)_d^{(1)} = \lim_{\epsilon\to 0}\left[i\frac{\partial}{\partial t}g_d^{(1)}\right]\Bigg|_{t=0} = \frac{1}{2}\sum_{\substack{j:\epsilon_j<\epsilon_F \\ k:\epsilon_k<\epsilon_F}} \langle jk \mid v \mid jk\rangle. \qquad (21.5)$$

Analogously, we obtain the exchange energy from the diagram $g_x^{(1)}$ (figure 21.7 (*b*)):

$$(\Delta E)_x^{(1)} = \lim_{\epsilon\to 0}\left[i\frac{\partial}{\partial t}g_x^{(1)}\right]\Bigg|_{t=0} = -\frac{1}{2}\sum_{\substack{j:\epsilon_j<\epsilon_F\\ k:\epsilon_k<\epsilon_F}}\langle jk\mid v\mid kj\rangle. \tag{21.6}$$

We now consider a term of second order; the diagram $g_2^{(2)}$ of figure 21.3 gives a contribution

$$\begin{aligned}
&(-)^2\frac{i}{2^2}\sum_{jkmn}\sum_{pqrs}\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\,\mathrm{e}^{-\epsilon(|t_1|+|t_2|)}\langle jk\mid v\mid mn\rangle\\
&\quad\times\langle pq\mid v\mid rs\rangle G^{(0)}(rt_2,jt_1)G^{(0)}(mt_1,pt_2)G^{(0)}(st_2,kt_1)G^{(0)}(nt_1,qt_2)\\
&=\frac{i^2}{2^2}\sum_{jkmn}\sum_{pqrs}\langle jk\mid v\mid mn\rangle\langle pq\mid v\mid rs\rangle\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\,\mathrm{e}^{+\epsilon(t_1+t_2)}\\
&\quad\times\left[-(-i)\delta_{rj}\mathrm{e}^{-i\epsilon_j(t_2-t_1)}\theta(\epsilon_F-\epsilon_j)\right]\left[(-i)\delta_{mp}\mathrm{e}^{-i\epsilon_m(t_1-t_2)}\theta(\epsilon_m-\epsilon_F)\right]\\
&\quad\times\left[-(-i)\delta_{sk}\mathrm{e}^{-i\epsilon_k(t_2-t_1)}\theta(\epsilon_F-\epsilon_k)\right]\left[(-i)\delta_{nq}\mathrm{e}^{-i\epsilon_n(t_1-t_2)}\theta(\epsilon_n-\epsilon_F)\right]\\
&=\frac{(-i)^2}{2^2}\sum_{\substack{\epsilon_j,\epsilon_k<\epsilon_F\\ \epsilon_m,\epsilon_n>\epsilon_F}}(-)^2\langle jk\mid v\mid mn\rangle\langle mn\mid v\mid jk\rangle\\
&\quad\times\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\,\mathrm{e}^{\epsilon(t_1+t_2)}\mathrm{e}^{-i(\epsilon_j+\epsilon_k-\epsilon_m-\epsilon_n)t_2}\mathrm{e}^{i(\epsilon_j+\epsilon_k-\epsilon_m-\epsilon_n)t_1}
\end{aligned}$$

where we used the fact that each hole-line gives an additional minus sign to arrive at the last expression. At this point we calculate the general limit needed for the energy shift:

$$\lim_{\epsilon\to 0}\left[i\frac{\partial}{\partial t}\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\ldots\int_{-\infty}^{t_{n-1}}\mathrm{d}t_n\,\mathrm{e}^{(\epsilon+i\beta_1)t_1}\mathrm{e}^{(\epsilon+i\beta_2)t_2}\ldots\mathrm{e}^{(\epsilon+i\beta_n)t_n}\right]$$

evaluated at $t=0$. From

$$\int_{-\infty}^{t_{n-1}}\mathrm{d}t_n\,\mathrm{e}^{(\epsilon+i\beta_n)t_n}=\frac{\mathrm{e}^{(\epsilon+i\beta_n)t_{n-1}}}{\epsilon+i\beta_n}$$

it follows that

$$\begin{aligned}
&\int_{-\infty}^{t_{n-2}}\mathrm{d}t_{n-1}\int_{-\infty}^{t_{n-1}}\mathrm{d}t_n\,\mathrm{e}^{(\epsilon+i\beta_{n-1})t_{n-1}}\mathrm{e}^{(\epsilon+i\beta_n)t_n}\\
&=\int_{-\infty}^{t_{n-2}}\mathrm{d}t_{n-1}\frac{\mathrm{e}^{[2\epsilon+i(\beta_{n-1}+\beta_n)]t_{n-2}}}{\epsilon+i\beta_n}\\
&=\frac{\mathrm{e}^{[2\epsilon+i(\beta_{n-1}+\beta_n)]t_{n-1}}}{[\epsilon+i\beta_n][2\epsilon+i(\beta_{n-1}+\beta_n)]},
\end{aligned}$$

and by induction we arrive at

$$\begin{aligned}
&\lim_{\epsilon\to 0}\left[i\frac{\partial}{\partial t}\int_{-\infty}^{t}\mathrm{d}t_1\ldots\int_{-\infty}^{t_{n-1}}\mathrm{d}t_n\,\mathrm{e}^{(\epsilon+i\beta_1)t_1}\ldots\mathrm{e}^{(\epsilon+i\beta_n)t_n}\right]_{t=0}\\
&\quad=\lim_{\epsilon\to 0}\left[i\frac{\partial}{\partial t}\bigg|_{t=0}\int_{-\infty}^{t}\mathrm{d}t_1\right.\\
&\quad\quad\times\left.\frac{\mathrm{e}^{[n\epsilon+i(\beta_1+\ldots+\beta_n)]t_1}}{[\epsilon+i\beta_n][2\epsilon+i(\beta_{n-1}+\beta_n)]\ldots[(n-1)\epsilon+i(\beta_2+\ldots+\beta_n)]}\right]\\
&\quad=\lim_{\epsilon\to 0} i\frac{1}{[\epsilon+i\beta_n]\,[2\epsilon+i(\beta_{n-1}+\beta_n)]\ldots[(n-1)\epsilon+i(\beta_2+\ldots+\beta_n)]}\\
&\quad=\frac{(-i)^{n-2}}{\beta_n(\beta_{n-1}+\beta_n)\ldots(\beta_2+\ldots+\beta_n)}. \qquad (21.7)
\end{aligned}$$

This gives the result for the second-order diagram $g_2^{(2)}$ above:

$$\lim_{\epsilon\to 0}\left[i\frac{\partial}{\partial t}g_2^{(2)}\right]\bigg|_{t=0}=-\frac{1}{4}\sum_{\substack{\epsilon_j\epsilon_k<\epsilon_F\\ \epsilon_m,\epsilon_n>\epsilon_F}}\frac{\langle jk\mid v\mid mn\rangle\langle mn\mid v\mid jk\rangle^*}{-(\epsilon_j+\epsilon_k-\epsilon_m-\epsilon_n)}.$$

The family of the two topologically equivalent diagrams in figure 21.5 then contributes

$$\begin{aligned}
(\Delta E)_2^{(2)}&=\lim_{\epsilon\to 0}\left\{i\frac{\partial}{\partial t}\left[g_2^{(2)}+\tilde{g}_2^{(2)}\right]\right\}\bigg|_{t=0}\\
&=2\lim_{\epsilon\to 0}\left\{i\frac{\partial}{\partial t}\left[g_2^{(2)}\right]\right\}\bigg|_{t=0}\\
&=\frac{1}{2}\sum_{\substack{\epsilon_j,\epsilon_k<\epsilon_F\\ \epsilon_m,\epsilon_n>\epsilon_F}}\frac{|\langle jk\mid v\mid mn\rangle|^2}{(\epsilon_j+\epsilon_k-\epsilon_m-\epsilon_n)}. \qquad (21.8)
\end{aligned}$$

For the so-called second-order exchange diagrams (see figure 21.8) we obtain in an analogous manner

$$\begin{aligned}
(\Delta E)_x^{(2)}&=\lim_{\epsilon\to 0}\left\{i\frac{\partial}{\partial t}\left[g_{x1}^{(2)}+g_{x2}^{(2)}\right]\right\}\bigg|_{t=0}\\
&=-\frac{1}{2}\sum_{\substack{\epsilon_j,\epsilon_k<\epsilon_F\\ \epsilon_m,\epsilon_n>\epsilon_F}}\frac{\langle jk\mid v\mid mn\rangle\langle nm\mid v\mid jk\rangle}{(\epsilon_j+\epsilon_k-\epsilon_m-\epsilon_n)}. \qquad (21.9)
\end{aligned}$$

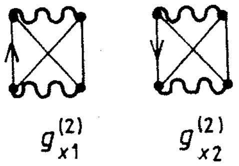


Figure 21.8 *The second-order exchange diagrams* $g^{(2)}_{x1}$ *and* $g^{(2)}_{x2}$.

We now finally consider an arbitrary connected diagram of nth order:

$$\begin{aligned} g^{(n)} &= (-)^{\ell}\frac{i^n}{2^n}\sum_{jkmn}\cdots\sum_{xywz}\langle jk\mid v\mid mn\rangle\ldots\langle xy\mid v\mid wz\rangle \\ &\quad\times\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\ldots\int_{-\infty}^{t_{n-1}}\mathrm{d}t_n\,\mathrm{e}^{-\epsilon(|t_1|+\ldots+|t_n|)} \\ &\quad\times\prod_{\text{all } G^{(0)}\text{-lines}} G^{(0)}(\alpha t_a,\beta t_b). \end{aligned}$$

The diagram contains h hole-lines and consequently $2n-h$ particle-lines. Here, $G^{(0)}$-lines with two equal-time arguments must be interpreted as hole-lines, on the basis of the limit-prescription rule (4). All summation indices that appear belong to either particle-lines or hole-lines. If we now use

$$iG^{(0)}(\alpha t_a,\beta t_b)=\delta_{\alpha\beta}\mathrm{e}^{-i\epsilon_\alpha(t_a-t_b)}\theta(\epsilon_\alpha-\epsilon_F)\quad\text{for particles}$$

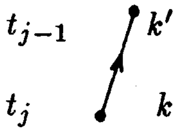
and

$$iG^{(0)}(\alpha t_a,\beta t_b)=-\delta_{\alpha\beta}^{-i\epsilon_\alpha(t_a-t_b)}\theta(\epsilon_F-\epsilon_\alpha)\quad\text{for holes}$$

so are the sums over the particle-indices and the sums over hole-indices to be performed above and below ϵ_F, respectively, because of the step-functions. Each $G^{(0)}$-line gives rise to a factor $(-i)$, and from each hole-line we obtain an additional factor of (-1):

$$\begin{aligned} g^{(n)} &= (-)^{\ell}\frac{i^n(-i)^{2n}}{2^n}(-)^h\sum_{\substack{\text{particle energies} > \epsilon_F\\ \text{hole energies} < \epsilon_F}}\langle jk\mid v\mid mn\rangle\ldots\langle xy\mid v\mid wz\rangle \\ &\quad\times\int_{-\infty}^{t}\mathrm{d}t_1\ldots\int_{-\infty}^{t_{n-1}}\mathrm{d}t_n\,\mathrm{e}^{\epsilon(t_1+t_2+\ldots+t_n)}\prod_{\text{all } G^{(0)}\text{-lines}}\delta_{\alpha\beta}\mathrm{e}^{-\epsilon_\alpha(t_a-t_b)}. \end{aligned}$$

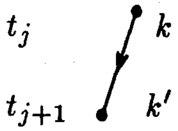
We rearrange the integrand to perform the time-integration. Consider a particular time t_j. Only four $G^{(0)}$-lines give a contribution to this time – the ones that are attached to the endpoints of the jth interaction line. For the line with index, say, k pointing away from the interaction line at t_j, the t_j-dependent contribution is $\exp(i\epsilon_k t_j)$, independent of whether the line is a particle line or a hole-line, since



$$= G^{(0)}(k't_{j-1}, kt_j) = (-i)\delta_{kk'}e^{-i\epsilon_k(t_{j-1}-t_j)}\theta(\epsilon_k - \epsilon_F)$$

$$\sim \exp\left(+i\epsilon_k t_j\right)$$

and



$$= G^{(0)}(k't_{j+1}, kt_j) = -(-i)\delta_{kk'}e^{-i\epsilon_k(t_{j+1}-t_j)}\theta(\epsilon_F - \epsilon_k)$$

$$\sim \exp(+i\epsilon_k t_j).$$

The t_j-dependent contribution from the line with index m pointing away from the interaction line is $\exp(-i\epsilon_m t_j)$. If we index the jth interaction line according to figure 21.9, the t_j-dependent factor in the integrand is*

$$\exp\left[-i\left(\epsilon_{m_j} + \epsilon_{n_j} - \epsilon_{k_j} - \epsilon_{\ell_j}\right)t_j\right].$$

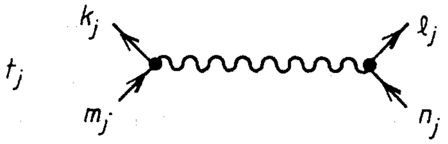


Figure 21.9 *Indexing of the jth interaction line at time t_j.*

If we set

$$\Delta_j \equiv \epsilon_{m_j} + \epsilon_{n_j} - \epsilon_{k_j} - \epsilon_{\ell_j} \quad \text{for } j = 1, \ldots, n \tag{21.10}$$

we can write the entire integrand as

$$e^{(\epsilon - i\Delta_1)t_1}e^{(\epsilon - i\Delta_2)t_2}\ldots e^{(\epsilon - i\Delta_n)t_n}.$$

By using the general formula equation (21.7), we can then write the contribution to the energy shift from the diagrams $g^{(n)}$ as

$$\begin{aligned}
&\lim_{\epsilon\to 0} i\left[\frac{\partial}{\partial t} g^{(n)}\right]\Bigg|_{t=0} \\
&= \frac{(-)^{\ell+h}}{2^n}(-i)^n(-i)^{n-2} \\
&\times \sum_{\substack{\text{particles above } \epsilon_F \\ \text{holes below } \epsilon_F}} \frac{\langle jk \mid v \mid mn\rangle \ldots \langle xy \mid v \mid wz\rangle \prod \delta_{\alpha\beta}}{(-)^{n-1}\Delta_n(\Delta_n+\Delta_{n-1})\ldots(\Delta_n+\Delta_{n-1}+\ldots+\Delta_2)}.
\end{aligned}$$

If we also use the fact that 2^n and 2^{n-1} diagrams, respectively, leave identical contributions, we obtain *for the entire family*:

$$\begin{aligned}
(\Delta E)_{g^{(n)}} &= \lim_{\epsilon\to 0}\left[i\frac{\partial}{\partial t}\left(g^{(n)} + \text{topologically equivalent diagrams}\right)\right]\Bigg|_{t=0} \\
&= \frac{(-)^{\ell+h}}{2^s} \sum_{\substack{\text{particles above } \epsilon_F \\ \text{holes below } \epsilon_F}} \frac{\langle jk \mid v \mid mn\rangle \ldots \langle xy \mid v \mid wx\rangle \prod_{\text{all } G^{(0)}\text{-lines}} \delta_{\alpha\beta}}{\Delta_n(\Delta_n+\Delta_{n-1})\ldots(\Delta_n+\Delta_{n-1}+\ldots+\Delta_2)}.
\end{aligned} \tag{21.11}$$

This is the main result of the present chapter. With it, it is very simple to calculate the contribution to the energy shift from a family of topologically equivalent diagrams. If the family is symmetric under reflection in a vertical line in the middle, $s = 1$. If the diagrams are asymmetric, $s = 0$. The Kroenecker-δ that appears can be read off by inspection of a representative of the family, and the reduction of indices can then be performed. Furthermore, there is an additional trick that can be used to determine the individual factors of the denominator (see figure 21.10). Imagine $(n-1)$ horizontal lines between the n interaction lines. Each of these lines leaves a factor to the denominator, by adding the energies of the hole-lines and then subtracting the energies of the particle-lines that are cut by this horizontal line. So long as no contractions appear (see figure 21.11 (a)), this is easy to see since the four endpoints of each layer of interaction lines just contributes one term to the sum $(\Delta_n + \Delta_{n-1} + \ldots)$. If a contraction appears, as in figure 21.11 (b), one particle line and one hole line has to be omitted per contraction. In this case, the corresponding particle and hole energies cancel out in the sum $(\Delta_n + \Delta_{n-1} + \ldots)$, since they are of equal magnitude but of opposite sign.

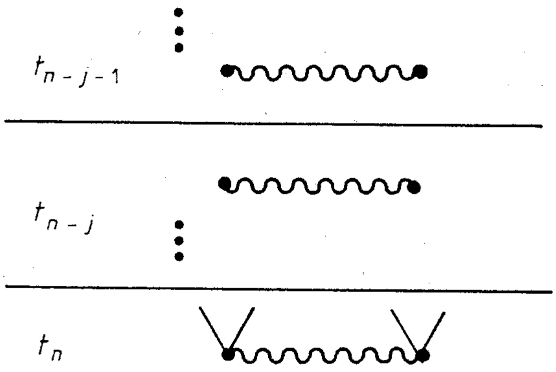


Figure 21.10 *Horizontal lines are inserted between the interaction lines.*

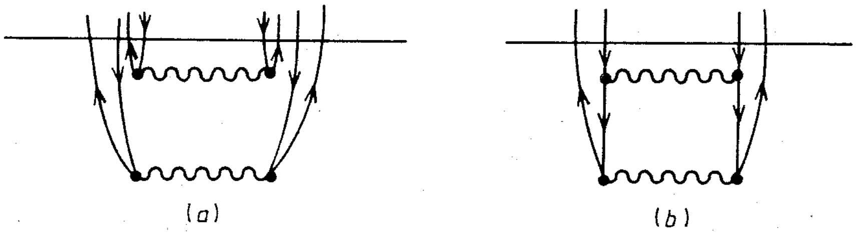


Figure 21.11 *In example (*a*), no contractions appear which directly connect the two interaction lines, whereas the result of the contractions in (*b*) is to eliminate one particle and one hole line.*

As an example, we will now calculate the contribution of the family of ring diagrams of third order shown in figure 21.5. As a representative of the family we choose the diagram in figure 21.12, for which

$$\begin{aligned}(\Delta_3 + \Delta_2) &= \epsilon_j + \epsilon_k - \epsilon_m - \epsilon_n \\ \Delta_3 &= \epsilon_j + \epsilon_p - \epsilon_m - \epsilon_r .\end{aligned}$$

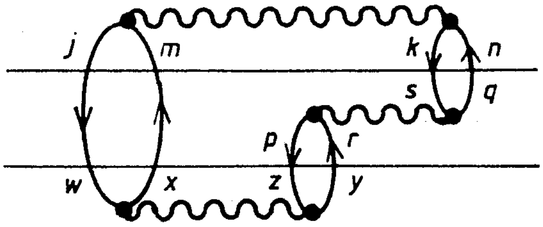


Figure 21.12 *We choose the following indexing for our representative third-order ring diagram.*

The energy shift from this diagram is

$$
\begin{aligned}
(\Delta E)^{(3)}_{\text{ring}} & \\
&= (-)^{3+3} \sum_{\substack{mxnqry:\epsilon>\epsilon_F \\ jwkspz:\epsilon<\epsilon_F}} \frac{\langle jk \mid v \mid mn\rangle\langle pq \mid v \mid rs\rangle\langle xy \mid v \mid wz\rangle}{\Delta_3(\Delta_3+\Delta_2)} \\
&\qquad \times \delta_{jw}\delta_{mx}\delta_{pz}\delta_{ry}\delta_{ks}\delta_{nq} \\
&= \sum_{\substack{mnr:\epsilon>\epsilon_F \\ jkp:\epsilon<\epsilon_F}} \frac{\langle jk \mid v \mid mn\rangle\langle pn \mid v \mid rk\rangle\langle mr \mid v \mid jp\rangle}{(\epsilon_j+\epsilon_k-\epsilon_m-\epsilon_n)(\epsilon_j+\epsilon_p-\epsilon_m\epsilon_r)}.
\end{aligned}
$$

With the help of the above representation of the denominator, it is easy to see that none of these factors can vanish: since all hole energies ϵ_h satisfy $\epsilon_h < \epsilon_F$, and all particle energies ϵ_p satisfy $\epsilon_p > \epsilon_F$, we must have $\sum \epsilon_h - \sum \epsilon_p \neq 0$. The value zero can be obtained at the most for disconnected diagrams, as shown in figure 21.13. But the disconnected diagrams were already summed out by the linked-cluster theorem.

The factors that appear in the denominators can clearly be interpreted as excitation energies of intermediate states, *e.g.*,

$$\Delta_n = \epsilon_{h_1} + \epsilon_{h_2} - \epsilon_{p_1} - \epsilon_{p_2} \equiv W_0 - W_1$$

where the W_i are energies of the unperturbed system. W_0 corresponds to the ground state, whereas the intermediate state with energy W_1 is obtained by occupying the levels p_1 and p_2 with energies above ϵ_F instead of the levels h_1 and h_2, which are occupied in the ground state:

$$W_1 = W_0 - \epsilon_{h_1} - \epsilon_{h_2} + \epsilon_{p_1} + \epsilon_{p_3}.$$

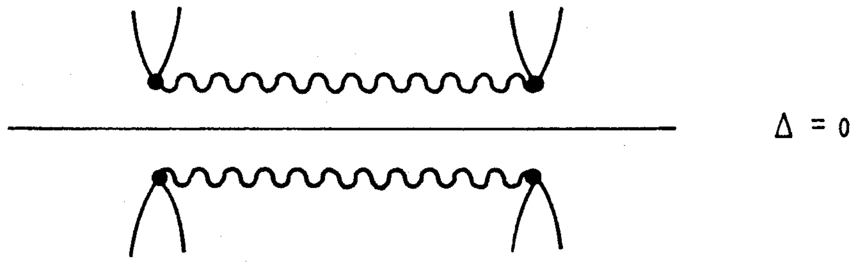


Figure 21.13 *The contribution to the energy shift can be zero only for disconnected diagrams.*

Similarly, we obtain for the other factors

$$\Delta_n + \Delta_{n-1} + \ldots + \Delta_{n-j+1} = \sum_h \epsilon_h^{(j)} - \sum_p \epsilon_p^{(j)} = W_0 - W_j$$

where

$$W_j = W_0 - \sum_h \epsilon_h^{(j)} + \sum_p \epsilon_p^{(p)}. \tag{21.12}$$

Since none of the factors is zero, the ground state itself can never appear as an intermediate state. The energy shift from a family of topologically equivalent diagrams g can then be written as

$$(\Delta E)_g^{(n)} = \frac{(-)^{\ell+h}}{2^s} \sum \frac{\langle v\rangle \ldots \langle v\rangle \prod \delta_{\alpha\beta}}{(W_0 - W_1)(W_0 - W_2)\ldots(W_0 - W_{n-1})}. \tag{21.13}$$

To further interpret this formula, we derive yet another equation for the energy shift. We start with the representation

$$\begin{aligned}\Delta E &= \lim_{\epsilon\to 0} i\frac{\partial}{\partial t}\langle \Phi_0 \mid U_\epsilon(t, -\infty) \mid \Phi_0\rangle_L \Big|_{t=0} \\ &= \sum_{n=0}^{\infty} \lim_{\epsilon\to 0} i\frac{\partial}{\partial t}\langle \Phi_0 \mid U_\epsilon^{(n)}(t, -\infty) \mid \Phi_0\rangle_L \Big|_{t=0}.\end{aligned}$$

Furthermore, we use

$$\begin{aligned}&\langle \Phi_0 \mid U_\epsilon^{(n)}(t, -\infty) \mid \Phi_0\rangle_L \\ &= \langle \Phi_0 \mid (-i)^n \int_{-\infty}^{t} \mathrm{d}t_1 \int_{-\infty}^{t_1} \ldots \\ &\quad \times \int_{-\infty}^{t_{n-1}} \mathrm{d}t_n \, \mathrm{e}^{-\epsilon(|t_1|+\ldots)} v(t_1)_I \ldots v(t_n)_I \mid \Phi_0\rangle_L.\end{aligned}$$

Since $0 > t > t_1 > \ldots > t_n$, we have

$$\mathrm{e}^{-\epsilon(|t_1|+\ldots+|t_n|)} = \mathrm{e}^{\epsilon(t_1+\ldots+t_n)}$$

so that we can write

$$\begin{aligned}
&\langle \Phi_0 \mid U_\epsilon^{(n)}(t,-\infty) \mid \Phi_0 \rangle_L \\
&\quad = \langle \Phi_0 \mid (-i)^n \int_{-\infty}^{t} \mathrm{d}t_1\, \mathrm{e}^{\epsilon t_1} v(t_1)_I \int_{-\infty}^{t_1} \mathrm{d}t_2\, \mathrm{e}^{\epsilon t_2} v(t_2)_I \ldots \\
&\qquad \times \int_{-\infty}^{t_{n-1}} \mathrm{d}t_n\, \mathrm{e}^{\epsilon t_n} v(t_n)_I \mid \Phi_0 \rangle_L .
\end{aligned}$$

In contrast to our earlier derivation, we will now perform the time integration at the operator level. For the last factor, we obtain

$$\begin{aligned}
&\int_{-\infty}^{t_{n-1}} \mathrm{d}t_n\, \mathrm{e}^{\epsilon t_n} v(t_n)_I \mid \Phi_0 \rangle \\
&\quad = \int_{-\infty}^{t_{n-1}} \mathrm{d}t_n\, \mathrm{e}^{(\epsilon+iH_0)t_n} v_S \underbrace{\mathrm{e}^{-iH_0 t_n} \mid \Phi_0 \rangle}_{\mathrm{e}^{-iW_0 t_n}|\Phi_0\rangle} \\
&\quad = \int_{-\infty}^{t_{n-1}} \mathrm{d}t_n\, \mathrm{e}^{[\epsilon+i(H_0-W_0)]t_n} v_S \mid \Phi_0 \rangle \\
&\quad = \frac{\mathrm{e}^{[\epsilon+i(H_0-W_0)]t_{n-1}}}{\epsilon + i(H_0 - W_0)} v_S \mid \Phi_0 \rangle \\
&\quad = \frac{\mathrm{e}^{[\epsilon+i(H_0-W_0)]t_{n-1}}}{\epsilon - i(W_0 - H_0)} v_S \mid \Phi_0 \rangle .
\end{aligned}$$

If we add the next factor to this, we obtain

$$\begin{aligned}
&\int_{-\infty}^{t_{n-2}} \mathrm{d}t_{n-1}\, \mathrm{e}^{\epsilon t_{n-1}} v(t_{n-1})_I \int_{-\infty}^{t_{n-1}} \mathrm{d}t_n\, \mathrm{e}^{\epsilon t_n} v(t_n)_I \mid \Phi_0 \rangle \\
&= \int_{-\infty}^{t_{n-2}} \mathrm{d}t_{n-1}\, \mathrm{e}^{(\epsilon+iH_0)t_{n-1}} v_S \mathrm{e}^{-iH_0 t_{n-1}} \frac{\mathrm{e}^{(\epsilon+iH_0-iW_0)t_{n-1}}}{\epsilon - i(W_0 - H_0)} v_S \mid \Phi_0 \rangle \\
&= \int_{-\infty}^{t_{n-2}} \mathrm{d}t_{n-1}\, \mathrm{e}^{2\epsilon+i(H_0-W_0)]t_{n-1}} v_S \frac{1}{\epsilon - i(W_0 - H_0)} v_S \mid \Phi_0 \rangle \\
&= \mathrm{e}^{[2\epsilon+i(H_0-W_0)]t_{n-2}} \frac{1}{2\epsilon - i(W_0 - H_0)} v_S \frac{1}{\epsilon - i(W_0 - H_0)} v_S \mid \Phi_0 \rangle .
\end{aligned}$$

The $(n-1)$-fold repetition of this procedure finally leads to

$$\begin{aligned}
& i\frac{\partial}{\partial t}\left.\langle\Phi_0 \mid U_\epsilon^{(n)}(t,-\infty) \mid \Phi_0\rangle_L\right|_{t=0} \\
&= (-i)^{(n-1)}\langle\Phi_0 \mid \underbrace{v(0)_I}_{=v_S}\int_{-\infty}^{0} \mathrm{d}t_2\, \mathrm{e}^{\epsilon t_2} v(t_2)_I \int_{-\infty}^{t_2} \mathrm{d}t_3 \ldots \\
&\quad \times \int_{-\infty}^{t_{n-1}} \mathrm{d}t_n\, \mathrm{e}^{\epsilon t_n} v(t_n)_I \mid \Phi_0\rangle_L \\
&= (-i)^{n-1}\langle\Phi_0 \mid v_S \frac{1}{(n-1)\epsilon - i(W_0 - H_0)} v_S \cdots \\
&\quad \times v_S \frac{1}{2\epsilon - i(W_0 - H_0)} v_S \frac{1}{\epsilon - i(W_0 - H_0)} v_S \mid \Phi_0\rangle_L .
\end{aligned}$$

The limit $\epsilon \to 0$ can then be performed with the result

$$\langle\Phi_0 \mid v_S \left(\frac{1}{W_0 - H_0} v_S\right)^{n-1} \mid \Phi_0\rangle_L .$$

If we now insert the completeness relation of the unperturbed eigenfunctions

$$1 = \sum_j \mid \Phi_j\rangle\langle\Phi_j \mid$$

between the potential operator v_S and the factors

$$\left(\frac{1}{W_0 - H_0} v_S\right)$$

a comparison with equation (21.13) shows that the energies W_j belong to the intermediate states. If we compare the result with the Rayleigh–Schrödinger formula

$$\Delta E = \sum_{n=0}^{\infty} \langle\Phi_0 \mid v_S \left(\frac{1}{W_0 - H_0} Q(v_S - \Delta E)\right)^n \mid \Phi_0\rangle$$

the restriction to connected diagrams has the same effect as the projection operator $Q = 1- \mid \Phi_0\rangle\langle\Phi_0 \mid$, namely, to prevent $\mid \Phi_0\rangle$ from appearing as an intermediate state, which would result in a zero denominator.

Chapter 22

An example: the Gell-Mann–Brueckner correlation energy of a dense electron gas

We will in this chapter use the methods discussed in the previous chapters in an important example: the calculation of the correlation energy of an electron gas in the limit of high density, according to Gell-Mann and Brueckner [16]. The interacting electron gas is, according to equation (10.10), described by the Hamiltonian

$$\begin{aligned} H &= \sum_{\mathbf{k}\sigma} \frac{\hbar^2 k^2}{2m} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} \\ &\quad + \frac{1}{2} \sum_{\substack{\mathbf{k}\sigma \\ \mathbf{k}'\sigma'}} \sum_{\mathbf{q}\neq 0} \frac{4\pi e^2}{\Omega q^2} c^\dagger_{(\mathbf{k}+\mathbf{q})\sigma} c^\dagger_{(\mathbf{k}'-\mathbf{q})\sigma'} c_{\mathbf{k}'\sigma'} c_{\mathbf{k}\sigma}. \end{aligned}$$

It is important that the the contribution from $\mathbf{q} = 0$ is explicitly removed from the sum over $\mathbf{q}$, since this Fourier component of the interaction potential is canceled out by the energy contribution from the uniform positive background charge density.

The matrix elements of the interaction have the form shown in figure 22.1, which is

$$\langle (\mathbf{k}+\mathbf{q})\sigma, (\mathbf{k}'-\mathbf{q})\sigma' \mid v \mid \mathbf{k}\sigma, \mathbf{k}'\sigma' \rangle = \frac{4\pi e^2}{\Omega q^2}.$$

This diagram can be interpreted as a momentum-transfer process: the first electron with momentum $\mathbf{k}'$ loses a momentum $\mathbf{q}$, which is transferred to a

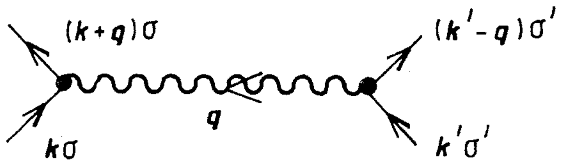


Figure 22.1 *Interaction diagram for the electron gas.*

second electron by the interaction. From this, it follows immediately that the diagrams which contain the part shown in figure 22.2 vanish, since they require $\mathbf{q} = 0$, and this term was omitted from the sum. In consequence,

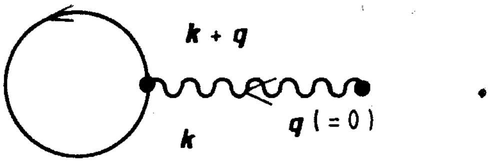


Figure 22.2 *Any diagram, which contains the so-called tadpole diagram, vanishes.*

the direct term in the Hartree–Fock energy, which was discussed earlier, vanishes:

$$(\Delta E)_d^{(1)} = 0. \tag{22.1}$$

In first-order perturbation theory, only the exchange terms represented in figure 22.3 remain. The energy contribution from these is

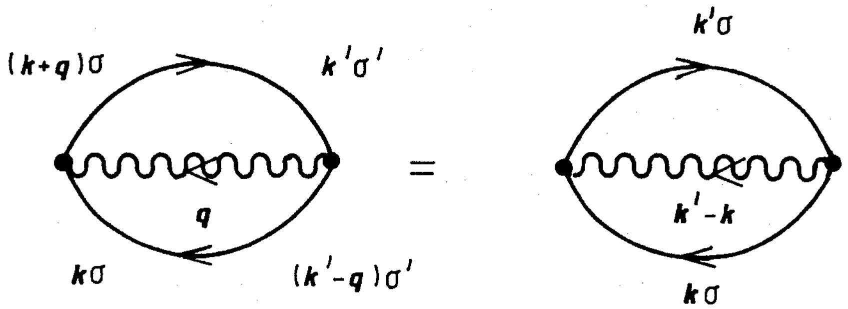


Figure 22.3 *The exchange diagrams of the electron gas.*

$$
\begin{aligned}
(\Delta E)_x^{(1)} &= \underbrace{\frac{(-)^{1+2}}{2^1}}_{\text{symmetric diagram}} \sum_{\mathbf{q}\neq 0} \sum_{\substack{\mathbf{k}\sigma \\ k<k_F}} \sum_{\substack{\mathbf{k}'\sigma' \\ k'<k_F}} \frac{4\pi e^2}{\Omega q^2} \underbrace{\delta_{(\mathbf{k}+\mathbf{q}),\mathbf{k}'}\delta_{\sigma,\sigma'}\delta_{\mathbf{k},(\mathbf{k}'-\mathbf{q})}\delta_{\sigma,\sigma'}}_{\delta_{\mathbf{q},(\mathbf{k}'-\mathbf{k})}\delta_{\sigma,\sigma'}} \\
&= \underbrace{-\frac{1}{2}\sum_{\sigma}}_{=-1} \sum_{\substack{\mathbf{k},\mathbf{k}' \\ \mathbf{k}\neq\mathbf{k}'}} \frac{4\pi e^2}{\Omega|\mathbf{k}-\mathbf{k}'|^2} \qquad (22.2) \\
&= \text{exchange energy as in Chapter 10.} \qquad (22.3)
\end{aligned}
$$

Here, both propagator lines are equal-time lines, *i.e.*, hole lines with $k, k' < k_F$, according to Feynman rule (4).

All higher-order diagrams which contain the elements in figure 22.4 also vanish, because $\delta_{(\mathbf{k}+\mathbf{q}),\mathbf{k}'} = \delta_{\mathbf{q},(\mathbf{k}'-\mathbf{k})}$ in the $G^{(0)}$-line above, from which we obtain the indices shown in figure 22.5. However, this cannot occur since one of the free lines corresponds to a hole (sum over $k < k_F$), and the other to a particle (sum over $k > k_F$), *i.e.*, their momenta cannot be equal. Therefore, the diagrams vanish. However, diagrams which contain the factors shown in figure 22.6 can appear. We have already encountered such diagrams as first-order contributions to the single-particle Green's function. In a connected diagram of second order for the vacuum amplitude of the electron gas, the bottom and top parts can only look like figure 22.7. When

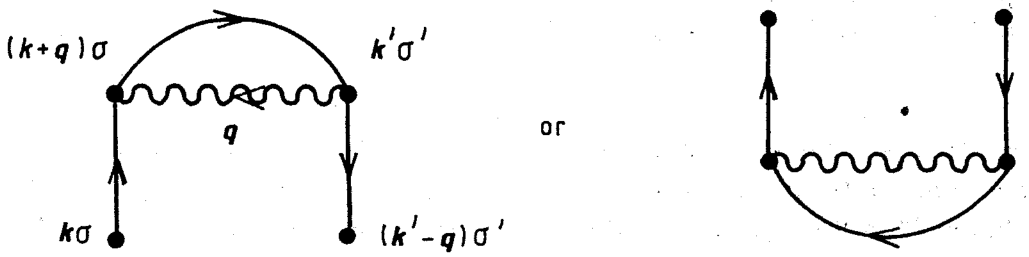


Figure 22.4 *Diagrams which contain these parts as factors also vanish.*

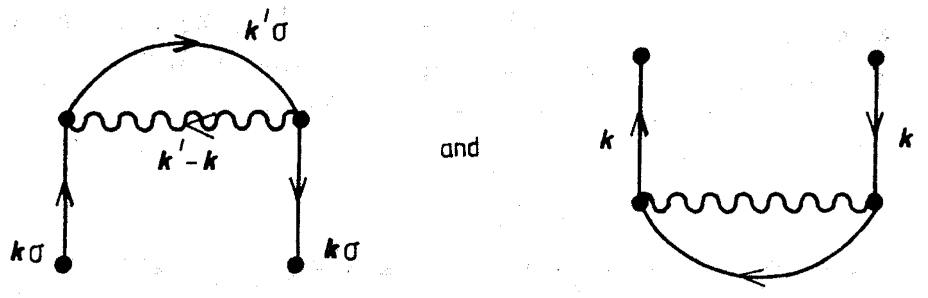


Figure 22.5 *Labeling of the $G^{(0)}$-lines in figure 22.4.*

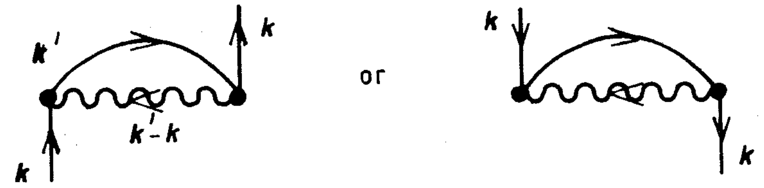


Figure 22.6 *Diagrams with these factors may give non-vanishing contributions.*

Figure 22.7 *Connected second-order diagrams for the vacuum amplitude can only have these bottom and top parts.*

these two are taken into account, of the 24 diagrams of second order, which were constructed in Chapter 20, only the four connected diagrams shown in figure 22.8 remain, and of these, only two are topologically distinct. We now label these according to figure 22.9, taking into account the momentum conservation. We eliminate $\mathbf{k}_1'$, $\mathbf{k}_2'$ and $\mathbf{q}$ by considering the unperturbed single-particle Green's functions labeled by the numbers 1 through 4:

$$
\begin{array}{lll}
1: & \delta_{\mathbf{k}_1',\mathbf{k}_1-\mathbf{q}}\delta_{\sigma_1'\sigma_1} & \Rightarrow \quad \mathbf{k}_1' = \mathbf{k}_1 - \mathbf{q} \\
2: & \delta_{\mathbf{k}_2,\mathbf{k}_1'-\mathbf{q}'}\delta_{\sigma_2\sigma_1'} & \Rightarrow \quad \mathbf{q}' = \mathbf{k}_1' - \mathbf{k}_2 = \mathbf{k}_1 - \mathbf{k}_2 - \mathbf{q} \\
3: & \delta_{\mathbf{k}_1,\mathbf{k}_2'+\mathbf{q}'}\delta_{\sigma_1\sigma_2'} & \Rightarrow \quad \mathbf{k}_2' = \mathbf{k}_1 - \mathbf{q}' = \mathbf{k}_1 - \mathbf{k}_1 + \mathbf{k}_2 + \mathbf{q} = \mathbf{k}_2 + \mathbf{q} \\
4: & \delta_{\mathbf{k}_2',\mathbf{k}_2+\mathbf{q}}\delta_{\sigma_2\sigma_2'} & \Rightarrow \quad \mathbf{k}_2' = \mathbf{k}_2 + \mathbf{q} \quad \text{consistent with 3} \\
 & & \Rightarrow \quad \sigma_1 = \sigma_1' = \sigma_2 = \sigma_2' \equiv \sigma
\end{array}
$$

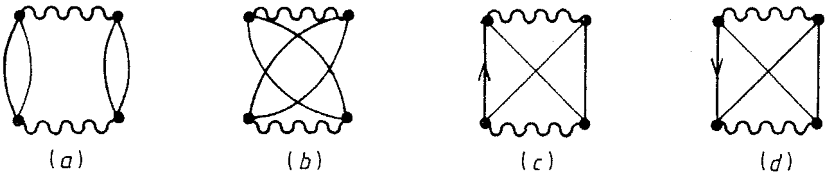


Figure 22.8 *The only connected second-order diagrams for the vacuum amplitude. The diagrams* (a) *and* (b), *and* (c) *and* (d) *are topologically equivalent.*

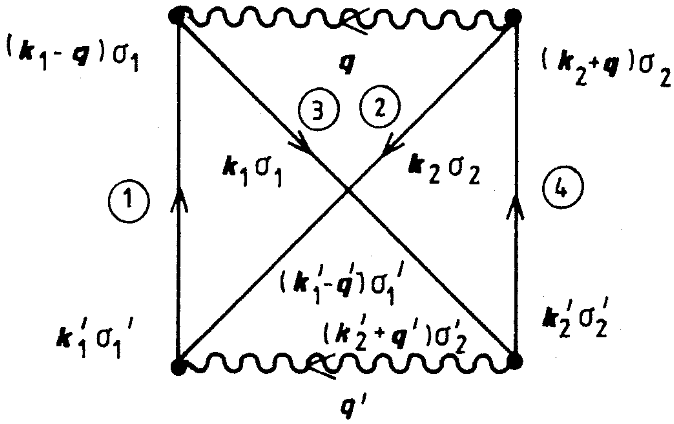


Figure 22.9 *Labeling of the diagrams in figure 22.8.*

Thus, we obtain indexing shown in figure 22.10. We also obtain

$$\begin{aligned}\Delta_2 &= \frac{1}{2m}\left\{k_1^2+k_2^2-(\mathbf{k}_1-\mathbf{q})^2-(\mathbf{k}_2+\mathbf{q})^2\right\} \\ &= \frac{1}{2m}\left\{k_1^2-k_1^2+k_2^2-k_2^2+2\mathbf{q}\cdot(\mathbf{k}_1-\mathbf{k}_2+\mathbf{q})\right\} \\ &= \frac{1}{m}\mathbf{q}\cdot(\mathbf{k}_1-\mathbf{k}_2-\mathbf{q}).\end{aligned}$$

This is a 'safe method', where the momentum conservation at each vertex

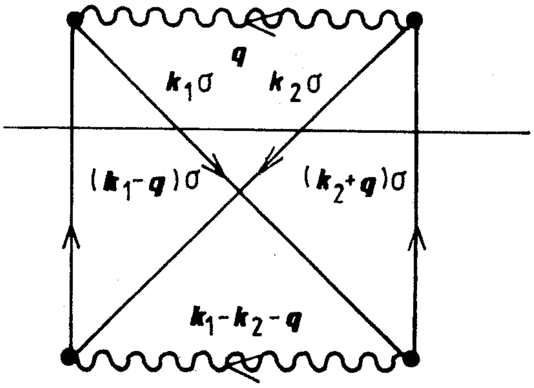


Figure 22.10 *Momentum conservation simplifies the indexing of figure 22.9.*

is taken into consideration. This method should be used for complicated diagrams and, in particular, in doubtful cases where it is not immediately clear if momentum conservation can be satisfied. In the case of simpler diagrams, the correct labeling can be found by inspection; see, for example, figure 22.11. In this figure

$$\begin{aligned}\Delta_2 &= \frac{1}{2m}\left\{k_1^2 + k_2^2 - (\mathbf{k}_1 + \mathbf{q})^2 - (\mathbf{k}_2 - \mathbf{q})^2\right\} \\ &= \frac{1}{m}\mathbf{q}\cdot(\mathbf{k}_2 - \mathbf{k}_1 - \mathbf{q}).\end{aligned}$$

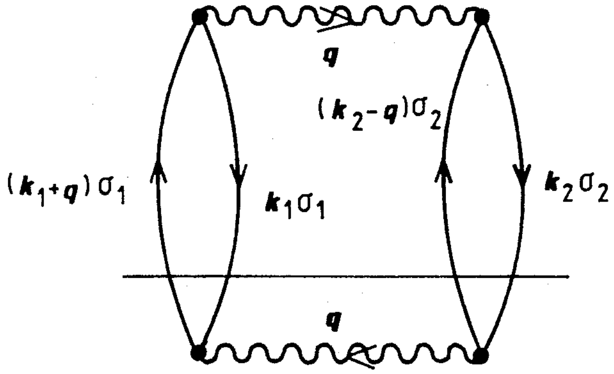


Figure 22.11 *In a diagram such as this one, it is straightforward to label the lines.*

We will now as an exercise label the ring diagram of third order in figure 22.12. A ring diagram is a diagram which is an uninterrupted sequence of interaction lines and particle–hole 'bubbles'. This example illustrates an important property of ring diagrams: the *same* momentum transfer **q** appears in all interaction lines.

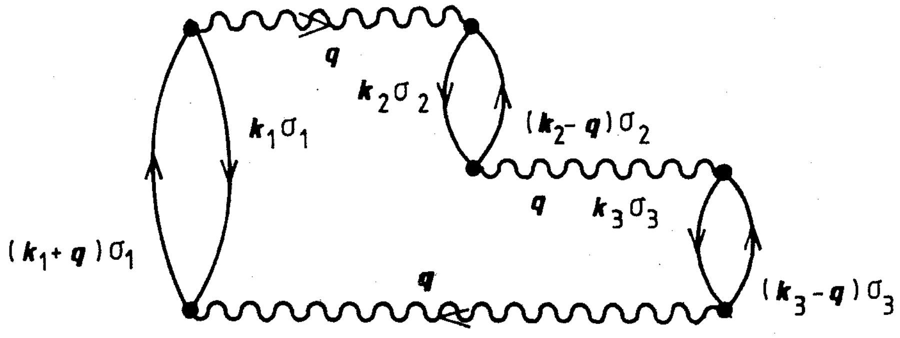


Figure 22.12 *A ring diagram only contains interaction lines and particle–hole 'bubbles'.*

Let us now calculate the energy contribution of the two topologically equivalent diagrams figure 22.8 (c) and 22.8 (d), according to equation (21.11):

$$
\begin{aligned}
&(\Delta E)^{(2)}_{(c)}\\
&\quad= \underbrace{(-)^3\frac{1}{2^1}\sum_{\sigma}}_{=-1}\sum_{\mathbf{q}\neq 0}\\
&\quad\times \sum_{\substack{k_1,k_2<k_F\\ |\mathbf{k}_1-\mathbf{q}|,|\mathbf{k}_2+\mathbf{q}|>k_F}} \left(\frac{4\pi e^2}{\Omega}\right)^2 \frac{1}{q^2}\,\frac{1}{|\mathbf{k}_1-\mathbf{k}_2-\mathbf{q}|^2}\,\frac{m}{\mathbf{q}\cdot(\mathbf{k}_1-\mathbf{k}_2-\mathbf{q})}.
\end{aligned}
$$

We go to the continuum limit

$$\frac{1}{\Omega}\sum_{\mathbf{k}} \to \frac{1}{(2\pi)^3}\int \mathrm{d}^3k$$

with the result

$$
\begin{aligned}
&(\Delta E)^{(2)}_{(c)}\\
&\quad= -16\pi^2 e^4 m\frac{\Omega}{(2\pi)^9}\int \mathrm{d}^3q\int \mathrm{d}^3k_1\int \mathrm{d}^3k_2\\
&\qquad\times\frac{1}{|\mathbf{k}_1-\mathbf{k}_2-\mathbf{q}|^2 q^2\left[\mathbf{q}\cdot(\mathbf{k}_1-\mathbf{k}_2-\mathbf{q})\right]}.
\end{aligned}
$$

and scale the variables by k_F

$$\mathbf{q}^{\text{new}} \equiv \frac{\mathbf{q}^{\text{old}}}{k_F}\quad \mathbf{k}_1^{\text{new}} \equiv \frac{\mathbf{k}_1^{\text{old}}}{k_F}\quad \mathbf{k}_2^{\text{new}} \equiv \frac{\mathbf{k}_2^{\text{old}}}{k_F}$$

which yields for $(\Delta E)^{(2)}_{(c)}$:

$$-\Omega\frac{e^4 m}{32\pi^7}k_F^3\int \mathrm{d}^3q\int \mathrm{d}^3k_1\int \mathrm{d}^3k_2\,\frac{1}{|\mathbf{k}_1-\mathbf{k}_2-\mathbf{q}|^2 q^2\left[\mathbf{q}\cdot(\mathbf{k}_1-\mathbf{k}_2-\mathbf{q})\right]}.$$

The integrations are to be performed over the regions

$$|\mathbf{k}_1|,|\mathbf{k}_2|<1\qquad |\mathbf{k}_1-\mathbf{q}|,|\mathbf{k}_2+\mathbf{q}|>1.$$

If we use

$$3\pi^2\left(\frac{N}{\Omega}\right)=k_F^3$$

and also make the substitutions

$$\mathbf{q}\to-\mathbf{q}\qquad \mathbf{k}_2\to-\mathbf{k}_2$$

and take into consideration that (with $\hbar\equiv 1$)

$$\frac{1}{2}e^4 m = 1\ \mathrm{Ry}$$

we obtain

$$(\Delta E)^{(2)}_{(c)} = +\frac{3N}{16\pi^5}\int\frac{\mathrm{d}^3q}{q^2}\int\mathrm{d}^3k_1\int\mathrm{d}^3k_2\,\frac{1}{|\mathbf{k}_1+\mathbf{k}_2+\mathbf{q}|^2}\frac{1}{\mathbf{q}\cdot(\mathbf{k}_1+\mathbf{k}_2+\mathbf{q})}\ \mathrm{Ry} \tag{22.4}$$

where $|\mathbf{k}_1|, |\mathbf{k}_2| < 1 < |\mathbf{k}_1+\mathbf{q}|, |\mathbf{k}_2+\mathbf{q}|$. The resulting expression can be integrated analytically [17], with the result

$$\begin{aligned}(\Delta E)^{(2)}_{(c)} &= \left[\frac{1}{3}\ln 2-\frac{3}{2\pi^2}\zeta(3)\right]N\ \mathrm{Ry}\\ &= 0.0484N\ \mathrm{Ry}.\end{aligned} \tag{22.5}$$

Here, $\zeta(3)$ is the Riemann zeta-function

$$\zeta(3)=\frac{1}{2}\int_0^\infty\frac{t^2\mathrm{d}t}{e^t-1}.$$

The important conclusion is that this energy contribution does not depend on k_F. Hence, it does not depend on the 'average atomic radius' r_s introduced earlier (*cf.* equation (10.6)):

$$\frac{1}{k_F}=\left[\frac{1}{3\pi^2}\left(\frac{\Omega}{N}\right)\right]^{1/3}=\left[\frac{1}{3\pi^2}\frac{4}{3}\pi r_s^3\right]^{1/3}=\left[\frac{4}{9\pi}\right]^{1/3}r_s. \tag{22.6}$$

We now calculate the other second-order energy contribution (the diagrams figure 22.8 (*a*) and (*b*)):

$$(\Delta E)^{(2)}_{(a)} = \underbrace{\frac{(-)^{2+2}}{2^1}\sum_{\sigma_1}\sum_{\sigma_2}}_{=2}\sum_{\mathbf{q}\neq 0}\sum_{\substack{k_1,k_2<k_F\\ |\mathbf{k}_1+\mathbf{q}|,|\mathbf{k}_2-\mathbf{q}|>k_F}}\left[\frac{4\pi e^2}{\Omega}\right]^2\frac{1}{q^4}\frac{m}{\mathbf{q}\cdot(\mathbf{k}_2-\mathbf{k}_1-\mathbf{q})}.$$

By going to the continuum limit and by making the substitutions

$$\mathbf{q}^{\text{new}}=-\mathbf{q}^{\text{old}}/k_F\ \mathbf{k}_1^{\text{new}}=-\mathbf{k}_1^{\text{old}}/k_F\ \mathbf{k}_2^{\text{new}}=\mathbf{k}_2^{\text{old}}/k_F$$

we obtain, analogously with $(\Delta E)^2_{(c)}$

$$(\Delta E)^{(2)}_{(a)}=-\frac{3N}{8\pi^5}\int\frac{\mathrm{d}^3q}{q^4}\int\mathrm{d}^3k_1\int\mathrm{d}^3k_2\,\frac{1}{\mathbf{q}\cdot(\mathbf{k}_1+\mathbf{k}_2+\mathbf{q})}\ \mathrm{Ry}. \tag{22.7}$$

Here, the integrals are performed over the region $k_1, k_2 < k_F$; $|\mathbf{k}_1+\mathbf{q}|, |\mathbf{k}_2+\mathbf{q}| > k_F$. This term, too, is independent of r_s. We will now proceed to show that the resulting integral diverges. Thus, we will prove the statement made in Chapter 10, that second-order perturbation theory diverges for the electron gas.

We consider the integral for $q \to 0$ and introduce the notation

$$x_i = \cos\sphericalangle(\mathbf{k}_i, \mathbf{q}) = \mathbf{k}_i \cdot \mathbf{q}/(k_i q) \quad i = 1, 2.$$

The integration region $|\mathbf{k}_i| < 1 < |\mathbf{k}_i + \mathbf{q}|$ of the $\mathbf{k}$-integrations becomes $1 - qx_i < k_i < 1$ for small q, since

$$\begin{aligned} |\mathbf{k} + \mathbf{q}| &= \sqrt{k^2 + 2kqx + q^2} = k\sqrt{1 + 2qx/k + q^2/k^2} \\ &= k\left[1 + \frac{qx}{k} + \mathrm{O}(q^2)\right] \approx k + qx. \end{aligned}$$

In the integral

$$I(q) = \int \mathrm{d}^3k_1 \int \mathrm{d}^3k_2 \, \frac{1}{\mathbf{q} \cdot (\mathbf{k}_1 + \mathbf{k}_2 + \mathbf{q})},$$

we take the z-axis parallel to $\mathbf{q}$, which leads to

$$I(q) = \int_0^1 2\pi \, \mathrm{d}x_1 \int_{1-qx_1}^1 k_1^2 \, \mathrm{d}k_1 \int_0^1 2\pi \, \mathrm{d}x_2 \int_{1-qx_2}^1 k_2^2 \, \mathrm{d}k_2 \, \frac{1}{qk_1x_1 + qk_2x_2 + q^2}$$

and, finally, by using the estimate above that $k_i = 1 + \mathrm{O}(q)$ and neglecting terms of order q^2, we arrive at

$$\begin{aligned} I(q) &= 4\pi^2 \int_0^1 \mathrm{d}x_1 \int_0^1 \mathrm{d}x_2 \int_{1-qx_1}^1 \mathrm{d}k_1 \int_{1-qx_2}^1 \mathrm{d}k_2 \, \frac{k_1^2 k_2^2}{q(x_1 + x_2)} \\ &= \frac{4\pi^2}{9} \int_0^1 \mathrm{d}x_1 \int_0^1 \mathrm{d}x_2 \frac{\left[1 - (1 - qx_1)^3\right]\left[1 - (1 - qx_2)^3\right]}{q(x_1 + x_2)} \\ &= \frac{4\pi^2}{9} \int_0^1 \mathrm{d}x_1 \int_0^1 \mathrm{d}x_2 \left\{ \frac{q^2}{q} \left[\frac{3x_1 3x_2}{x_1 + x_2}\right] + \frac{\mathrm{O}(q^3)}{q} \right\} \\ &= \frac{8\pi^2}{3} (1 - \ln 2)\, q + \mathrm{O}(q^2). \end{aligned}$$

It remains to perform the $\mathbf{q}$-integration:

$$(\Delta E)^{(2)}_{(a)} = -\frac{3N}{8\pi^5} \int_0^\infty \frac{I(q)}{q^4} 4\pi q^2 \, \mathrm{d}q \approx -\frac{4N}{\pi^2} \int_0^\infty \frac{\mathrm{d}q}{q}. \qquad (22.8)$$

This integral diverges at the lower limit.

At the upper limit of the integration, *i.e.*, for $q \to \infty$, our estimate does not hold. However, a glance at the term q^4 in the denominator of the original integral shows that no problem arises at the upper limit.

Let us look at what happens in third-order perturbation theory. Consider the third-order ring diagram shown in figure 22.13, with

$$\begin{aligned}\Delta_3+\Delta_2 &= \frac{1}{m}\mathbf{q}\cdot(\mathbf{k}_2-\mathbf{k}_1-\mathbf{q})\\ \Delta_3 &= \frac{1}{2m}\left[k_1^2+k_3^2-(\mathbf{k}_1+\mathbf{q})^2-(\mathbf{k}_3-\mathbf{q})^2\right]\\ &= \frac{1}{m}\mathbf{q}\cdot(\mathbf{k}_3-\mathbf{k}_1-\mathbf{q}).\end{aligned}$$

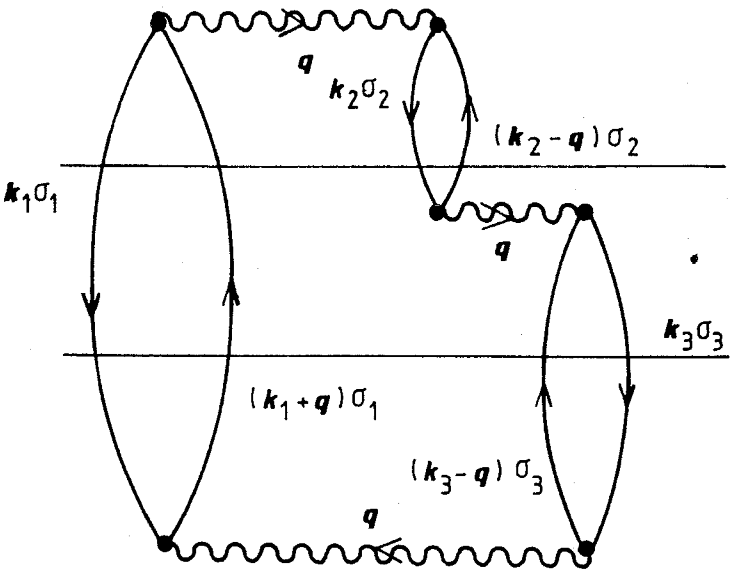


Figure 22.13 *A third-order ring diagram.*

The energy contribution is

$$(\Delta E)^{(3)}_{\text{ring}} = \underbrace{\frac{(-)^{3+3}}{2^0}\sum_{\sigma_1}\sum_{\sigma_2}\sum_{\sigma_3}}_{=8} \times \sum_{\substack{|\mathbf{k}_1|<k_F<|\mathbf{k}_1+\mathbf{q}|\\ |\mathbf{k}_2|<k_F<|\mathbf{k}_2-\mathbf{q}|\\ |\mathbf{k}_3|<k_F<|\mathbf{k}_3-\mathbf{q}|}} \frac{(4\pi e^2/\Omega)^3}{q^6}\,\frac{m}{\mathbf{q}\cdot(\mathbf{k}_2-\mathbf{k}_1-\mathbf{q})}\,\frac{m}{\mathbf{q}\cdot(\mathbf{k}_3-\mathbf{k}_1-\mathbf{q})}.$$

By now, it is clear how to proceed from here: we go over to the continuum limit, scale the wavevectors by k_F, change the signs of $\mathbf{k}_1$ and $\mathbf{q}$ to obtain

$$(\Delta E)^{(3)}_{\text{ring}} = \frac{3N}{4\pi^7 k_F}\,\text{Ry} \tag{22.9}$$

$$\times \int \frac{\mathrm{d}^3 q}{q^6} \underbrace{\int\int\int \mathrm{d}^3k_1 \mathrm{d}^3k_2 \mathrm{d}^3k_3 \frac{1}{[\mathbf{q}\cdot(\mathbf{k}_1+\mathbf{k}_2+\mathbf{q})]\,[\mathbf{q}\cdot(\mathbf{k}_1+\mathbf{k}_3+\mathbf{q})]}}_{\equiv I(q)} \tag{22.10}$$

with the usual integration limits

$$|\mathbf{k}_i| < 1 < |\mathbf{k}_i + \mathbf{q}| \quad i = 1, 2, 3.$$

We can establish the following important facts:

(1) The total expression is proportional to r_s, due to the factor of $1/k_F$ (*cf.* equation (22.6)).

(2) It is easy to establish that $I(q)$ goes linearly to zero as $q \to 0$, by using the scheme above. This means that the third-order ring diagram diverges strongly at the lower limit:

$$(\Delta E)^{(3)}_{\text{ring}} \sim \int_0 \frac{\mathrm{d}q}{q^3}.$$

In complete analogy, we obtain

$$(\Delta E)^{(n)}_{\text{ring}} \sim \int_0 \frac{\mathrm{d}q}{q^{2n-3}}. \tag{22.11}$$

The r_s-dependence is easy to determine for an arbitrary energy contribution, irrespectively whether or not it is a ring diagram. We have already established that all contributions of second order are independent of r_s. For each *additional* order, we obtain

- a matrix element $\langle \ | v | \ \rangle = 4\pi e^2/(\Omega k^2)$, *i.e.*, a factor of k_F^{-2};
- a factor $(\Delta + \ldots + \Delta) \sim k^2$ in the denominator, *i.e.*, another factor of k_F^{-2};
- a sum $\sum_{\mathbf{k}}$, which after the replacement $\frac{1}{\Omega}\sum_{\mathbf{k}} \to \int \mathrm{d}^3k$ and scaling by k_F, $\mathbf{k}^{\text{new}} \equiv \mathbf{k}^{\text{old}}/k_F$, gives a factor of k_F^3.

Thus, an additional factor of k_F^{-1}, or rather a factor r_s^{+1}, appears for each order:

$$(\Delta E)^{(n)}_{\text{ring}} \sim r_s^{n-2}. \tag{22.12}$$

Our goal is to calculate the energy for high densities, *i.e.*, for $r_s \to 0$. If the individual energy terms $(\Delta E)^{(n)}$ did not diverge, this would be straightforward (provided the perturbation theory would converge); we would simply take the constant second-order term and eventually also include a higher-order correction. However, we must consider the divergence in detail: since the total correlation energy must be finite, we can assume that by summing up all terms, the divergence will be removed. Thus, the task will be to obtain a sensible limit value of such a series of divergent terms. It is clear what happens physically: the electrons screen themselves, so that the long range of the interaction, *i.e.*, the $q \to 0$-contribution, is eliminated. The ring diagrams have the strongest divergences in each order. It is then natural to sum these dominant contributions in each order:

$$\Delta E^{(n)} \approx (\Delta E)^{(n)}_{\text{ring}} = \int_0 \frac{\mathrm{d}q}{q^{2n-3}} I_{n,1}(q) \quad \text{where } \lim_{q\to 0} I_{n,1}(q) = \text{constant}.$$

This procedure seems plausible. However, we must be aware that there are divergent diagrams other than the ring diagrams, for example the third-order diagram shown in figure 22.14. Because of the two identical momentum transfers, this diagram is as divergent as the second-order ring diagram, and it is not at all obvious that this diagram can be omitted, but that the diagram figure 22.10 (a) must be included.

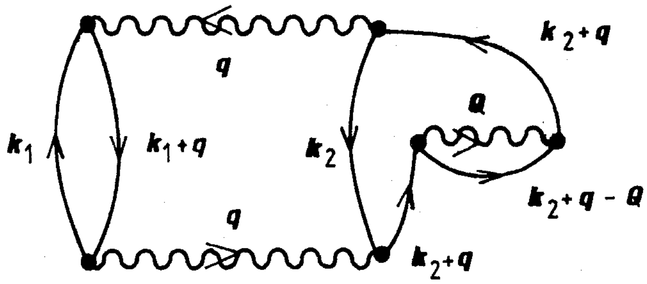


Figure 22.14 *A third-order ring diagram which is not maximally divergent.*

In total, the perturbation series can be written in the following way:

$$\begin{aligned}
\Delta E^{(2)} &= \int_0 \frac{\mathrm{d}q}{q} I_{2,1}(q) + \int_0 q I_{2,2}(q) dq \\
\Delta E^{(3)} &= \left[\int_0 \frac{\mathrm{d}q}{q^3} I_{3,1}(q) + \int_0 \frac{\mathrm{d}q}{q} I_{3,2}(q) + \int_0 q I_{3,3}(q) \mathrm{d}q\right] r_s \\
\Delta E^{(4)} &= \left[\int_0 \frac{\mathrm{d}q}{q^5} I_{4,1}(q) + \ldots + \int_0 q I_{4,4}(q)\right] r_s^2 \\
&\vdots \quad \vdots \quad \vdots
\end{aligned}$$

where $\lim_{q\to 0} I_{n,m}(q) = \text{constant}$.

We will now argue why it is necessary only to consider the ring diagrams. The reason why the divergences appear is the long range of the Coulomb potential. However, we may expect that an effective screening-effect appears in the electron gas, so that the Fourier components are only important to a minimal value k_c. Provided k_c is small, this results in

$$\begin{aligned}\int_{k_c} \frac{dq}{q} I_{n,m}(q) &\sim \ln k_c\\ \int_{k_c} \frac{dq}{q^3} I_{n,m}(q) &\sim 1/k_c^2\\ \int_{k_c} \frac{dq}{q^5} I_{n,m}(q) &\sim 1/k_c^4\end{aligned}$$

and so on. If we recall from our discussion of plasmon theory, that the effective screening comes into effect at

$$k_c \sim r_s^{1/2}$$

the expressions that we have already calculated are proportional to $\ln(r_s)$, $1/r_s$, and $1/r_s^2$, respectively. If we insert these into the individual energy contributions, we obtain, together with the explicit r_s-dependences:

$$\begin{aligned}(\Delta E)^{(2)}_{\text{ring}} &\sim \ln r_s\\ (\Delta E)^{(n)}_{\text{ring}} &\sim \text{constant}\\ (\Delta E)^{(2)}_{(c)} &\sim \text{constant}\end{aligned} \tag{22.13}$$

All other contributions go to zero at least as $(r_s \ln r_s)$ as $r_s \to 0$. Therefore, it should be reasonable to put the correlation energy in the following form for high densities:

$$E_{\text{corr}} \approx \sum_{n=2}^{\infty} (\Delta E)^{(n)}_{\text{ring}} + (\Delta E)^{(2)}_{(c)}.$$

We will now start with the summation of all ring diagrams. We first make the following representation of the contributions from the ring diagrams plausible:

$$(\Delta E)^{(n)}_{\text{ring}} = (-)^{n+1} \frac{3N}{8\pi^5} \left[\frac{\alpha r_s}{\pi^2}\right]^{n-2} \int \frac{J_n}{q^{2n}} d^3q \ \text{Ry} \tag{22.14}$$

with

$$\alpha = (4/9\pi)^{1/2}$$

and

$$J_n = \frac{1}{n}\int_{-\infty}^{+\infty} \mathrm{d}t_1 \int_{-\infty}^{+\infty} \mathrm{d}t_2 \ldots \int_{-\infty}^{+\infty} \mathrm{d}t_n \, F_q(t_1)\cdot \ldots \cdot F_q(t_n)\delta(t_1 + \ldots + t_n)$$

and[†]

$$F_q(t) = \int_{|\mathbf{p}|<1<|\mathbf{p}+\mathbf{q}|} \exp\left[-|t|\left(\frac{1}{2}q^2 + \mathbf{q}\cdot\mathbf{p}\right)\right] \mathrm{d}^3p.$$

The statement holds for $n = 2$:

$$\begin{aligned}
J_2 &= \frac{1}{2}\int_{-\infty}^{+\infty} \mathrm{d}t_1 \int_{-\infty}^{+\infty} \mathrm{d}t_2 \, F_q(t_1)F_q(t_2)\delta(t_1+t_2) \\
&= \frac{1}{2}\int_{-\infty}^{+\infty} \mathrm{d}t_1 \, F_q(t_1)F_q(-t_1) = \int_0^{\infty} F_q(t)F_q(-t)\mathrm{d}t \\
&= \int \mathrm{d}^3p_1 \int \mathrm{d}^3p_2 \int_0^{\infty} \mathrm{d}t \, \mathrm{e}^{-t(\mathbf{q}\cdot\mathbf{p}_1)+q^2/2)}\mathrm{e}^{-t(\mathbf{q}\cdot\mathbf{p}_2+q^2/2)} \\
&= \int \mathrm{d}^3p_1 \int \mathrm{d}^3p_2 \left[-\frac{\mathrm{e}^{-t\mathbf{q}\cdot(\mathbf{p}_1+\mathbf{p}_2+\mathbf{q})}}{\mathbf{q}\cdot(\mathbf{p}_1+\mathbf{p}_2+\mathbf{q})}\right]\Bigg|_0^{\infty} \\
&= \int \mathrm{d}^3p_1 \int \mathrm{d}^3p_2 \frac{1}{\mathbf{q}\cdot(\mathbf{p}_1+\mathbf{p}_2+\mathbf{q})}
\end{aligned}$$

(*cf.* equation (22.7)), and for $n = 3$:

$$\begin{aligned}
J_3 &= \frac{1}{3}\int_{-\infty}^{\infty} \mathrm{d}t_1 \int_{-\infty}^{\infty} \mathrm{d}t_2 \int_{-\infty}^{\infty} \mathrm{d}t_3 \, F_q(t_1)F_q(t_2)F_q(t_3)\delta(t_1+t_2+t_3) \\
&= \frac{1}{3}\int_{-\infty}^{\infty} \mathrm{d}t_1 \int_{-\infty}^{\infty} \mathrm{d}t_2 \, F_q(t_1)F_q(t_2)F_q(-t_1-t_2) \\
&= \frac{1}{3}\int \mathrm{d}^3p_1 \int \mathrm{d}^3p_2 \int \mathrm{d}^3p_3 \int_{-\infty}^{\infty} \mathrm{d}t_1 \int_{-\infty}^{\infty} \mathrm{d}t_2 \\
&\quad \times \mathrm{e}^{-|t_1|(\mathbf{q}\cdot\mathbf{p}_1+q^2/2)}\mathrm{e}^{-|t_2|(\mathbf{q}\cdot\mathbf{p}_2+q^2/2)}\mathrm{e}^{-|t_1+t_2|(\mathbf{q}\cdot\mathbf{p}_3+q^2/2)}.
\end{aligned}$$

To evaluate this expression, we partition the integration regions in six pieces:

1) $|t_1| = t_1$, $|t_2| = t_2$, $|t_1+t_2| = t_1+t_2$
2) $|t_1| = t_1$, $|t_2| = -t_2$, $|t_1+t_2| = t_1+t_2$ *i.e.*, $t_1 > |t_2|$
3) $|t_1| = t_1$, $|t_2| = -t_2$, $|t_1+t_2| = -t_1-t_2$ *i.e.*, $t_1 < |t_2|$
4) $|t_1| = -t_1$, $|t_2| = -t_2$, $|t_1+t_2| = -t_1-t_2$
5) $|t_1| = -t_1$, $|t_2| = t_2$, $|t_1+t_2| = -t_1-t_2$ *i.e.*, $t_2 < |t_1|$
6) $|t_1| = -t_1$, $|t_2| = t_2$, $|t_1+t_2| = t_1+t_2$ *i.e.*, $t_2 > |t_1|$.

[†] $F_q(it)$ corresponds to the zero-order polarization propagator $i\Pi^{(0)}(\mathbf{q},t)$, which will be discussed in detail in Chapter 27.

By making the substitutions $t_1 \to -t_1$, $t_2 \to -t_2$, we see that the contributions 1) and 4), the contributions 2) and 5), as well as the contributions 3) and 6) are pairwise identical. Furthermore, we can calculate that, with the abbreviation $D_i \equiv (\mathbf{q} \cdot \mathbf{p}_i + q^2/2)$, we have

$$\begin{aligned}
\text{contribution 1)} &= \int_0^\infty \mathrm{d}t_1 \int_0^\infty \mathrm{d}t_2\, \mathrm{e}^{-t_1 D_1} \mathrm{e}^{-t_2 D_2} \mathrm{e}^{(-t_1-t_2)D_3} \\
&= \int_0^\infty \mathrm{d}t_1 \int_0^\infty \mathrm{d}t_2\, \mathrm{e}^{-t_1(D_1+D_3)} \mathrm{e}^{-t_2(D_2+D_3)} \\
\text{contribution 2)} &= \int_{-\infty}^0 \mathrm{d}t_2 \int_{-t_2}^0 \mathrm{d}t_1\, \mathrm{e}^{-t_1 D_1} \mathrm{e}^{+t_2 D_2} \mathrm{e}^{-(t_1-t_2)D_3} \\
& \quad (t_2^{\text{new}} \equiv -t_2^{\text{old}}\; t_1^{\text{new}} \equiv t_1^{\text{old}} + t_2^{\text{old}}\; t_1^{\text{new}} + t_2^{\text{new}} = t_1^{\text{old}}) \\
&= \int_0^\infty \mathrm{d}t_2 \int_0^\infty \mathrm{d}t_1\, \mathrm{e}^{(-t_1-t_2)D_1} \mathrm{e}^{-t_2 D_2} \mathrm{e}^{-t_1 D_3} \\
&= \int_0^\infty \mathrm{d}t_1 \int_0^\infty \mathrm{d}t_2\, \mathrm{e}^{-t_1(D_1+D_3)} \mathrm{e}^{-t_2(D_2+D_3)}.
\end{aligned}$$

If we also interchange $\mathbf{p}_1 \leftrightarrow \mathbf{p}_3$, so that we interchange $D_1 \leftrightarrow D_3$, we see that

$$\text{contribution 1)} = \text{contribution 2)}.$$

A completely analogous calculations shows that

$$\text{contribution 3)} = \text{contribution 1)}.$$

Thus, the contributions from the six different integrations are equal, and we obtain for J_3 (with the notation of the calculation for contribution 2)):

$$\begin{aligned}
J_3 &= 6\frac{1}{3} \int \mathrm{d}^3 p_1 \int \mathrm{d}^3 p_2 \int \mathrm{d}^3 p_3 \int_0^\infty \mathrm{d}t_1 \int_0^\infty \mathrm{d}t_2\, \mathrm{e}^{-t_1(D_1+D_3)} \mathrm{e}^{-t_2(D_1+D_2)} \\
&= 2 \int \mathrm{d}^3 p_1 \int \mathrm{d}^3 p_2 \int \mathrm{d}^3 p_3 \\
& \quad \times \int_0^\infty \mathrm{d}t_1 \mathrm{e}^{-t_1 \mathbf{q}\cdot(\mathbf{p}_1+\mathbf{p}_3+\mathbf{q})} \int_0^\infty \mathrm{d}t_2 \mathrm{e}^{-t_2 \mathbf{q}\cdot(\mathbf{p}_1+\mathbf{p}_2+\mathbf{q})} \\
&= 2 \int\int\int_{\substack{|\mathbf{p}_i|<1<|\mathbf{p}_i+\mathbf{q}| \\ \text{for } i=1,2,3}} \mathrm{d}^3 p_1 \mathrm{d}^3 p_2 \mathrm{d}^3 p_3 \\
& \quad \times \frac{1}{\mathbf{q}\cdot(\mathbf{p}_1+\mathbf{p}_2+\mathbf{q})} \frac{1}{\mathbf{q}\cdot(\mathbf{p}_1+\mathbf{p}_2+\mathbf{q})}
\end{aligned}$$

in agreement with the expression equation (22.10) that we obtained earlier for $(\Delta E)^{(3)}_{\text{ring}}$.

We will not here further pursue the proof of equation (22.14) for arbitrary n. The correctness of the hypothesis is fairly clear, on the basis of the analogy between the function $F_q(t)$ and the Feynman propagator of quantum field theory (see [16]). However, we should note that in the fourth order, different topologically *non*-equivalent types of ring diagrams start to appear. These lead to new energy denominators. In fourth order, we have for example a contribution from the diagrams shown in figure 22.15:

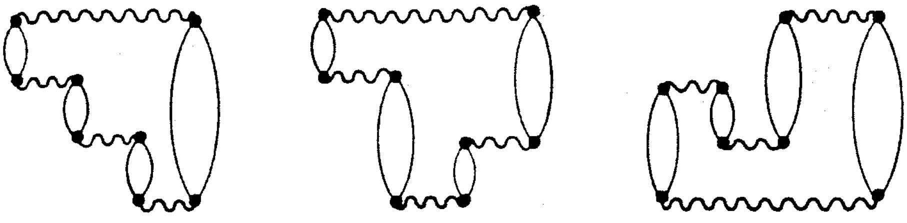


Figure 22.15 *In fourth order, there are topologically non-equivalent diagrams.*

$$
\begin{aligned}
(\Delta E)^{(4)}_{\mathrm{ring}} \\
= & -\frac{3N}{4\pi^5}\left[\frac{\alpha r_s}{\pi^2}\right]^2 \int \frac{\mathrm{d}^3 q}{q^8} \int\int\int\int_{\substack{|\mathbf{p}_i|<1<|\mathbf{p}_i+\mathbf{q}| \\ \text{for } i=1,..,4}} \mathrm{d}^3 p_1 \mathrm{d}^3 p_2 \mathrm{d}^3 p_3 \mathrm{d}^3 p_4 \\
& \times \left[\frac{1}{\mathbf{q}\cdot(\mathbf{p}_1+\mathbf{p}_2+\mathbf{q})}\frac{1}{\mathbf{q}\cdot(\mathbf{p}_1+\mathbf{p}_3+\mathbf{q})}\frac{1}{\mathbf{q}\cdot(\mathbf{p}_1+\mathbf{p}_4+\mathbf{q})}\right. \\
& +\frac{1}{\mathbf{q}\cdot(\mathbf{p}_1+\mathbf{p}_2+\mathbf{q})}\frac{1}{\mathbf{q}\cdot(\mathbf{p}_1+\mathbf{p}_3+\mathbf{q})}\frac{1}{\mathbf{q}\cdot(\mathbf{p}_3+\mathbf{p}_4+\mathbf{q})} \\
& \left.+\frac{1}{\mathbf{q}\cdot(\mathbf{p}_1+\mathbf{p}_2+\mathbf{q})}\frac{1}{\mathbf{q}\cdot(\mathbf{p}_1+\mathbf{p}_2+\mathbf{p}_3+\mathbf{p}_4+2\mathbf{q})}\frac{1}{\mathbf{q}\cdot(\mathbf{p}_1+\mathbf{p}_3+\mathbf{q})}\right].
\end{aligned}
$$

We will hereafter assume that the hypothesis equation (22.14) is correct.

We insert the representation

$$\delta(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{d}u\, \mathrm{e}^{iux} = \frac{q}{2\pi}\int_{-\infty}^{\infty} \mathrm{d}u\, \mathrm{e}^{iqux}$$

in the definition of J_n. This yields

$$
\begin{aligned}
J_n &= \frac{q}{2\pi n}\int_{-\infty}^{+\infty} \mathrm{d}u \int_{-\infty}^{+\infty} \mathrm{d}t_1 \ldots \int_{-\infty}^{+\infty} \mathrm{d}t_n\, F_q(t_1)\ldots F_q(t_n) \mathrm{e}^{iqu(t_1+\ldots t_n)} \\
&= \frac{q}{2\pi n}\int_{-\infty}^{+\infty} \mathrm{d}u\, \left[Q_q(u)\right]^n
\end{aligned}
$$

where

$$\begin{aligned} Q_q(u) &\equiv \int_{-\infty}^{+\infty} \mathrm{d}t\, F_q(t) \mathrm{e}^{iqut} \\ &= \int_{|\mathbf{p}|<1<|\mathbf{p}+\mathbf{q}|} \mathrm{d}^3p \int_{-\infty}^{+\infty} \mathrm{d}t\, \mathrm{e}^{iqut} \mathrm{e}^{-|t|(\mathbf{q}\cdot\mathbf{p}+q^2/2)} \\ &= 2\pi \left\{ 1 + \frac{1}{2q}\left(1 - \frac{1}{4}q^2 + u^2\right) \ln\left[\frac{\left(1+\frac{1}{2}q\right)^2 + u^2}{\left(1-\frac{1}{2}q\right)^2 + u^2}\right] \right. \\ &\qquad \left. - u \arctan\left[\frac{1+\frac{1}{2}q}{u}\right] - u \arctan\left[\frac{1-\frac{1}{2}q}{u}\right] \right\}. \end{aligned} \tag{22.15}$$

The total contribution from the ring diagrams is then

$$\begin{aligned} \Delta E_{\text{ring}} &= \sum_{n=2}^{\infty} (\Delta E)^{(n)}_{\text{ring}} \\ &= -\frac{3N}{16\pi^6}\left[\frac{\pi^2}{\alpha r_s}\right]^2 \int \mathrm{d}^3q\, q \int_{-\infty}^{+\infty} \mathrm{d}u \sum_{n=2}^{\infty} \frac{(-)^n}{n}\left[\frac{Q_q(u)\alpha r_s}{\pi^2 q^2}\right]^n \\ &= \frac{3N}{16\pi^6}\left[\frac{\pi^2}{\alpha r_s}\right]^2 \int \mathrm{d}^3q\, q \int_{-\infty}^{+\infty} \mathrm{d}u \left\{ \ln\left[1 + \frac{Q_q(u)\alpha r_s}{\pi^2 q^2}\right] - \frac{Q_q(u)\alpha r_s}{\pi^2 q^2} \right\}. \end{aligned}$$

Strictly speaking, the series in the integrand converges only for

$$-1 < \frac{Q_q(u)\alpha r_s}{\pi^2 q^2} < 1.$$

The small q-values are interesting. We calculate the value of $Q_q(u)$ for $q \to 0$. With

$$\begin{aligned} \ln\left[\frac{1+q+\frac{q^2}{4}+u^2}{1-q+\frac{q^2}{4}+u^2}\right] &= \ln\left[1 + \frac{q+q^2/4}{1+u^2}\right] - \ln\left[1 - \frac{q-q^2/4}{1+u^2}\right] \\ &\approx \frac{q}{1+u^2} + \frac{q}{1+u^2} = \frac{2q}{1+u^2} \end{aligned}$$

as $q \to 0$, we obtain from equation (22.15)

$$\begin{aligned} Q_0(u) \equiv \lim_{q\to 0} Q_q(u) &= \lim_{q\to 0} 2\pi \left[1 + \frac{1+u^2+0}{2q}\frac{2q}{1+u^2} - 2u \arctan\left(\frac{1}{u}\right)\right] \\ &= 4\pi\left[1 - u\arctan\left(\frac{1}{u}\right)\right]. \end{aligned}$$

It is clear that we may end up outside the convergence radius of the logarithm for small q. Nevertheless, we will

(1) further use the logarithm-function, and

(2) approximate Q_q by Q_0 since the small q-values dominate the contribution to the integral.

In this approximation, we obtain

$$\Delta E_{\text{ring}} = \left[\frac{2}{\pi^2}(1-\ln 2)\ln(r_s) - 0.142 + \mathrm{O}\left(r_s \ln(r_s)\right)\right] N \text{ Ry} \qquad (22.16)$$

for the resulting multi-dimensional integral. Together with the earlier result

$$(\Delta E)^{(2)}_{(c)} \approx 0.048N \text{ Ry}$$

we obtain

$$E_{\text{corr}}/N = \{0.0622\ln(r_s) - 0.094 + \mathrm{O}\left(r_s\ln(r_s)\right)\} \text{ Ry}. \qquad (22.17)$$

This is the final result of the long calculation.

Gell-Mann and Brueckner [16] provided the correction to the approximation (2) for the second-order term in figure 22.8 (a), which can be calculated exactly. The result is a small correction term which is independent of r_s, and which has been incorporated in the value 0.142 in equation (22.16). Further corrections correspond to powers of r_s, which have been consistently neglected here. The 'approximation' and the procedure (1) can be shown to hold exactly. This is done with the so-called *Sawada method* [18], which we will now briefly indicate. The idea is the following: Once it is known that the ring diagrams dominate in the limiting case of high density, one can try to construct a Hamiltonian, for which the perturbation expansion from the outset only contains the ring diagrams, or a related class of diagrams. The complete fermion interaction potential is (with conservation of momentum taken into account):

$$v = \frac{1}{2}\sum_{\mathbf{q}\neq 0}\ \sum_{\substack{\mathbf{k}_1'-\mathbf{k}=\mathbf{q}\\ \mathbf{k}_2-\mathbf{k}_2'=\mathbf{q}}}\ \sum_{\sigma_1,\sigma_2} v(q)\, a^\dagger_{\mathbf{k}_1'\sigma_1} a^\dagger_{\mathbf{k}_2'\sigma_2} a_{\mathbf{k}_2\sigma_2} a_{\mathbf{k}_1\sigma_1}.$$

We obtain a drastic reduction if we instead of *all* momentum-conserving processes, as shown in figure 22.16, only include the following:

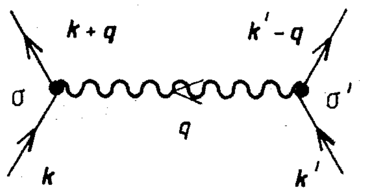


Figure 22.16 *A general diagram for the complete Coulomb interaction.*

$$\widetilde{v} = \frac{1}{2}\sum_{\mathbf{q}\neq 0}\sum_{\sigma_1\sigma_2}\left[\sum_{\substack{k_1',k_2'<k_F\\ k_1,k_2>k_F}} + \sum_{\substack{k_1',k_2<k_F\\ k_2',k_1>k_F}} + \sum_{\substack{k_1,k_2'<k_F\\ k_2,k_1'>k_F}} + \sum_{\substack{k_1,k_2<k_F\\ k_1',k_2'>k_F}}\right]$$
$$\times v(q) a^{\dagger}_{\mathbf{k}_1'\sigma_1} a^{\dagger}_{\mathbf{k}_2'\sigma_2} a_{\mathbf{k}_2\sigma_2} a_{\mathbf{k}_1\sigma_1}\,.$$

This operator can be illustrated diagrammatically as shown in figure 22.17 (where the direction relative to the imagined time axis *is* of importance, in contrast to earlier). The perturbation expansion of these operators contains diagrams other than the ring diagrams, *e.g.*, the diagram shown in figure 22.18. However, the contribution of these diagrams vanishes in the limit $r_s \to 0$.

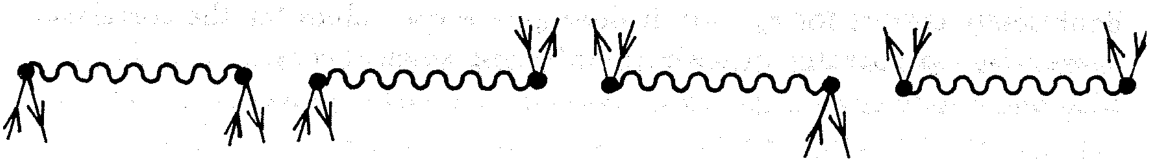


Figure 22.17 *The effective Sawada interaction contains only theses diagrams.*

The pictorial representation lets us assume that the Sawada potential can be expressed in terms of an electron–hole pair creation operator

$$d_{\mathbf{q}}(\mathbf{k},\sigma) \equiv a^{\dagger}_{\mathbf{k},\sigma} a_{\mathbf{k}+\mathbf{q},\sigma}\,.$$

We then obtain

$$\widetilde{v} = \frac{1}{2}\sum_{\mathbf{q}\neq 0}\sum_{\mathbf{k},\sigma}\sum_{\mathbf{k}',\sigma'}\left[d_{\mathbf{q}}(\mathbf{k},\sigma) + d^{\dagger}_{-\mathbf{q}}(-\mathbf{k},\sigma)\right]\left[d_{-\mathbf{q}}(-\mathbf{k}',\sigma') + d^{\dagger}_{\mathbf{q}}(\mathbf{k}',\sigma')\right].$$

The Hamiltonian with this interaction can then be treated *exactly*. In all fairness, it must be said that in spite of the elegance of the idea of the

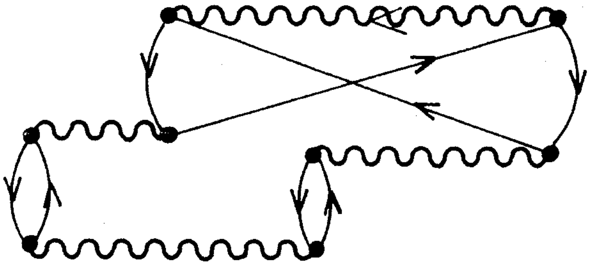


Figure 22.18 *In addition to all ring diagrams, the Sawada interaction also gives rise to diagrams such as this one.*

exact treatment of this Hamiltonian, the important application is in the Gell-Mann–Brueckner summation. However, the exact treatment of $\widetilde{v}$ does give additional information on the excited states. In the case of the ground state, the Sawada-method confirms the correctness of replacing the series by the logarithm (as done by Gell-Mann and Brueckner).

We close this chapter by comparing the result equation (22.17) with the result from plasmon theory, equation (11.10):

$$E_{\text{corr}}/N = [0.0622 \ln(r_s) - 0.158]\ \text{Ry}.$$

The coefficient of the logarithm is identical in both expressions. This is not surprising, since this term comes from the short-range part in the second order, which is treated correctly by both methods. The r_s-dependent term differs clearly. Even though the Gell-Mann–Brueckner calculation is doubtlessly correct for $r_s \rightarrow 0$, it does give worse values for the correlation energy for real metallic densities than the plasmon theory.

Chapter 23

Diagrammatic calculation of the single-particle Green's function: Dyson's equation

The representation

$$
\begin{aligned}
&iG_{\alpha\beta}(\mathbf{r}t,\mathbf{r}'t')\\
&\quad= \lim_{\epsilon\to 0}\frac{1}{\langle\Phi_0 \mid U_\epsilon(-\infty,\infty)\mid\Phi_0\rangle}\sum_{n=0}^{\infty}\frac{(-i)^n}{n!}\int_{-\infty}^{\infty}\mathrm{d}t_1\ldots\int_{-\infty}^{\infty}\mathrm{d}t_n\\
&\qquad\times \mathrm{e}^{-\epsilon(|t_1|+\ldots+|t_n|)}\langle\Phi_0 \mid T\left[v(t_1)_I\ldots v(t_n)_I\underline{\psi_\alpha(\mathbf{r}t)_I\psi^\dagger_\beta(\mathbf{r}'t')_I}\right]\mid\Phi_0\rangle
\end{aligned}
$$

which we proved in Chapter 18, provides the basis for the diagrammatic analysis of the single-particle Green's function. If we replace the underlined field operators by other creation and annihilation operators, for example $c_{\mathbf{k}\alpha}(t)_I$ and $c^\dagger_{\mathbf{k}'\beta}(t')_I$, we obtain the representations for other Green's functions, in this example $G_{\alpha\beta}(\mathbf{k}t,\mathbf{k}'t')$. The denominator in this representation of the Green's functions corresponds to the vacuum amplitude, the diagrammatic calculation of which was discussed in Chapter 21. If the second-quantized representation of the interaction $v(t_i)_I$ is inserted and Wick's theorem is used, the numerator can also be represented diagrammatically with the Feynman rules of Chapter 20. In first order, we obtain the six diagrams of figure 23.1. The two arguments of the Green's function appear as external endpoints of the diagrams. We have here only depicted the diagrams for particle propagation. The corresponding diagrams for hole propagation are obtained by interchanging the endpoint indices and changing the directions of all arrows. The diagrams (3) and (4), as well as the diagrams (5) and (6) in figure 23.1 are topologically equivalent, in the sense of our earlier definition, *i.e.*, they can be obtained from one another by interchanging the

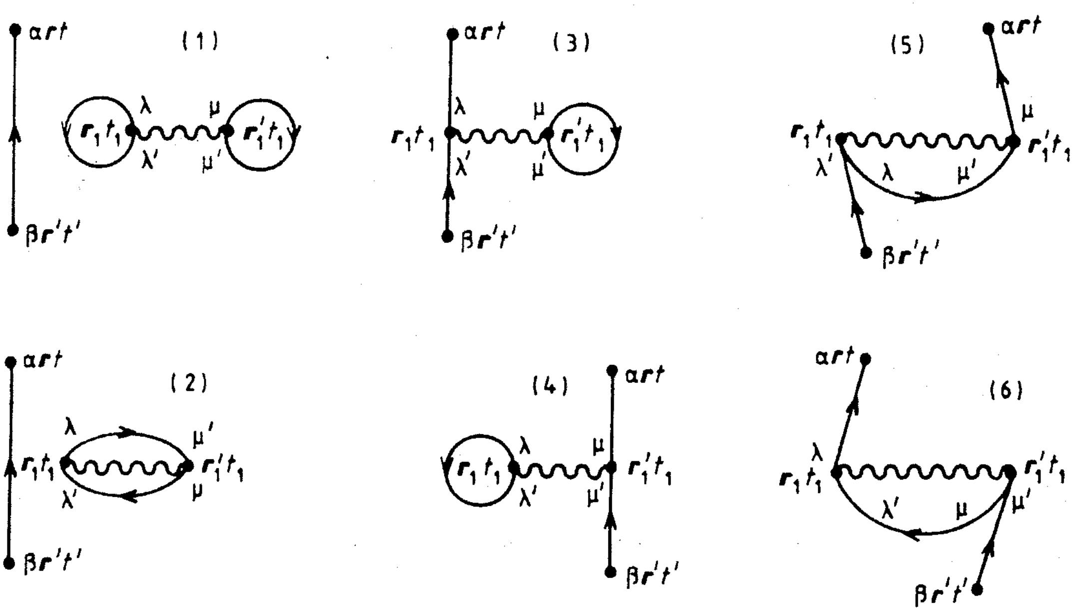


Figure 23.1 *The first-order diagrams of the numerator of the Green's function.*

indices on the vertices of *one* interaction line. The diagrams (1) and (2) are disconnected. It is clear, after translation to formal language, that such diagrams factorize into contributions from connected sub-diagrams. In what follows, we will prove that all terms in the numerator of the single-particle Green's function are obtained from the product of all connected digrams which connect the two external endpoints with all diagrams of the vacuum amplitude (see figure 23.2). All there is to do is simply to combine all diagrams which are connected between the two external endpoints with all other loose pieces, the sum total of which is the vacuum amplitude. In this

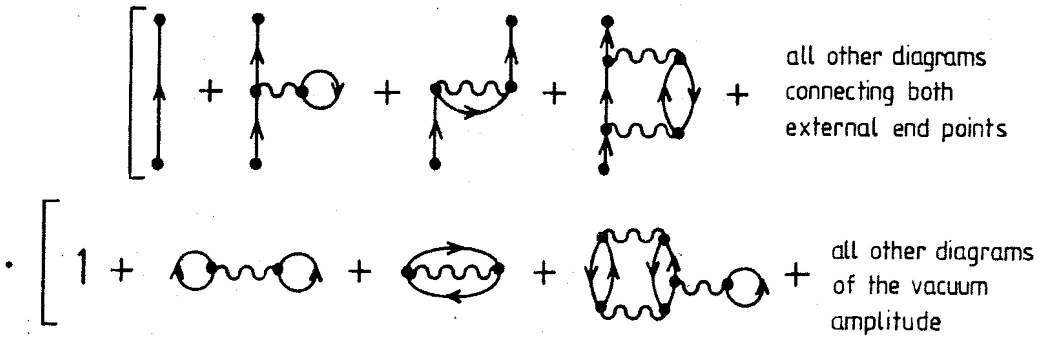


Figure 23.2 *Diagrammatic representation of the numerator of the Green's function.*

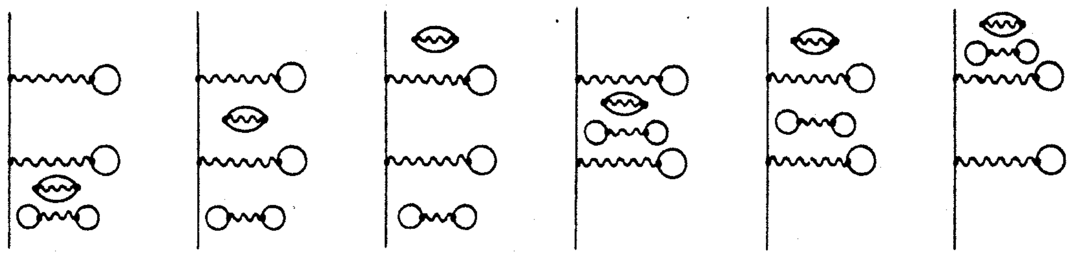


Figure 23.3 *Six diagrams of the numerator of the Green's function.*

way, we obtain all topologically distinct diagrams. However, it also remains to be shown that the prefactors agree. As an example, we first consider the six diagrams in figure 23.3, which all contribute to the perturbation expansion of the numerator. These diagrams all give the same contribution, namely (in a transparent notation):

$$\begin{aligned}&\frac{(-)^5 i^4}{4!2^4}\left[\sum G^{(0)}vG^{(0)}\right]_{g_x^{(1)}}\left[\sum G^{(0)}vG^{(0)}\right]_{g_d^{(1)}}\\ &\quad\times\left[\sum G^{(0)}(t,.)vG^{(0)}G^{(0)}vG^{(0)}G^{(0)}(.,t')\right]_{g_t^{(2)}}.\end{aligned}$$

On the other hand, the product of $g_t^{(2)}$, and $g_x^{(1)}$ and $g_d^{(1)}$ (figure 23.4) is

$$\begin{aligned}&\left\{\frac{(-)^2 i^2}{2!2^2}\left[\sum G^{(0)}(t,.)vG^{(0)}G^{(0)}vG^{(0)}G^{(0)}(.,t')\right]_{g_t^{(2)}}\right\}\\ &\quad\times\left\{\frac{(-)^3 i^2}{2!2^2}\left[\sum G^{(0)}vG^{(0)}\right]_{g_x^{(1)}}\left[\sum G^{(0)}vG^{(0)}\right]_{g_d^{(1)}}\right\}\\ &= \frac{(-)^5 i^4}{2!2!2^4}[\quad]_{g_x^{(1)}}[\quad]_{g_d^{(1)}}[\quad]_{g_t^{(2)}}\\ &= 6\frac{(-)^5 i^4}{4!2^4}[\quad]_{g_x^{(1)}}[\quad]_{g_d^{(1)}}[\quad]_{g_t^{(2)}}.\end{aligned}$$

Thus, we obtain the sum of the diagrams in figure 23.3. We now have to generalize this calculation to diagrams of arbitrary order. Once we have succeeded with that task, the statement is proved.

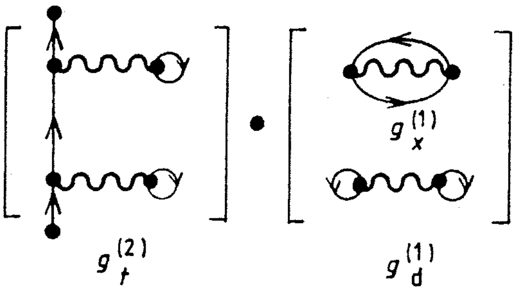


Figure 23.4 *All diagrams of figure 23.3 can be produced by the connected diagrams* $g_t^{(2)}$, $g_x^{(1)}$ *and* $g_d^{(1)}$.

We consider a general term of order ν in the numerator of G. This term will consist of a uniquely determined connected piece $G_L^{(n)}$ of nth order, which connects both endpoints, and furthermore of a loose piece $g^{(\nu-n)}$ of order $(\nu - n)$. This latter piece is also uniquely determined. This one may be partitioned into connected sub-diagrams, as in the example above; this is however meaningless for the present proof. There are precisely $\binom{\nu}{n}$ possibilities to choose n interaction lines out of the ν ones connected to the times $t_1, \ldots t_\nu$ in order to construct the connected diagrams $G_L^{(n)}$. The remaining $(\nu - n)$ interaction lines result in the disconnected vacuum amplitude diagrams $g^{(\nu-n)}$. Each possible combination apparently corresponds to a diagram which contributes to the numerator of the Green's function. All these $\binom{\nu}{n}$ diagrams give the same contribution. Thus, the sum of them contributes

$$
\begin{aligned}
&\frac{\nu!}{n!(\nu-n)!}\left\{\frac{(-)^{\ell} i^{\nu}}{\nu! 2^{\nu}}\left[\sum G^{(0)} v \ldots\right]_{G_L^{(n)}}\left[\sum G^{(0)} v \ldots\right]_{g^{(\nu-n)}}\right\} \\
&= (-)^{\ell_1} \frac{i^n}{n! 2^n}\left[\sum G^{(0)} v \ldots\right]_{G_L^{(n)}} \\
&\quad \times (-)^{(\ell-\ell_1)} \frac{i^{(\nu-n)}}{(\nu-n)! 2^{\nu-n}}\left[\sum G^{(0)} v \ldots\right]_{g^{(\nu-n)}} \\
&= \left(G_L^{(n)}\right) \times \left(g^{(\nu-n)}\right).
\end{aligned}
$$

We have here used the easily shown fact, that the number of fermion hole lines (denoted by ℓ, ℓ_1 and $\ell - \ell_1$) is additive. The hypothesis is then proved. We can cancel the denominator of the Green's function with the vacuum amplitude factor of the numerator and obtain the important result (see figure 23.5)

$$
\begin{aligned}
&G_{\alpha\beta}(\mathbf{r}t, \mathbf{r}'t') \\
&= \lim_{\epsilon\to 0}(-i)\sum_{n=0}^{\infty}\frac{(-i)^n}{n!}\int_{-\infty}^{+\infty}dt_1\ldots\int_{-\infty}^{+\infty}dt_n e^{-\epsilon(|t_1|+\ldots+|t_n|)} \\
&\quad\times\langle\Phi_0\mid T\left[v(t_1)_I\ldots v(t_n)_I\psi_\alpha(\mathbf{r}t)_I\psi_\beta^\dagger(\mathbf{r}'t')_I\right]\mid\Phi_0\rangle_L.
\end{aligned}
\tag{23.1}
$$

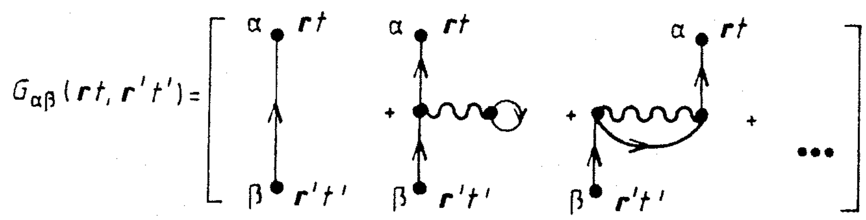


Figure 23.5 *In the series expansion for the Green's function, only diagrams connecting the external endpoints need to be included.*

The index L means that only the connected diagrams are to be summed over. Equation (23.1) is, if we wish, the 'linked-cluster theorem' for the single-particle Green's function.

In the remaining terms of the perturbation expansion, many degeneracies in the diagrams appear

(1) through the interchange of entire interaction lines (figure 23.6). This gives in all $n!$ permutation possibilities for nth order diagrams.

(2) By topological degeneracy (figure 23.7). There are two such possibilities per interaction line. This means an additional degeneracy factor of 2^n for nth order diagrams. In contrast to the vacuum amplitude, there are in the present case only asymmetric diagrams, so that we do not count any diagrams twice.

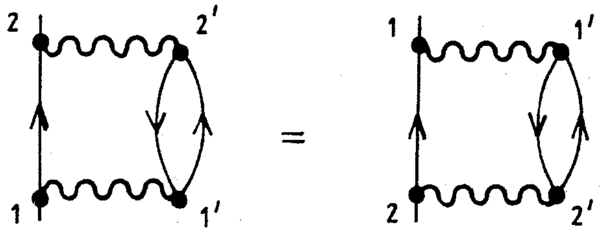


Figure 23.6 *Diagrams which can be obtained from one another by interchanging entire interaction lines leave identical contributions.*

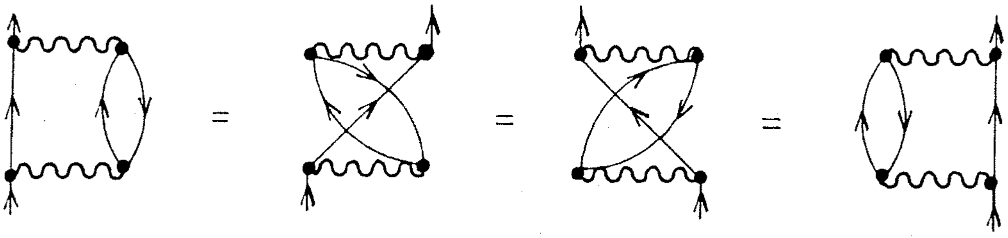


Figure 23.7 *These diagrams are topologically equivalent and give identical contributions.*

At this point, we agree to represent the entire family of $(n!2^n)$ degenerate diagrams by a single diagram *without indices*. At the same time, we establish a new Feynman rule.

> Feynman rule (7) for the prefactor of the unindexed connected Green's function diagrams:
>
> $$\text{prefactor} = i^n.$$

The degeneracy factor $(n!2^n)$ cancels out with the denominator of the earlier shown prefactors of the indexed diagrams.

All connected second-order diagrams for the Green's function are shown in figure 23.8. Each of these unindexed diagrams represents a family of $2^2 2!$ diagrams. Some of these unindexed diagrams clearly vanish in the momentum representation of a translationally invariant system.

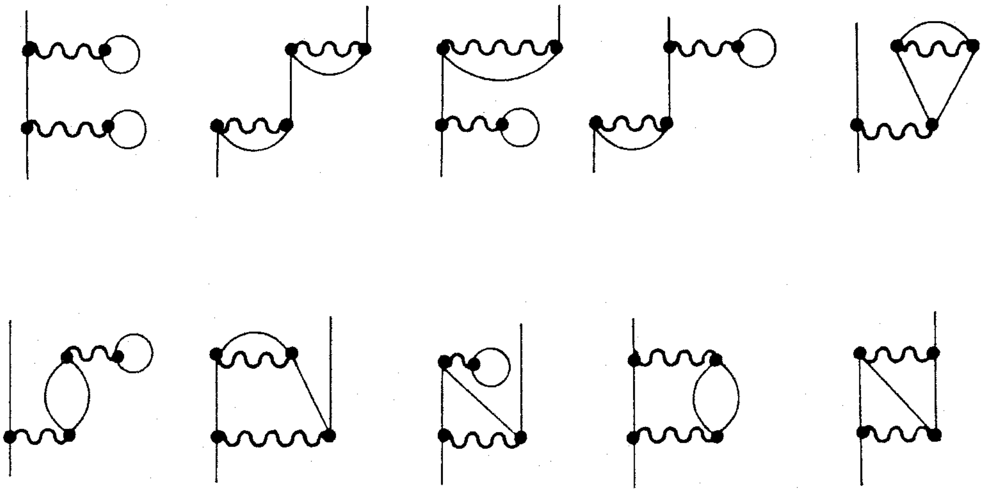


Figure 23.8 *All second-order connected diagrams for the Green's function.*

We now have a rough idea of what the perturbation expansion of the single-particle Green's function looks like. As the illustration of the second-order diagrams in figure 23.8 shows, many diagrams are constructed from a few simple 'building blocks'. This is the basis for what is maybe the most important equation in the entire perturbation theory: Dyson's equation. We will now derive this equation. If the full Green's function is depicted by a thick line, the perturbation series can be summarized by figure 23.9.

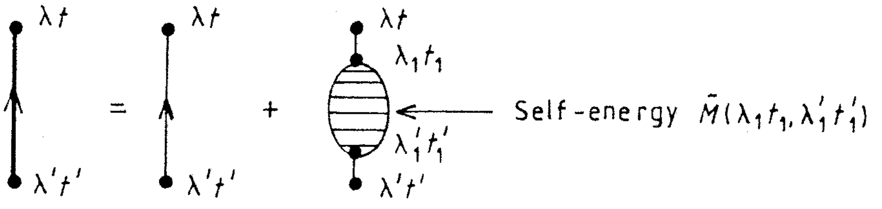


Figure 23.9 *The self-energy $\widetilde{M}$ allows for a compact representation of the perturbation series for G.*

The self-energy $\widetilde{M}$ denotes the sum of all *self-energy insertions* (figure 23.10). These are any part of a diagram which is connected to the rest

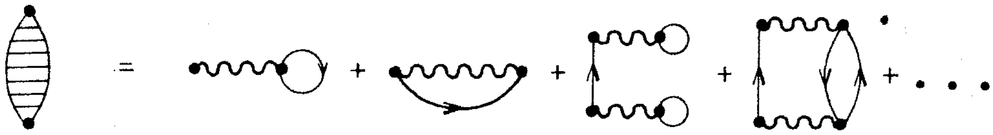


Figure 23.10 *The self-energy is obtained by summing all self-energy insertions, as shown here.*

of the diagram only by one incoming and one outgoing $G^{(0)}$-line. Furthermore, we classify self-energy insertions as *reducible* if they can be partitioned into lower-order self-energy insertions by cutting a single $G^{(0)}$-line. For example, the diagrams on the top row in figure 23.11 are irreducible, whereas the diagrams on the bottom row are reducible. The sum of of all irreducible self-energy insertions is called the *proper self-energy*, and is denoted by M (without a ~). It is clear that we obtain the total self-energy from the sum of all possible repetitions of the proper self-energy connected with Green's function line, as shown diagrammatically in figure 23.12. Formally, figure 23.12 can be written

$$\begin{aligned}\widetilde{M}(\lambda_1 t_1, \lambda_1' t_1') &= M(\lambda_1 t_1, \lambda_1' t_1') + \int \mathrm{d}t_2 \int \mathrm{d}t_2' \sum_{\lambda_2 \lambda_2'} M(\lambda_1 t_1, \lambda_2, t_2) \\ &\quad \times G^{(0)}(\lambda_2 t_2, \lambda_2' t_2') M(\lambda_2' t_2', \lambda_1' t_1') + \ldots\end{aligned}$$

Convergence factors $e^{-\epsilon|t|}$ which may possibly appear have been omitted from these definitions of M and $\widetilde{M}$, respectively.

and

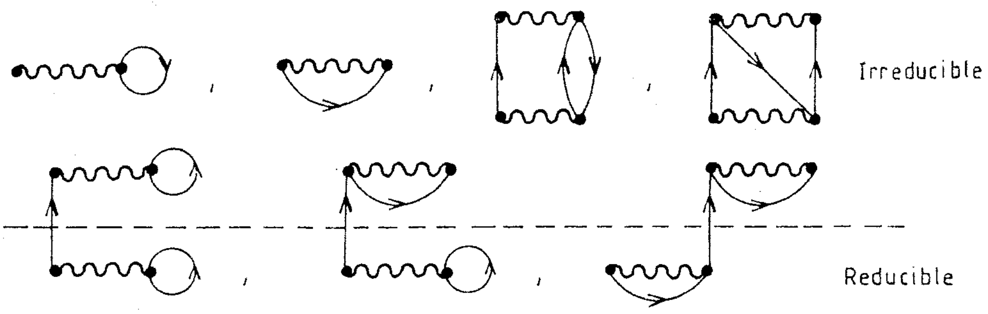


Figure 23.11 *Examples of irreducible and reducible self-energy insertions. The reducible ones can be cut into lower-order diagrams by cutting a single $G^{(0)}$-line as indicated by the dashed line.*

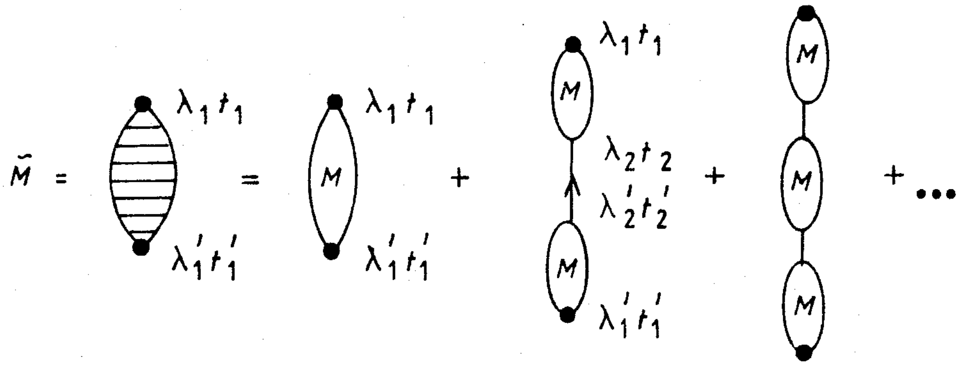


Figure 23.12 *The self-energy $\widetilde{M}$ is obtained as a series in the proper self-energy.*

The equation for the Green's function can then be represented as shown in figure 23.13.

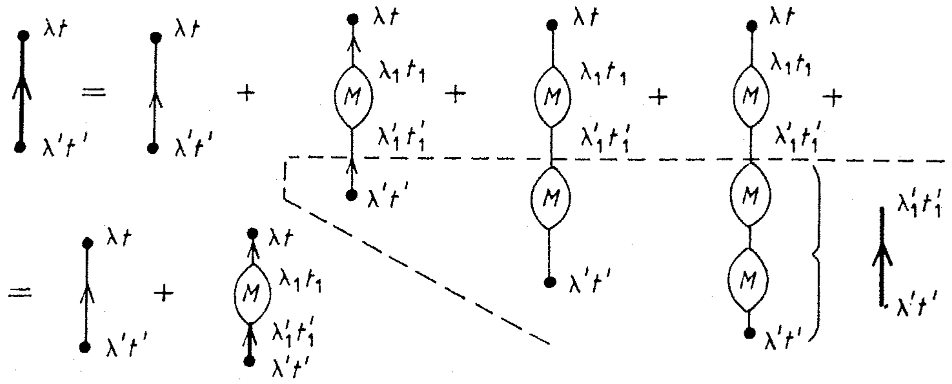


Figure 23.13 *Dyson's equation for the Green's function.*

This is *Dyson's equation.* Formally, it is written

$$
\begin{aligned}
&G(\lambda t\lambda' t') \\
&\quad = \quad G^{(0)}(\lambda t, \lambda' t') \\
&\qquad + \sum_{\lambda_1} \sum_{\lambda_1'} \int \mathrm{d}t_1 \int \mathrm{d}t_1' G^{(0)}(\lambda t, \lambda_1 t_1) M(\lambda_1 t_1, \lambda_1' t_1') G(\lambda_1' t_1', \lambda' t').
\end{aligned}
\tag{23.2}
$$

At first sight this equation seems astonishing, since we have seen earlier that the single-particle Green's function is calculated from the two-particle Green's function, and so on, and here it appears that we obtain the single-particle Green's function from an integral equation in which there is a seemingly independent quantity, the self-energy. However, we could have shown before that the single-particle Green's function satisfies such an equation. In Chapter 16, we found the equation of motion for the Green's functions:

$$\left[i\frac{\partial}{\partial t} + \frac{\nabla_r^2}{2m}\right] G^{(0)}(\mathbf{r}t, \mathbf{r}'t') = \delta(t-t')\delta(\mathbf{r}-\mathbf{r}')$$

and

$$
\begin{aligned}
&\left[i\frac{\partial}{\partial t} + \frac{\nabla_r^2}{2m}\right] G(\mathbf{r}t, \mathbf{r}'t') \\
&\quad = \quad \delta(t-t')\delta(\mathbf{r}-\mathbf{r}') - i\int \mathrm{d}^3y\, v(\mathbf{r},\mathbf{y}) G_2(\mathbf{r}t, \mathbf{y}t, \mathbf{y}t^+, \mathbf{r}'t').
\end{aligned}
$$

In this approach, M is introduced by

$$\begin{aligned}
&-i\int \mathrm{d}^3y\, v(\mathbf{r},\mathbf{y})G_2(\mathbf{r}t,\mathbf{y}t,\mathbf{y}t^+,\mathbf{r}'t')\\
&\equiv \int \mathrm{d}\tau' \int \mathrm{d}^3y'\, M(\mathbf{r}t,\mathbf{y}'\tau')G(\mathbf{y}'\tau',\mathbf{r}'t').
\end{aligned} \tag{23.3}$$

This equation shows the relation between M and G_2. We must now identify the M introduced in this way as the proper self-energy. We can do this by convincing ourselves that the equation of motion

$$\begin{aligned}
&\left[i\frac{\partial}{\partial t}+\frac{\nabla_r^2}{2m}\right]G(\mathbf{r}t,\mathbf{r}'t')\\
&= \delta(t-t')\delta(\mathbf{r}-\mathbf{r}')+\int \mathrm{d}\tau' \int \mathrm{d}^3y'\, M(\mathbf{r}t,\mathbf{y}'\tau')G(\mathbf{y}'\tau,\mathbf{r}'t')
\end{aligned}$$

is satisfied by the solution of Dyson's equation

$$\begin{aligned}
&G(\mathbf{r}t,\mathbf{r}'t')\\
&= G^{(0)}(\mathbf{r}t,\mathbf{r}'t')+\int \mathrm{d}\tau' \int \mathrm{d}^3y' \int \mathrm{d}\tau \int \mathrm{d}^3y\, G^{(0)}(\mathbf{r}t,\mathbf{y}\tau)\\
&\quad \times M(\mathbf{y}\tau,\mathbf{y}'\tau')G(\mathbf{y}'\tau',\mathbf{r}'t').
\end{aligned}$$

Chapter 24

Diagrammatic analysis of the Green's function $G(\mathbf{k},\omega)$

We start by re-writing the perturbation expansion of the Green's function in the space-representation in a manifestly covariant notation. As is customary in relativistic problems, we define

$$\begin{aligned} x &\equiv (\mathbf{r},t) \qquad & \mathrm{d}^4x &= \mathrm{d}^3r\,\mathrm{d}t \\ k &\equiv (\mathbf{k},\omega) \qquad & \mathrm{d}^4k &= \mathrm{d}^3k\mathrm{d}\omega \end{aligned}$$

and use the 'Minkowski scalar product'

$$k\cdot x = \mathbf{k}\cdot\mathbf{r} - \omega t.$$

The use of the single letter k for $(\mathbf{k},\omega)$ should not lead to any confusion. However, as a precaution we will only abbreviate $|\mathbf{k}|$ with k in unambiguous cases, such as in combination with d^3k.

Up to this point, we had established that each interaction line gives a contribution (see figure 24.1)

$$\int \mathrm{d}t\,\mathrm{e}^{-\epsilon|t|}\int \mathrm{d}^3r\int \mathrm{d}^3r'\,v(\mathbf{r},\mathbf{r}').$$

If we now set

Figure 24.1 *A general interaction line with its vertices.*

$$u(x,x') \equiv v(\mathbf{r},\mathbf{r}')\delta(t-t')$$

the diagrammatic representation in figure 24.2 becomes

$$\int \mathrm{d}x \int \mathrm{d}x'\, u(x,x')$$

by modifying Feynman rule (5) (which says that *all* indices must be integrated over). This agrees of course with our earlier expression,

$$\begin{aligned}\int \mathrm{d}x \int \mathrm{d}x'\, u(x,x') &= \int \mathrm{d}t \int \mathrm{d}^3r \int \mathrm{d}t' \int \mathrm{d}^3r' v(\mathbf{r},\mathbf{r}')\delta(t-t') \\ &= \int \mathrm{d}t \int \mathrm{d}^3r \int \mathrm{d}^3r'\, v(\mathbf{r},\mathbf{r}').\end{aligned}$$

The convergence fator $\mathrm{e}^{-\epsilon|t|}$ will hereafter be omitted for ease of notation; it must of course be reinserted when any expression is actually calculated explicitly.

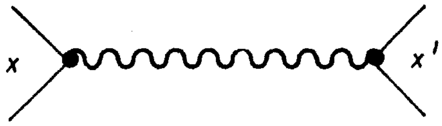


Figure 24.2 *The vertices* $\mathbf{r}t$ *and* $\mathbf{r}'t'$ *of an interaction line are relabeled in the covariant notation.*

It is evident that this notation makes a covariant formulation for relativistic systems possible, where the interaction has a finite speed of propagation and is no longer described merely by a delta-function in time. In this context, the time does not play a special role any longer; we can omit Feynman rule (1) as well as the requirement that the interaction lines must be horizontal. The diagrams that we have studied so far are frequently drawn in a different way; some examples are shown in figure 24.3. From here on, we will make use of both representations.

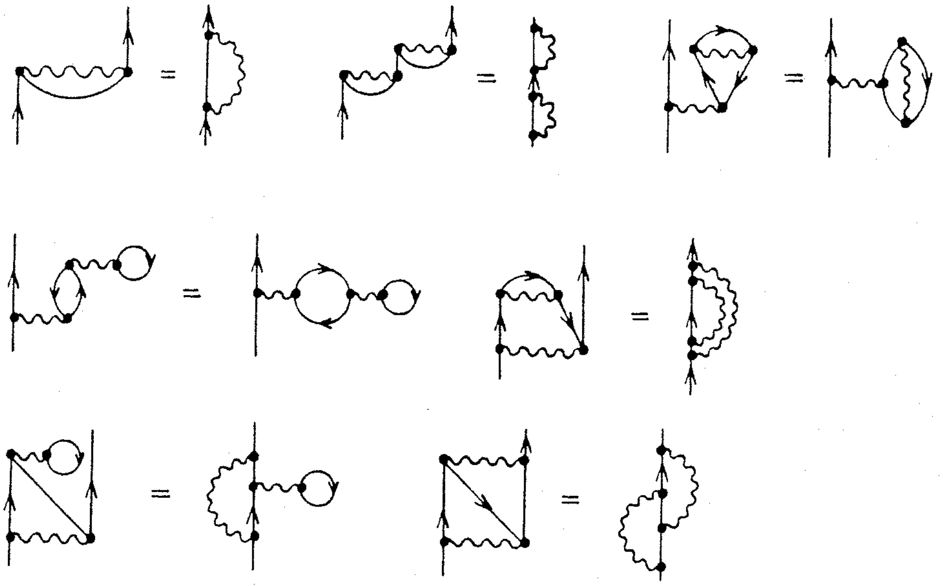


Figure 24.3 *When Feynamn rule (1) can be omitted, time loses its special meaning and many diagrams can be drawn differently by allowing for the interaction line not to be horizontal.*

In what folloes, we will restrict ourselves to translationally invariant systems, which do not explicitly depend on time. We said in Chapter 15 that in this case, the single-particle Green's function only depends on the difference between the space and time coordinates, and that we can use four-dimensional Fourier transforms given by

$$G_{\alpha\beta}(x,y) = \frac{1}{(2\pi)^4} \int \mathrm{d}^4k \, \mathrm{e}^{i(x-y)k} G_{\alpha\beta}(k)$$

and

$$G_{\alpha\beta}(k) = \int \mathrm{d}^4(x-y) \, \mathrm{e}^{-i(x-y)k} G_{\alpha\beta}(x,y).$$

We Fourier transform the interaction potential in the same way:

$$u(x-x') = \frac{1}{(2\pi)^4} \int \mathrm{d}^4k \, \mathrm{e}^{-ik(x-x')} u(k)$$

where the Fourier transform

$$u(k) = \int \mathrm{d}^4(x-x') \, \mathrm{e}^{-ik(x-x')} u(x-x')$$

for non-relativistic systems becomes

$$\begin{aligned} u(k) &= \int \mathrm{d}^3(\mathbf{r}-\mathbf{r}')\,\mathrm{e}^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')}v(\mathbf{r}-\mathbf{r}')\underbrace{\int \mathrm{d}(t-t')\,\delta(t-t')}_{=1} \\ &= v(\mathbf{k}). \end{aligned}$$

In order to derive the Feynman rules for the Green's function $G_{\alpha\beta}(k)$, we must first Fourier transform the diagrams which appear in the space-representation. We do that in the example shown in figure 24.4. The contribution from this diagram is

$$\begin{aligned} &\frac{i^1}{1!2^1}\sum_{\substack{\lambda\lambda'\\ \mu\mu'}}\int \mathrm{d}^4x_1\int \mathrm{d}^4x_1'\,G^{(0)}_{\alpha\lambda}(x,x_1) \\ &\qquad \times u(x_1,x_1')_{\substack{\lambda\lambda'\\ \mu\mu'}}\left[\lim_{t_1'\to t_1^+} G^{(0)}_{\lambda'\mu}(x_1,x_1')\right]G^{(0)}_{\mu'\beta}(x_1',y) \\ &= \frac{i}{2}\sum_{\substack{\lambda\lambda'\\ \mu\mu'}}\int \mathrm{d}^4x_1\int \mathrm{d}^4x_1'\int\frac{\mathrm{d}^4k}{(2\pi)^4}\mathrm{e}^{ik(x-x_1)}G^{(0)}_{\alpha\lambda}(k) \\ &\qquad \times\int\frac{\mathrm{d}^4q}{(2\pi)^4}\mathrm{e}^{iq(x_1-x_1')}u(q)_{\substack{\lambda\lambda'\\ \mu\mu'}}\int\frac{\mathrm{d}^4p}{(2\pi)^4}G^{(0)}_{\lambda'\mu}(p)\underline{\mathrm{e}^{i\mathbf{p}\cdot(\mathbf{x}_1-\mathbf{x}_1')}} \\ &\qquad \times\left[\lim_{t_1'\to t_1^+}\mathrm{e}^{-i\omega_p(t_1-t_1')}\right]\int\frac{\mathrm{d}^4p'}{(2\pi)^4}\mathrm{e}^{ip'(x_1'-y)}G^{(0)}_{\mu'\beta}(p'). \end{aligned}$$

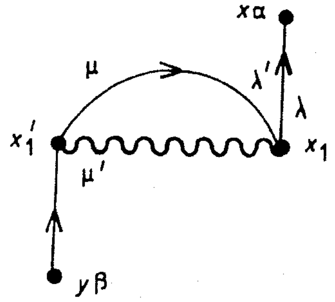


Figure 24.4 *A first-order diagram for the Green's function.*

We replace the time limit by

$$\lim_{t_1'\to t_1^+}\mathrm{e}^{-i\omega_p(t_1-t_1')} = \lim_{\eta\to 0^+}\mathrm{e}^{i\omega_p\eta}$$

where we agree to take the limit $\eta\to 0^+$ at the end of the calculation. After this manipulation we can, for esthetic reasons, insert a *new* additional factor $\exp\left[-i\omega_p(t_1-t_1')\right]$, since this factor is unity anyhow, due to the delta function $\delta(t_1 - t_1')$ contained in $u(x_1, x_1')$. This transforms the underlined usual scalar product to a Minkowski scalar product, and we can then write for the whole expression

$$\lim_{\eta \to 0^+} \frac{i}{2} \frac{1}{(2\pi)^{16}} \sum_{\substack{\lambda\lambda' \\ \mu\mu'}} \int \mathrm{d}^4k \int \mathrm{d}^4q \int \mathrm{d}^4p \int \mathrm{d}^4p' \, \mathrm{e}^{i(kx - p'y)} G^{(0)}_{\alpha\beta}(k)$$
$$\times u(q)_{\substack{\lambda\lambda' \\ \mu\mu'}} \left[\mathrm{e}^{i\omega_p\eta} G^{(0)}_{\lambda'\mu}(\mathbf{p}, \omega_p)\right] G^{(0)}_{\mu'\beta}(p')$$
$$\times \underbrace{\int \mathrm{d}^4x_1 \mathrm{e}^{i(q-k+p)x_1}}_{(2\pi)^4\delta^{(4)}(q-k+p)} \underbrace{\int \mathrm{d}^4x_1' \, \mathrm{e}^{i(-q-p+p')x_1'}}_{(2\pi)^4\delta^{(4)}(p'-q-p)} .$$

Thus, we obtain a four-momentum delta-function at each of the two vertices at x_1 and x_1'. This results in

$$\lim_{\eta \to 0^+} \frac{i}{2} \sum_{\substack{\lambda\lambda' \\ \mu\mu'}} \int \frac{\mathrm{d}^4k}{(2\pi)^4} \int \frac{\mathrm{d}^4p}{(2\pi)^4} \mathrm{e}^{ik\cdot(x-y)} G^{(0)}_{\alpha\lambda}(k) u(k-p)_{\substack{\lambda\lambda' \\ \mu\mu'}}$$
$$\times \left[\mathrm{e}^{i\eta\omega_p} G^{(0)}_{\lambda'\mu}(\mathbf{p}, \omega_p)\right] G^{(0)}_{\mu'\beta}(k).$$

Since the full Green's function is obtained from the Fourier transform

$$G_{\alpha\beta}(x, y) = \int \frac{\mathrm{d}^4k}{(2\pi)^4} \mathrm{e}^{ik\cdot(x-y)} G_{\alpha\beta}(k)$$

we can interpret the expression

$$\lim_{\eta \to 0^+} \frac{i}{2} \sum_{\substack{\lambda\lambda' \\ \mu\mu'}} \int \frac{\mathrm{d}^4p}{(2\pi)^4} G^{(0)}_{\alpha\lambda}(k) u(k-p)_{\substack{\lambda\lambda' \\ \mu\mu'}} \left[\mathrm{e}^{i\eta\omega_p} G^{(0)}_{\lambda'\mu}(\mathbf{p}, \omega_p)\right] G^{(0)}_{\mu'\beta}(k) \quad (24.1)$$

as the diagram in figure 24.5, which contributes to $G_{\alpha\beta}(k)$.

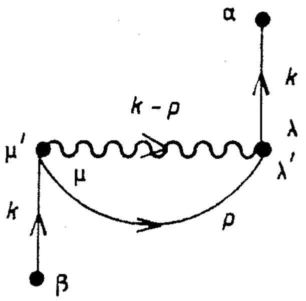


Figure 24.5 *After Fourier transforming the contribution from the diagram in figure 24.4, the contribution can be represented by this diagram for* $G_{\alpha\beta}(k)$.

This example lets us deduce the contribution of a general diagram to the Green's function:

(1) For each $u(x,x')$, there is a $u(q)$.

(2) Each $G^{(0)}(x,y)$ gives a $G^{(0)}(k)$.

(3) The prefactors and signs arising from the topological structure and the number of interaction lines remain unchanged by the Fourier transform.

(4) In the example, the momentum was conserved at the internal vertices. It is easy to prove the assumption that this holds for general diagrams. For example, the diagram in figure 24.6 gives

$$\begin{aligned} & G^{(0)}(b,x)u(x,c)G^{(0)}(x,a) \\ &= \frac{1}{(2\pi)^{12}} \int \mathrm{d}^4x \int \mathrm{d}^4k\, \mathrm{e}^{ik\cdot(b-x)} G^{(0)}(k) \int \mathrm{d}^4q\, \mathrm{e}^{iq\cdot(x-c)} u(q) \\ & \quad \times \int \mathrm{d}^4p\, \mathrm{e}^{ip\cdot(x-a)} G^{(0)}(p). \end{aligned}$$

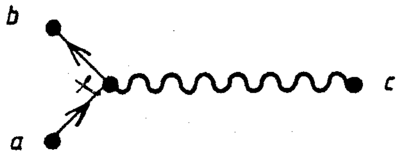


Figure 24.6 *A general vertex of an interaction line.*

The integration variable x does not appear in any Green's function, and the integral over x can be performed with the result

$$\frac{1}{(2\pi)^8}\int d^4k\int d^4q\int d^4p\, e^{i(k\cdot b-q\cdot c-p\cdot a)}G^{(0)}(k)u(q)G^{(0)}(p)$$
$$\underbrace{\times\frac{1}{(2\pi)^4}\int d^4x\, e^{i(-k+q+p)\cdot x}}_{=\delta^{(4)}(q-k+p)}\,.$$

All integrations $\int d^4x$ which belong to internal vertices can then be performed explicitly, and leave a momentum- and energy-conserving delta function $\delta^{(4)}$ at the corresponding vertices. We note that precisely the exponential factors that are necessary for the corresponding calculation of the adjacent vertices remain in this equation.

(5) Because of the δ-functions, several of the momentum integrals which arise from the Fourier transforms can be performed. A few integrals which are independent from one another, for example integrals over momentum running through particle loops, remain and yield each a factor of $(2\pi)^{-4}$.

(6) In each diagram, there is a sequence of $G^{(0)}$-lines which connect the external endpoints with one another. Since all vertices inbetween conserve momentum, performing the integrations over the δ-functions at the endpoints results in the same momentum on the external legs. The two remaining exponential factors can then be combined. Hence, all diagrams that contribute to the Green's function have a common factor of

$$\frac{1}{(4\pi)^4}\int d^4k\, e^{ik\cdot(x-y)}\ldots$$

(This also holds for the diagram that consists of a single $G^{(0)}$-line.) Since the sum of all these diagrams yields the full Green's function

$$G(x,y)=\frac{1}{(2\pi)^4}\int d^4k\, e^{ik\cdot(x-y)}G(\mathbf{k},\omega)$$

we obtain by comparison with the Fourier components the sought-for perturbation expansion of $G(\mathbf{k},\omega)$.

After these considerations, we can formulate the *Feynman rules for* $G(\mathbf{k},\omega)$:

(1) The Green's function $G^{(0)}_{\alpha\beta}(k)$ is represented by a line labeled by the momentum $\mathbf{k}$ and with the spin-indices α and β labeling the end-points (figure 24.7). Each such line gives a factor

$$G^{(0)}_{\alpha\beta}(k) \;=\; \lim_{\xi\to 0^+}\delta_{\alpha\beta}\left[\frac{\theta(|\mathbf{k}|-k_F)}{\omega-\epsilon^{(0)}_k+i\xi}+\frac{\theta(k_F-|\mathbf{k}|)}{\omega-\epsilon^{(0)}_k-i\xi}\right]$$

where, for example

$$\epsilon_k^{(0)} = |\mathbf{k}|^2/2m.$$

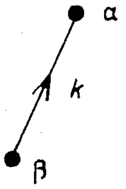


Figure 24.7 *The Green's function* $G^{(0)}_{\alpha\beta}(k)$.

(2) An interaction line is labeled by the momentum q transferred by the interaction, and the vertices are labeled by spin-indices α, α' (first vertex) and β, β' (second vertex) (see figure 24.8). Each interaction line contributes a factor $u(q)_{\substack{\alpha\alpha'\\ \beta\beta'}}$.

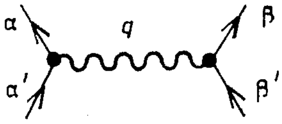


Figure 24.8 *Labeling of an interaction line and its vertices.*

(3) $G^{(0)}$-lines which begin and end on the same interaction line are interpreted as $e^{i\omega\eta}G^{(0)}(\mathbf{k},\omega)$, where the limit $\eta \to 0^+$ is taken at the end of the calculation (figure 24.9).

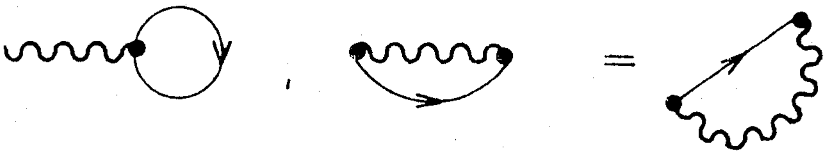


Figure 24.9 *Examples of diagrams in which the Green's function has its endpoints on the same interaction line.*

(4) Momentum is conserved at each vertex. This is illustrated in figure 24.10.

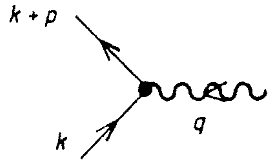


Figure 24.10 *A momentum q is transferred by the interaction to the Green's function connected at one vertex.*

(5) All four-momenta that appear (after satisfying momentum conservation) are integrated over. When the integrals are performed, each is multiplied by a phase-space factor:

$$(2\pi)^{-4}\int \mathrm{d}^4 p.$$

(The four-momentum k, which enters with the Green's function $G(k)$ at one endpoint and leaves at the other, is of course not integrated over.)

(6) The sign of the diagram is given by $(-)^{\ell}$, where ℓ is the number of closed $G^{(0)}$-loops.

(7) The prefactor of a diagram of order n is

$$\begin{cases} \dfrac{(i)^n}{2^n n!} & \text{for an indexed diagram of order } n \\ (i)^n & \text{for an unindexed diagram of order } n \end{cases}$$

With these rules, we can easily translate the connected Green's function diagram of first order shown in figure 24.11. The result is

$$(-1)\frac{1}{2}\sum_{\substack{\lambda\lambda' \\ \mu\mu'}} \frac{1}{(2\pi)^4}\int \mathrm{d}^4 k_1\, u(0)_{\substack{\lambda\lambda' \\ \mu\mu'}} \times G^{(0)}_{\alpha\lambda}(k) G^{(0)}_{\lambda'\beta}(k) \lim_{\eta\to 0+} \mathrm{e}^{i\omega_1\eta} G^{(0)}_{\mu\mu'}(k_1).$$

Because of momentum conservation, only the $q = 0$ Fourier component of the interaction potential appears. (In the case of the electron gas, this one is explicitly omitted, since it is canceled by the positive ionic background.) We also note that the two $G^{(0)}(k)$-factors only couple to the third one through the spin-indices. Hence, the Green's functions factor out for spin-independent interactions.

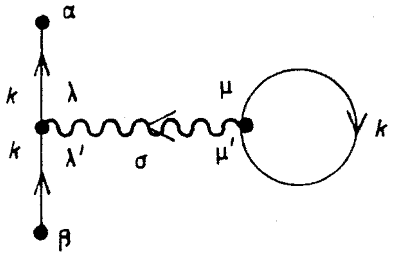


Figure 24.11 *The so-called tadpole diagram of the Green's function.*

Next, we consider Dyson's equation for translationally invariant systems. In the space-representation, this equation is

$$\begin{aligned} G_{\alpha\beta}(x-y) \\ &= G^{(0}_{\alpha\beta}(x-y) \\ &\quad + \sum_{\lambda\mu} \int \mathrm{d}^4 x_1 \int \mathrm{d}^4 x_1' \, G^{(0)}_{\alpha\lambda}(x-x_1) M_{\lambda\mu}(x_1 - x_1') G_{\mu\beta}(x_1' - y). \end{aligned} \tag{24.2}$$

We emphasize through the notation $G(x-y)$ *etc.*, that for such systems, G, $G^{(0)}$ and consequently also M, only depend on the difference between the arguments. A simple direct calculation, or the convolution theorem for Fourier transforms, show that by Fourier transforming, the (convolution) integrals become ordinary products:

$$G_{\alpha\beta}(k) = G^{(0)}_{\alpha\beta}(k) + \sum_{\lambda} \sum_{\mu} G^{(0)}_{\alpha\lambda}(k) M_{\lambda\mu}(k) G_{\mu\beta}(k) \tag{24.3}$$

where $M_{\lambda\mu}(k)$ is the four-dimensional Fourier transform of $M_{\lambda\mu}(x-y)$.

If the interaction is *spin-independent*, G, $G^{(0)}$ and M have the form

$$G_{\alpha\beta}(k) = \delta_{\alpha\beta} G(k) \quad G^{(0)}_{\alpha\beta}(k) = \delta_{\alpha\beta} G^{(0)}(k) \quad M_{\alpha\beta}(k) = \delta_{\alpha\beta} M(k).$$

In this case, Dyson's equation has the simple form

$$G(k) = G^{(0)}(k) + G^{(0)}(k) M(k) G(k) \tag{24.4}$$

from which we can solve directly for G:

$$G(k) = \frac{G^{(0)}(k)}{1 - G^{(0)}(k) M(k)} = \frac{1}{\left[G^{(0)}(k)\right]^{-1} - M(k)}.$$

The function $G^{(0)}$ is given by

$$G^{(0)}(k) = \lim_{\xi \to 0^+} \left[\frac{\theta(|\mathbf{k}| - k_F)}{\omega - \epsilon^{(0)}_k + i\xi} + \frac{\theta(k_F - |\mathbf{k}|)}{\omega - \epsilon^{(0)}_k - i\xi} \right].$$

The inverse is

$$\left[G^{(0)}(\mathbf{k},\omega)\right]^{-1} = \omega - \epsilon_k^{(0)} \quad \text{where, for example } \epsilon_k^{(0)} = |\mathbf{k}|^2/2m$$

irrespectively of whether $|\mathbf{k}| > k_F$ or $|\mathbf{k}| < k_F$. We then obtain the important representation

$$G(\mathbf{k},\omega) = \frac{1}{\omega - \epsilon_k^{(0)} - M(\mathbf{k},\omega)}. \tag{24.5}$$

This is an exact representation of the full Green's function for translationally invariant, spin-independent and not explicitly time-dependent systems. Since we know that the poles of the Green's function give the exact excitation energies of the system, the problem of finding these is reduced to solving the equation

$$\omega - \epsilon_k^{(0)} - M(\mathbf{k},\omega) = 0.$$

It is important to emphasize that any approximation that is used for the self-energy means a summation of infinitely many diagrams for the Green's function. If we for example take only the first-order diagrams $g_t^{(1)}$ and $g_x^{(1)}$ in the proper self-energy, $M \approx M^{(1)}$, we obtain the approximation for the Green's function shown in figure 24.12.

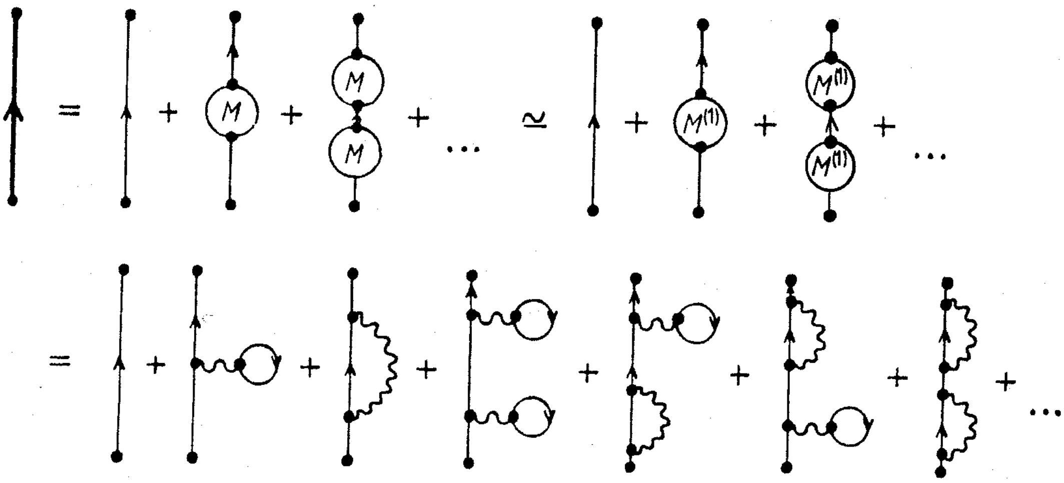


Figure 24.12 *Even the simplest first-order approximation for the self-energy means that an infinity of diagrams are included in the Green's function.*

Finally, we will also express the total energy of an interacting system through the self-energy. In Chapter 15, we derived the equation

$$E_0 = -\frac{i}{2}\frac{\Omega}{(2\pi)^4}\lim_{\tau\to 0^+}\int \mathrm{d}^3k \int \mathrm{d}^3\omega \, \mathrm{e}^{i\omega\tau}\left[\frac{|\mathbf{k}|^2}{2m} + \omega\right] \mathrm{Tr}\left\{G_{\alpha\beta}(\mathbf{k},\omega)\right\}.$$

With Dyson's equation and $\mathrm{Tr}\left\{G_{\alpha\beta}(k)\right\} = \mathrm{Tr}\left\{\delta_{\alpha\beta}G(k)\right\} = 2G(k)$, this equation becomes

$$E_0 = -i\frac{\Omega}{(2\pi)^4}\lim_{\tau\to 0^+}\int \mathrm{d}^3k \int \mathrm{d}\omega\, \mathrm{e}^{i\omega\tau}\frac{\frac{k^2}{2m}+\omega}{\omega-\frac{k^2}{2m}-M(\mathbf{k},\omega)}. \tag{24.6}$$

Chapter 25

Self-consistent perturbation theory, an advanced perspective on Hartree–Fock theory

In what follows, a self-energy diagram that does not contain any self-energy insertions other than itself will be called a skeleton. Examples of skeletons and diagrams that are not skeletons are given in figure 25.1. These skeletons are 'dressed' by inserting all possible self-energy insertions in each $G^{(0)}$-line and summing (see figure 25.2). Finally, by the summation all $G^{(0)}$-lines are replaced by full G-lines. One can easily convince oneself that the sum of all

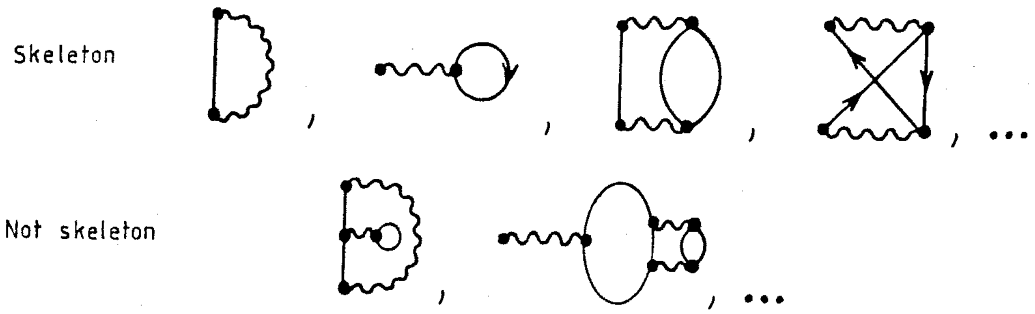
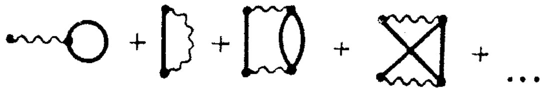


Figure 25.1 *The diagrams in the top row are skeleton diagrams. The diagrams in the bottom row consist of several self-energy insertions and are not skeletons.*

such dressed skeletons produces the full irreducible self-energy:

$$M = \sum_{\text{all dressed skeletons}} =$$



(25.1)

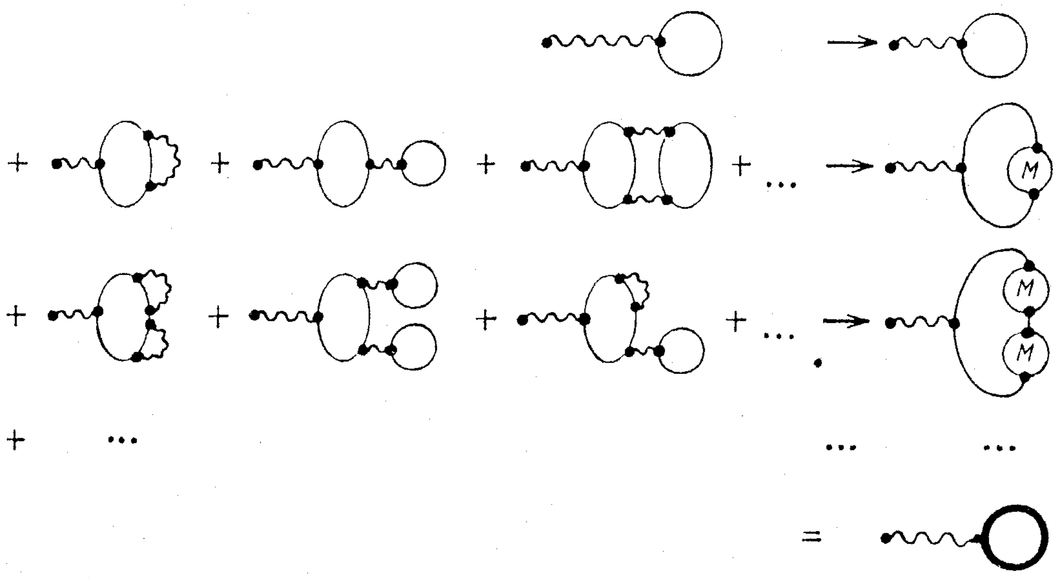
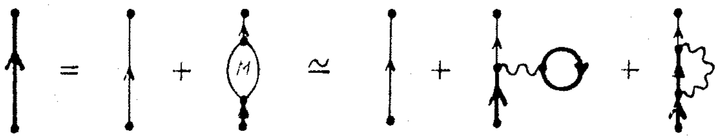


Figure 25.2 *The skeletons are dressed by inserting all possible self-energy insertions at all $G^{(0)}$-lines.*

If the sum is truncated after a finite number of dressed skeletons, for example after the two first-order dressed skeletons, we obtain through Dyson's equation an integral equation for the Green's function:



(25.2)

This equation must then be solved self-consistently; such approximations are called 'self-consistent perturbation theory'.

In what follows, we let

$$\begin{aligned} H_0 &= \int \mathrm{d}x\, \psi^\dagger(x) \left[-\frac{\nabla^2}{2m} + u(x)\right] \psi(x) \\ V &= \frac{1}{2}\int \mathrm{d}x \int \mathrm{d}x'\, \psi^\dagger(x)\psi^\dagger(x')v(x,x')\psi(x')\psi(x). \end{aligned}$$

(Here x denotes both space and spin variables as before; $x = (\mathbf{r}, s)$.) The Hamiltonian $H = H_0 + V$ does not depend on time. Therefore, it is suitable to go over to a Fourier representation with respect to $(t - t')$:

$$\begin{aligned} G(xt, x't') &= \int \frac{\mathrm{d}\omega}{2\pi} \mathrm{e}^{-i\omega(t-t')} G(x, x', \omega) \\ G^{(0)}(xt, x't') &= \int \frac{\mathrm{d}\omega}{2\pi} \mathrm{e}^{-i\omega(t-t')} G^{(0)}(x, x', \omega) \\ M(xt, x't') &= \int \frac{\mathrm{d}\omega}{2\pi} \mathrm{e}^{-i\omega(t-t')} M(x, x', \omega). \end{aligned}$$

If these expressions are inserted in the space–spin representation of Dyson's equation, we obtain a corresponding Dyson's equation for the Fourier components:

$$\begin{aligned} &G(x, x', \omega) \\ &= G^{(0)}(x, x', \omega) + \int \mathrm{d}y' \int \mathrm{d}y\, G^{(0)}(x, y', \omega) M(y', y, \omega) G(y, x', \omega) \end{aligned} \qquad (25.3)$$

We will now prove that Dyson's equation in this approximation, equation (25.3), is equivalent to the Hartree–Fock procedure derived in Chapter 7. The approximation for the self-energy can be represented as shown in figure 25.3. These diagrams are equivalent to the equation

$$\begin{aligned} &M(xt, x't') \\ &= (-)^1 i\delta(t-t')\delta(x-x') \int \mathrm{d}x_1 \int \mathrm{d}t_1\, G(x_1t_1, x_1t_1^+) v(x, x_1)\delta(t-t_1) \\ &\quad + (-)^0 iv(x, x')\delta(t-t')G(xt, x't') \\ &= \delta(t-t')\Big[-i\delta(x-x') \int \mathrm{d}x_1\, G(x_1t, x_1t^+) v(x, x_1) \\ &\quad + iv(x, x')G(xt, x't^+)\Big]. \end{aligned}$$

If we use $G(t, t^+) = G(0, (t^+ - t)) = G(0, 0^+)$, and perform the trivial Fourier transform with respect to $(t - t')$, we obtain the following expression for the irreducible self-energy:

$$\begin{aligned} M(x, x') &= \delta(x-x') \int \mathrm{d}x_1 \left[-iG(x_10, x_10^+)\right] v(x, x_1) \\ &\quad - v(x, x')\left[-iG(x0, x'0^+)\right] \end{aligned}$$

which is frequency-independent Furthermore, from the relation equation (15.15) between the Green's function and the density matrix we obtain

$$M(x, x') = \delta(x-x') \int \mathrm{d}x_1\, \rho(x_1) v(x, x_1) - v(x, x')\rho(x, x'). \qquad (25.4)$$

In this approximation, the irreducible self-energy corresponds precisely to the Hartree–Fock potential, equation (7.3) (disregarding the external part $u(x)$).

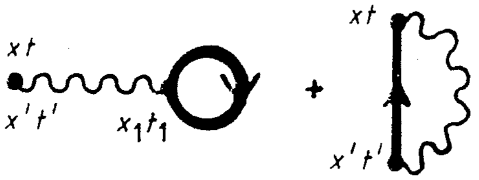


Figure 25.3 *Self-consistent first-order approximation for the self-energy.*

With the operator

$$h_0(x) = -\frac{\nabla^2}{2m} + u(x)$$

the Green's function $G^{(0)}(xt, x't')$ satisfies the equation of motion (*cf.* equations (16.8) and (16.9)):

$$\left[i\frac{\partial}{\partial t} - h_0(x)\right] G^{(0)}(xt, x't') = \delta(x - x')\delta(t - t').$$

By Fourier transforming with respect to $(t - t')$ it follows that

$$[\omega - h_0(x)]\, G^{(0)}(x, x', \omega) = \delta(x - x'). \tag{25.5}$$

If we operate with $(\omega - h_0(x))$ on Dyson's equation equation (25.3) and use equation (25.5), we obtain

$$[\omega - h_0(x)]\, G(x, x', \omega) - \int \mathrm{d}y\, M(x, y, \omega) G(y, x', \omega) = \delta(x - x'). \tag{25.6}$$

If we insert the approximation equation (25.4) in this equation, we obtain

$$[\omega - h_{HF}]\, G = 1. \tag{25.7}$$

This is the equation of motion for the Green's function for a system of *independent* particles, which move in an effective, self-consistently determined potential, which is precisely the Hartree–Fock potential. Thus, the statement is proved. For the sake of completeness, we will now also express the Greens' functions obtained from equation (25.7), which we will denote by G_{HF}, in terms of the Hartree–Fock single-particle orbitals. We have

$$h_{HF}\varphi_j(x) = \epsilon_j \varphi_j(x).$$

If we denote by $c_j^\dagger$ and c_j the creation and annihilation operators for these single-particle orbitals, we can express the field operators through these orbitals:

$$\psi(x) = \sum_j \varphi_j(x) c_j \quad \text{and} \quad \psi^\dagger(x) = \sum_j \varphi_j^*(x) c_k^\dagger.$$

In the Heisenberg picture, which is identical to the interaction picture for independent particles, we then have

$$\psi(xt)_H = \psi(xt)_I = \sum_j \varphi_j(x) c_j(t)_I = \sum_j \varphi_j(x) \mathrm{e}^{-i\epsilon_j t} c_j,$$

and, correspondingly,

$$\psi^\dagger(xt)_H = \sum_k \varphi_k^*(x) \mathrm{e}^{+i\epsilon_k t} c_k^\dagger.$$

The Green's function is then

$$\begin{aligned} & iG_{HF}(xt, x't') \\ &= \langle \Phi_0 \mid T\left[\psi(xt)_H \psi^\dagger(x't')_H\right] \mid \Phi_0\rangle \\ &= \sum_{jk} \mathrm{e}^{-i(\epsilon_j t - \epsilon_k t')} \varphi_j(x) \varphi_k^*(x') \\ &\quad \times \left[\theta(t-t') \underbrace{\langle \Phi_0 \mid c_j c_k^\dagger \mid \Phi_0\rangle}_{=\delta_{jk}\theta(\epsilon_j - \epsilon_F)} - \theta(t'-t) \underbrace{\langle \Phi_0 \mid c_k^\dagger c_j \mid \Phi_0\rangle}_{=\delta_{jk}\theta(\epsilon_F - \epsilon_j)}\right]. \end{aligned}$$

Thus, if the orbitals in the ground-state Slater determinants are occupied up to the maximum single-particle energy ϵ_F, we obtain for the Hartree–Fock Green's function:

$$\begin{aligned} & iG_{HF}(xt, x't') \\ &= \sum_j \varphi_j(x) \varphi_j^*(x') \mathrm{e}^{-\epsilon_j (t-t')} \\ &\quad \times \left[\theta(t-t')\theta(\epsilon_j - \epsilon_F) - \theta(t'-t)\theta(\epsilon_F - \epsilon_j)\right]. \end{aligned} \tag{25.8}$$

Finally, we obtain by Fourier transforming

$$G_{HF}(x, x'\omega) = \lim_{\eta \to 0^+} \sum_j \varphi_j(x) \varphi_j^*(x') \left[\frac{\theta(\epsilon_j - \epsilon_F)}{\omega - \epsilon_j + i\eta} + \frac{\theta(\epsilon_F - \epsilon_j)}{\omega - \epsilon_j - i\eta}\right]. \tag{25.9}$$

It can be verified by direct substitution that this Green's function satisfies the equation of motion equation (25.7). The only thing needed is the completeness of the Hartree–Fock single-particle basis.

The expansion of M in a series of dressed skeletons presents an interesting possibility for generalizing the usual Hartree–Fock procedure by including higher orders, for example as shown in figure 25.4. This diagram corresponds to

$$(-)^1 i^2 G(xt, x't') \int \mathrm{d}y \int \mathrm{d}y'\, v(x,y) v(x',y') G(yt, y't') G(y't', yt).$$

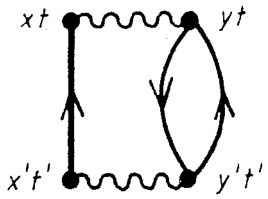


Figure 25.4 *This second-order diagram can be included in the equation for M to yield a higher-order Hartree–Fock approximation.*

In this case, M does really depend on the time difference $(t - t')$, *i.e.*, the Fourier transform will, in contrast to the Hartree–Fock approximation equation (25.4), depend on the frequency ω. It should be noted, that by such an approximation the integral operator $\int M(x,y,\omega)\_\_\_\mathrm{d}y$ in general is not hermitian, so that the corresponding term in equation (25.6) cannot readily be interpreted as an effective non-local single-particle potential. In spite of this, we can also in this case obtain a representation of the Green's function analogous to equation (25.9). To obtain this, the eigenvalue problems

$$[\epsilon_n(\omega) - h_0(x)]\, f_n(x,\omega) - \int \mathrm{d}y\, M(x,y,\omega) f_n(y,\omega) = 0 \qquad (25.10)$$

and

$$[\tilde{\epsilon}_n(\omega) - h_0(x)]\, \tilde{f}_n(x,\omega) - \int \mathrm{d}y\, M(y,x,\omega)^* \tilde{f}_n(y,\omega) = 0. \qquad (25.11)$$

are first solved for arbitrary ω. A simple calculation [19], shows that

$$\begin{aligned} \tilde{\epsilon}_n(\omega) &= \epsilon_n^*(\omega) && (25.12)\\ \int \mathrm{d}y\, \tilde{f}_n(y,\omega) f_{n'}(y,\omega) &= \delta_{n,n'} && (25.13)\\ \sum_n \tilde{f}_n(y',\omega) f_n(y,\omega) &= \delta(y-y'). && (25.14) \end{aligned}$$

In contrast to the eigenvalues (*cf.* equation (25.12)), the left and right eigenvectors in general are not complex conjugate:

$$\tilde{f}_n(y,\omega) \neq f_n(y,\omega)^*.$$

The Green's function then has the representation

$$G(x,x',\omega)=\sum_n \frac{f_n(x,\omega)\tilde{f}_n(x',\omega)}{\omega-\epsilon_n(\omega)} \tag{25.15}$$

which is readily demonstrated by substitution in equation (25.6) and using equations (25.10) and (25.14). If the equation

$$\omega-\epsilon_n(\omega)=0 \tag{25.16}$$

has solutions $\omega_{n\nu}$ for fixed n, the Green's function has, according to equation (25.15), poles at $\omega_{n\nu}$. These poles are in general complex. In the next chapter we will thoroughly discuss under which conditions the real and imaginary parts of these poles can be interpreted as excitation energies and inverse life-times of quasi-particles.

The equation (25.15) is an *exact* representation of the Green's function if the *exact* irreducible self-energy is inserted in equations(25.10) and (25.11). In this case, we can compare with the (also exact) Lehmann-representation of the Green's function, which was derived in Chapter 15 for translationally invariant systems (*cf.* equation (15.28)):

$$\begin{aligned} G(x,x',\omega) & \\ = \lim_{\eta\to 0^+} & \left[\sum_m \frac{\langle\Psi_0^N \mid \psi(x) \mid \Psi_m^{N+1}\rangle\langle\Psi_m^{N+1} \mid \psi^\dagger(x') \mid \Psi_0^N\rangle}{\omega-\mu-(E_m^{N+1}-E_0^{N+1})+i\eta}\right. \\ & \left.+\sum_m \frac{\langle\Psi_0^N \mid \psi^\dagger(x') \mid \Psi_m^{N-1}\rangle\langle\Psi_m^{N-1} \mid \psi(x) \mid \Psi_0^N\rangle}{\omega-\mu+(E_m^{N-1}-E_0^{N-1})-i\eta}\right]. \end{aligned} \tag{25.17}$$

Since the poles in equations (25.17) and (25.15) agree, the values $\omega_{n\nu}=\epsilon_n(\omega_{n\nu})\equiv\epsilon_m$ obtained from equation (25.16) must correspond to the exact excitation energies, reckoned from the chemical potential, for the $(N+1)$-particle system

$$\epsilon_m=\mu+(E_m^{N+1}-E_0^{N+1})-i\eta \tag{25.18}$$

or for the $(N-1)$-particle system

$$\epsilon_m=\mu-(E_m^{N-1}-E_0^{N-1})+i\eta. \tag{25.19}$$

Similarly, for the corresponding eigenvectors $f_n(x,\omega_{n\nu})\equiv\varphi_m(x)$ and $\tilde{f}_n(x,\omega_{n\nu})\equiv\tilde{\varphi}_m(x)$, we must have

$$\left.\begin{aligned} \varphi_m(x) &= \langle\Psi_0^N \mid \psi(x) \mid \Psi_m^{N+1}\rangle \\ \tilde{\varphi}_m(x) &= \langle\Psi_m^{N+1} \mid \psi^\dagger(x) \mid \Psi_0^N\rangle=\varphi_m^*(x) \end{aligned}\right\} \text{ for } \epsilon_m>\mu \tag{25.20}$$

and

$$\left.\begin{aligned} \varphi_m(x) &= \langle \Psi_m^{N-1} \mid \psi(x) \mid \Psi_0^N \rangle \\ \widetilde{\varphi}_m(x) &= \langle \Psi_0^N \mid \psi^\dagger(x) \mid \Psi_m^{N-1} \rangle = \varphi_m^*(x) \end{aligned}\right\} \text{ for } \epsilon_m \leq \mu. \tag{25.21}$$

We then obtain the following representation for the Green's function:

$$G(x, x', \omega) = \sum_m \frac{\varphi_m(x)\varphi_m^*(x')}{\omega - \epsilon_m}. \tag{25.22}$$

If we consider equation (25.10) at the frequencies $\omega = \epsilon_m (= \omega_{n\nu})$, we obtain

$$h_0(x)\varphi_m(x) + \int dy\, M(x, y, \epsilon_m)\varphi_m(y) = \epsilon_m \varphi_m(x). \tag{25.23}$$

This 'non-linear eigenvalue problem' gives an important re-formulation of Dyson's equation. It was first obtained by Schwinger [20].

Chapter 26

The quasi-particle concept

We recall that in Part I the first part of this book, which was concerned with the foundations of many-particle physics, we several times used various mathematical tricks to go from an interacting many-particle system to a system of non-interacting 'quasi-particles'. At this point it is now possible for us to introduce these in a systematic way and to understand them correctly.

The Green's function for free particles is (*cf.* equation (15.23))

$$\begin{aligned} iG^{(0)}(\mathbf{k},t) &= \theta(t)\left[e^{-i\epsilon_k t}\theta(|\mathbf{k}|-k_F)\right] \text{ (particle contribution)} \\ &\quad -\theta(-t)\left[e^{-i\epsilon_k t}\theta(k_F-|\mathbf{k}|)\right] \text{ (hole contribution).} \end{aligned}$$

This Green's function consists essentially of a time-dependent exponential function $\exp(-i\epsilon_k t)$, which says that a particle, or a hole, with a well-defined energy ϵ_k propagates in time. If a particle which has been added to the ground state of a many-particle system interacts with all other particles, the Green's function will in general be very complicated. However, we may ask under what conditions the time development of such a system can be interpreted as the propagation of a 'particle' with a reasonably well defined energy and a sufficiently long life-time. In other words, we ask under what conditions the propagator has the form

$$G(\mathbf{k},t) \approx e^{-i\epsilon(\mathbf{k})t}e^{-\Gamma(\mathbf{k})t}.$$

The dispersion relation $\epsilon(\mathbf{k})$ and the life-time $1/\Gamma(\mathbf{k})$ then reflect the interactions with the other particles; the effect of these interactions can be called the polarization of the medium. The initially 'bare' particle to a certain extent drags a polarization cloud with it and so becomes a 'dressed' particle with a different dispersion relation and life-time. We have already learnt about one such quasi-particle: the Hartree–Fock electron, which drags with it the exchange hole and consequently has a modified dispersion relation $\epsilon(\mathbf{k})$.

To answer the question whether the Green's function of an interacting system can be interpreted as a quasi-particle propagator, we must backtrack a little. We consider once again the Lehmann-representation of the Green's function for translationally invariant systems (*cf.* equation (15.28)):

$$\begin{aligned} G(\mathbf{k},\omega) \;=\; \lim_{\eta\to 0^+} & \left[\sum_n \frac{\left|\langle \Psi_n^{(N+1)}(\mathbf{k}) \mid c_{\mathbf{k}}^\dagger \mid \Psi_0^N\rangle\right|^2 / \langle \Psi_0^N \mid \Psi_0^N\rangle}{\omega-\mu-w_{n,\mathbf{k}}^{(N+1)}+i\eta} \right. \\ & \left. +\sum_n \frac{\left|\langle \Psi_n^{(N-1)}(-\mathbf{k}) \mid c_{\mathbf{k}} \mid \Psi_0^N\rangle\right|^2 / \langle \Psi_0^N \mid \Psi_0^N\rangle}{\omega-\mu+w_{n,-\mathbf{k}}^{(N-1)}-i\eta} \right]. \end{aligned}$$

Here

$$w_{n,\pm\mathbf{k}}^{(N\pm 1)} \equiv E_n^{(N\pm 1)}(\pm\mathbf{k}) - E_0^{(N\pm 1)} > 0.$$

The first term in the expression for G has a pole at

$$\omega = \mu + w_{n,\mathbf{k}}^{(N+1)} - i\eta$$

and the second term has a pole at

$$\omega = \mu - w_{n,-\mathbf{k}}^{(N-1)} + i\eta.$$

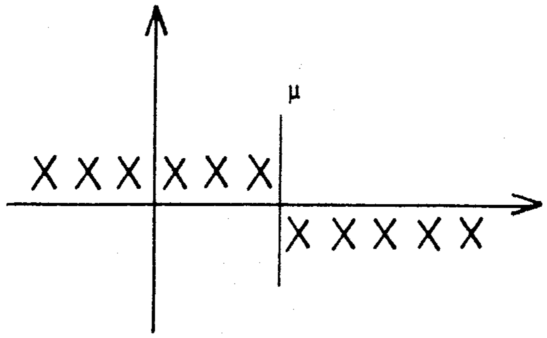


Figure 26.1 *Location of the poles of the Green's function in the complex ω-plane.*

We introduce the *retarded* and *advanced* Green's functions:

$$iG^R(\mathbf{r}t,\mathbf{r}'t') \;\equiv\; \theta(t-t')\frac{\langle \Psi_0 \mid \left\{\psi(\mathbf{r}t)_H,\psi^\dagger(\mathbf{r}'t')_H\right\} \mid \Psi_0\rangle}{\langle \Psi_0 \mid \Psi_0\rangle} \tag{26.1}$$

$$iG^A(\mathbf{r}t,\mathbf{r}'t') \;\equiv\; -\theta(t'-t)\frac{\langle \Psi_0 \mid \left\{\psi(\mathbf{r}t)_H,\psi^\dagger(\mathbf{r}'t')_H\right\} \mid \Psi_0\rangle}{\langle \Psi_0 \mid \Psi_0\rangle} \tag{26.2}$$

where the curly brackets denote the anti-commutator of the field operators, as usual. The Lehmann representation of G and $G^{R/A}$ only differ in the sign of the small imaginary part in the denominator:

$$\begin{aligned} G^R(\mathbf{k},\omega) &= \lim_{\eta\to 0+}\left[\sum_n \frac{\left|\langle\Psi_n^{(N+1)}(\mathbf{k}) \mid c_{\mathbf{k}}^{\dagger} \mid \Psi_0^N\rangle\right|^2/\langle\Psi_0^N \mid \Psi_0^N\rangle}{\omega-\mu-w_{n,\mathbf{k}}^{(N+1)}+i\eta}\right. \\ &\quad \left. +\sum_n \frac{\left|\langle\Psi_n^{(N-1)}(-\mathbf{k}) \mid c_{\mathbf{k}} \mid \Psi_0^N\rangle\right|^2/\langle\Psi_0^N \mid \Psi_0^N\rangle}{\omega-\mu+w_{n,-\mathbf{k}}^{(N-1)}+i\eta}\right] \end{aligned}$$

with poles at

$$\omega=\mu+w_{n,\mathbf{k}}^{(N+1)}-i\eta$$

and

$$\omega=\mu-w_{n,-\mathbf{k}}^{(N-1)}-i\eta;$$

$$\begin{aligned} G^A(\mathbf{k},\omega) &= \lim_{\eta\to 0+}\left[\sum_n \frac{\left|\langle\Psi_n^{(N+1)}(\mathbf{k}) \mid c_{\mathbf{k}}^{\dagger} \mid \Psi_0^N\rangle\right|^2/\langle\Psi_0^N \mid \Psi_0^N\rangle}{\omega-\mu-w_{n,\mathbf{k}}^{(N+1)}-i\eta}\right. \\ &\quad \left. +\sum_n \frac{\left|\langle\Psi_n^{(N-1)}(-\mathbf{k}) \mid c_{\mathbf{k}} \mid \Psi_0^N\rangle\right|^2/\langle\Psi_0^N \mid \Psi_0^N\rangle}{\omega-\mu+w_{n,-\mathbf{k}}^{(N-1)}-i\eta}\right] \end{aligned}$$

with poles at

$$\omega=\mu+w_{n,\mathbf{k}}^{(N+1)}+i\eta$$

and

$$\omega=\mu-w_{n,-\mathbf{k}}^{(N-1)}+i\eta.$$

In contrast to G, the Green's functions G^R and G^A are analytic in the upper and lower ω-plane, respectively. We note that

$$G^R(\mathbf{k},\omega)^*=G^A(\mathbf{k},\omega) \quad \text{for } \omega\in\mathcal{R}. \tag{26.3}$$

For $\mu\neq\omega$ and $\mu\in\mathcal{R}$ we can in each case calculate the limit $\eta\to 0$ with the result

$$\mu<\omega \;:\; G(\mathbf{k},\omega)=G^R(\mathbf{k},\omega) \quad \mu\in\mathcal{R} \tag{26.4}$$

$$\mu>\omega \;:\; G(\mathbf{k},\omega)=G^A(\mathbf{k},\omega) \quad \mu\in\mathcal{R}. \tag{26.5}$$

We insert these relations in

$$G(\mathbf{k},t)=\int_{-\infty}^{+\infty}\frac{\mathrm{d}\omega}{2\pi}\mathrm{e}^{-i\omega t}G(\mathbf{k},\omega)$$

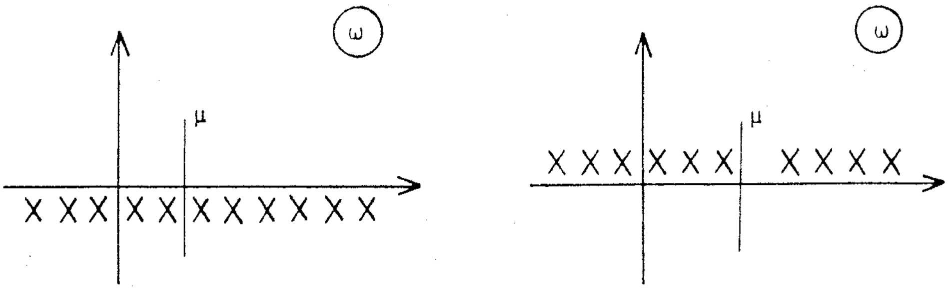


Figure 26.2 *Location of the poles of the retarded and advanced Green's function.*

which yields

$$G(\mathbf{k},t)=\int_{-\infty}^{\mu}\frac{\mathrm{d}\omega}{2\pi}\mathrm{e}^{-i\omega t}G^{A}(\mathbf{k},\omega)+\int_{\mu}^{+\infty}\frac{\mathrm{d}\omega}{2\pi}\mathrm{e}^{-i\omega t}G^{R}(\mathbf{k},\omega). \tag{26.6}$$

We use the integration path in the complex ω-plane shown in figure 26.3 to further evaluate these integrals.

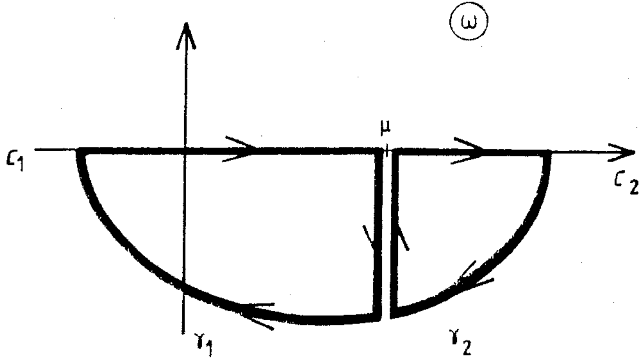


Figure 26.3 *Integration path for equation (26.6). The integration path is divided into two pieces C_1 and C_2 with circular arcs γ_1 and γ_2, respectively.*

We have

$$\begin{aligned}\int_{C_1}&\frac{\mathrm{d}\omega}{2\pi}\mathrm{e}^{-i\omega t}G^{A}(\mathbf{k},\omega)\\ &=\int_{-\infty}^{\mu}\frac{\mathrm{d}\omega}{2\pi}\mathrm{e}^{-i\omega t}G^{A}(\mathbf{k},\omega)+\int_{\mu}^{\mu-i\infty}\frac{\mathrm{d}\omega}{2\pi}\mathrm{e}^{-i\omega t}G^{A}(\mathbf{k},\omega)\\ &\quad+\int_{\gamma_1}\frac{\mathrm{d}\omega}{2\pi}\mathrm{e}^{-i\omega t}G^{A}(\mathbf{k},\omega)=0\end{aligned}$$

since $G^{A}(\mathbf{k},\omega)$ has no poles below the real axis. The exponential makes the integral over the circular arc go to zero in the limit of infinite radius so that the first term for $G(\mathbf{k},t)$ becomes

$$\int_{-\infty}^{\mu}\frac{\mathrm{d}\omega}{2\pi}\mathrm{e}^{-i\omega t}G^A(\mathbf{k},\omega)=\int_{\mu-i\infty}^{\mu}\frac{\mathrm{d}\omega}{2\pi}\mathrm{e}^{-i\omega t}G^A(\mathbf{k},\omega).$$

We rewrite the second term of $G(\mathbf{k},t)$ in equation (26.6) in a corresponding way, but now we have to take into account the fact that G^R may have poles at ω_ν with residues z_ν in the enclosed area:

$$\begin{aligned}
&\int_{C_2}\frac{\mathrm{d}\omega}{2\pi}\mathrm{e}^{-i\omega t}G^R(\mathbf{k},\omega)\\
&= \int_{\mu}^{\infty}\frac{\mathrm{d}\omega}{2\pi}\mathrm{e}^{-i\omega t}G^R(\mathbf{k},\omega)+\underbrace{\int_{\gamma_2}\frac{\mathrm{d}\omega}{2\pi}\mathrm{e}^{-i\omega t}G^R(\mathbf{k},\omega)}_{=0}\\
&\quad+\int_{\mu-i\infty}^{\mu}\frac{\mathrm{d}\omega}{2\pi}\mathrm{e}^{-i\omega t}G^R(\mathbf{k},\omega)\\
&= -i\sum_{\nu}z_\nu\mathrm{e}^{-i\omega_n ut}.
\end{aligned}$$

Thus,

$$\int_{\mu}^{\infty}\frac{\mathrm{d}\omega}{2\pi}\mathrm{e}^{-i\omega t}G^R(\mathbf{k},\omega)=-i\sum_{\nu}z_\nu\mathrm{e}^{-i\omega_\nu t}-\int_{\mu-i\infty}^{\mu}\frac{\mathrm{d}\omega}{2\pi}\mathrm{e}^{-i\omega t}G^R(\mathbf{k},\omega).$$

From these expressions, we obtain the following result for the Green's function $G(\mathbf{k},\omega)$ after separating ω_ν in real and imaginary parts $\omega_\nu=\epsilon_\nu-i\Gamma_\nu$:

$$G(\mathbf{k},t)=-i\sum_{\nu}z_\nu\mathrm{e}^{-i\epsilon_\nu t}\mathrm{e}^{-\Gamma_\nu t}+\int_{\mu-i\infty}^{\mu}\frac{\mathrm{d}\omega}{2\pi}\mathrm{e}^{-i\omega t}\left[G^A(\mathbf{k},\omega)-G^R(\mathbf{k},\omega)\right].$$

Suppose now that the pole at $\omega_0=\epsilon_0-i\Gamma_0$ is closest to the real axis of all poles, *i.e.*, $\Gamma_0<\Gamma_\nu$ for $\nu\neq 0$. For sufficiently large times, we can then write

$$-i\sum_{\nu}z_\nu\mathrm{e}^{-i\epsilon_\nu t}\mathrm{e}^{-\Gamma_\nu t}\approx -iz_0\mathrm{e}^{-i\epsilon_0 t}\mathrm{e}^{-\Gamma_0 t}.$$

Of course, we cannot wait so long that the contribution from this pole dies out; thus, we consider times of the order

$$\frac{1}{\Gamma_\nu}<t\lesssim\frac{1}{\Gamma_0}. \tag{26.7}$$

For such times, the Green's function $G(\mathbf{k},t)$ is

$$G(\mathbf{k},t)\approx -iz_0\mathrm{e}^{-i\epsilon_0 t}\mathrm{e}^{-\Gamma_0 t}+\int_{\mu-i\infty}^{\mu}\frac{\mathrm{d}\omega}{2\pi}\mathrm{e}^{-i\omega t}\left[G^A(\mathbf{k},\omega)-G^R(\mathbf{k},\omega)\right]. \tag{26.8}$$

All that remains is to investigate under what conditions the integral may be neglected.

The quantity $(\epsilon_0 - \mu) > 0$, *i.e.*, the distance from the Fermi energy to the quasi-particle energy, is a measure of the energy and hence of the deviation from the ground state to which the quasi-particle is related. In order to guarantee a reasonably well-defined energy, the quasi-particle must propagate at least for a time $t \gg 1/(\epsilon_0 - \mu)$, according to the energy-time uncertainty principle. We will now show that this condition together with equation (26.7), *i.e.*,

$$\frac{1}{\epsilon_0 - \mu} \ll t \lesssim \frac{1}{\Gamma_0} \tag{26.9}$$

are sufficent conditions to let us neglect the integral term. The condition $\Gamma_0 \ll \epsilon - \mu$ is contained implicitly in this inequality, *i.e.*, the life-time of the quasi-particle must be large enough for an accurate measurement of the quasi-particle to be at all possible. Hence, the pole must be *very close* to the real axis.

The integrand vanishes for large imaginary parts of ω. Hence, only the contributions close to the real axis play any role. For an estimate of the integrand, we can then take ω to be real

$$G^{R/A}(\mathbf{k},\omega) \approx G^{R/A}(\mathbf{k},\omega_{\mathrm{real}}).$$

Under the assumption discussed above, *i.e.*, that the pole is very close to the real axis, the poles dominate the integrals for real values of ω, so we have

$$G^R(\mathbf{k},\omega) \approx \frac{z_0}{\omega - \epsilon_0 + i\Gamma_0}$$

and by using equation (26.3):

$$G^A(\mathbf{k},\omega) = \left[G^R(\mathbf{k},\omega)\right]^* \approx \frac{z_0}{\omega - \epsilon_0 - i\Gamma_0}.$$

Hence, the integral in equation (26.8) is approximately

$$\begin{aligned} I &\equiv \int_{\mu-i\infty}^{\mu} \frac{\mathrm{d}\omega}{2\pi} \mathrm{e}^{-i\omega t} \left[G^A(\mathbf{k},\omega) - G^R(\mathbf{k},\omega)\right] \\ &\approx 2iz_0\Gamma_0 \int_{\mu-i\infty}^{\mu} \frac{\mathrm{d}\omega}{2\pi} \frac{\mathrm{e}^{-i\omega t}}{(\omega - \epsilon_0)^2 + \Gamma_0^2} \end{aligned}$$

and with the substitution $y \equiv i(\omega - \mu)$, $\omega = \mu - iy$, $\mathrm{d}\omega = -i\,\mathrm{d}y$ the integral I becomes

$$-\frac{z_0\Gamma_0}{\pi}\mathrm{e}^{-i\mu t} \int_0^{\infty} \mathrm{d}y \frac{\mathrm{e}^{-yt}}{\Gamma_0^2 + (\epsilon_0 - \mu + iy)^2}.$$

If now $t \gg 1/(\epsilon_0 - \mu)$, then $\exp(-yt)$ is different from zero essentially only if $y \ll \epsilon_0 - \mu$. However, in this region the denominator is

$$\Gamma_0^2 + (\epsilon_0 - \mu + iy)^2 \approx \Gamma_0^2 + (\epsilon_0 - \mu)^2 \approx (\epsilon_0 - \mu)^2$$

so that

$$\begin{aligned} I &\approx -\frac{z_0\Gamma_0}{\pi} e^{-i\mu t} \int_0^\infty dy \frac{e^{-yt}}{(\epsilon_0 - \mu)^2} = -\frac{z_0\Gamma_0}{\pi} \frac{e^{-i\mu t}}{t(\epsilon_0 - \mu)^2} \\ &\approx -\frac{z_0}{\pi} e^{-i\mu t} \underbrace{t^{-2}(\epsilon_0 - \mu)^{-2}}_{\ll 1} \end{aligned}$$

for $t \approx 1/\Gamma_0$. Thus, the integral is much smaller than $|z_0|$ under the given assumptions, whereas $\exp(-\Gamma_0 t) \approx 1$ in the time interval under consideration, so that

$$\left| -iz_0 e^{-i\epsilon_0 t} e^{-\Gamma_0 t} \right| \approx |z_0|.$$

The contribution from the integral in equation (26.8) can then be neglected. Only the contributions from the poles next to the real axis remain:

$$G(\mathbf{k}, t) \approx -iz(\mathbf{k}) e^{-i\epsilon(\mathbf{k})t} e^{-\Gamma(\mathbf{k})t} \text{ for } t > 0.$$

In this equation, the dependence of the position and residue of the pole on **k** are emphasized by a transparent change in notation.

In the considerations above, it was assumed that $t > 0$. For $t < 0$, one obtains a completely analogous expression for the propagation of 'quasi-holes'. In the derivation, the integration path must in this case close in the upper complex ω-plane. In all, the final result is

$$\begin{aligned} G(\mathbf{k}, t) &= -iz(\mathbf{k}) \Big[\theta(t)\theta(\epsilon(\mathbf{k}) - \mu) e^{-i\epsilon(\mathbf{k})t} e^{-\Gamma(\mathbf{k})t} \\ &\quad - \theta(-t)\theta(\mu - \epsilon(\mathbf{k})) e^{-i\epsilon(\mathbf{k})t} e^{-\Gamma(\mathbf{k})t} \Big] + I(\mathbf{k}, t) \qquad (26.10) \end{aligned}$$

where all terms discussed which are negligible under the condition equation (26.9) are included in $I(\mathbf{k}, t)$.

Any approximation for the irreducible self-energy gives an approximation for the Green's function. From the representation given in equation (24.5)

$$G(\mathbf{k}, \omega) = \frac{1}{\omega - \frac{k^2}{2m} - M(\mathbf{k}, \omega)} \qquad (26.11)$$

the pole, and consequently the dispersion relation and the life-time of the resulting quasi-particle, can be read off immediately. We will now investigate the approximation

$$M \approx M^{(1)} \qquad (26.12)$$

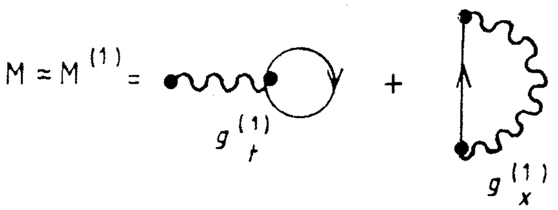


Figure 26.4 *The self-energy diagrams* $g_t^{(1)}$ *and* $g_x^{(1)}$ *in the Hartree–Fock approximation for* M.

where $M^{(1)}$ is the self-energy in the Hartree–Fock approximation (see figure 26.4), in detail. Since the Hartree–Fock equation for translationally invariant systems is satisfied by plane waves, it is clear from the considerations in the previous chapters that the approximation equation (26.12) will give the dispersion relation and life-time for the Hartree–Fock quasi-particles. In what follows, we will explicitly prove this.

The first diagram, $g_t^{(1)}$, only gives a contribution for the $q = 0$ Fourier component, because of momentum conservation:

$$\begin{aligned}
g_t^{(1)} &= (-1)^1 i \lim_{\eta\to 0^+} \int \frac{\mathrm{d}^3 q'}{(2\pi)^3} \int \frac{\mathrm{d}\omega}{2\pi} v(q=0) \mathrm{e}^{i\omega\eta} G^{(0)}(\mathbf{q}',\omega) \\
&= -iv(q=0) \int \frac{\mathrm{d}^3 q'}{(2\pi)^3} G^{(0)}(\mathbf{q}', t=0^+) \\
&= -iv(q=0) \underbrace{\lim_{(\mathbf{r}-\mathbf{r}')\to 0} \int \frac{\mathrm{d}^3 q'}{(2\pi)^3} \mathrm{e}^{i\mathbf{q}'\cdot(\mathbf{r}-\mathbf{r}')} G^{(0)}(\mathbf{q}', t=0^+)}_{=G^{(0)}(\mathbf{r},\mathbf{r}',t=0^+)} \\
&= v(q=0)\left[-iG^{(0)}(\mathbf{r},\mathbf{r},t=0^+)\right] \\
&= v(q=0)\left[\frac{N}{\Omega}\right]
\end{aligned}$$

where in the last step we used the relation between the Green's function and the particle density, which we proved in Chapter 15.

The second diagram, $g_x^{(1)}$, yields (for instantaneous, *i.e.*, frequency-independent, interactions)

$$g_x^{(1)} = (-)^0 i \lim_{\eta\to 0^+} \int \frac{\mathrm{d}^3 q}{(2\pi)^3} \int \frac{\mathrm{d}\omega}{2\pi} \mathrm{e}^{i\omega\eta} G^{(0)}(\mathbf{q},\omega) v(\mathbf{k}-\mathbf{q}).$$

Insertion of the explicit expression equation (15.26) for $G^{(0)}$ in this equation yields

$$i \lim_{\eta\to 0^+} \int \frac{\mathrm{d}^3 q}{(2\pi)^3} \int \frac{\mathrm{d}\omega}{2\pi} \mathrm{e}^{i\omega\eta} \lim_{\xi\to 0^+} \left[\frac{\theta(|\mathbf{q}|-k_F)}{\omega-\epsilon_q^{(0)}+i\xi} + \frac{\theta(k_F-|\mathbf{q}|)}{\omega-\epsilon_q^{(0)}-i\xi} \right] v(\mathbf{k}-\mathbf{q}).$$

By making the substitution $\omega^{(\mathrm{new})} \equiv \epsilon_q^{(0)} - \omega^{(\mathrm{old})}$ together with the representation equation (15.24) of the step-function we finally obtain

$$\begin{aligned} g_x^{(1)} &= i\int \frac{\mathrm{d}^3q}{(2\pi)^3}\left[\theta(|\mathbf{q}|-k_F)\lim_{\eta\to 0^+} \mathrm{e}^{i\eta\epsilon_q^{(0)}} \underbrace{\lim_{\xi\to 0^+}\int \frac{\mathrm{d}\omega}{2\pi}\frac{\mathrm{e}^{-i\omega\eta}}{-\omega+i\xi}}_{=-i\theta(-\eta)=0}\right. \\ &\quad \left. -\,\theta(k_F-|\mathbf{q}|)\lim_{\eta\to 0^+} \mathrm{e}^{i\eta\epsilon_q^{(0)}} \underbrace{\lim_{\xi\to 0^+}\int \frac{\mathrm{d}\omega}{2\pi}\frac{\mathrm{e}^{-i\omega\eta}}{+\omega+i\xi}}_{=-i\theta(+\eta)=-i}\right] v(\mathbf{k}-\mathbf{q}). \end{aligned}$$

We obtain in total

$$M^{(1)}(\mathbf{k},w) = M^{(1)}(\mathbf{k}) = v(q=0)\left[\frac{N}{\Omega}\right] - \int \frac{\mathrm{d}^3q}{(2\pi)^3}\theta(k_F-|\mathbf{q}|)v(\mathbf{k}-\mathbf{q}). \tag{26.13}$$

Thus, the pole of the Greens' function equation (26.11) is at

$$\omega = \frac{k^2}{2m} + M^{(1)}(\mathbf{k})$$

i.e., we have a quasi-particle with

- a dispersion relation

  $$\epsilon(\mathbf{k}) = \frac{k^2}{2m} + v(q=0)\left[\frac{N}{\Omega}\right] - \int \frac{\mathrm{d}^3}{(2\pi)^3}\theta(k_F-|\mathbf{q}|)v(\mathbf{k}-\mathbf{q}).$$

  This is precisely the dispersion relation equation (9.4) (for $k_+ = k_- = k_F$) that we derived for translationally invariant system in the Hartree–Fock approximation;

- an imaginary part $\Gamma(\mathbf{k}) = 0$, *i.e.*, the life-time of the Hartree–Fock quasi-particle is infinite.

We end this example by quoting from Chapter 10 the value of the integral in equation (26.13) for the electron gas:

$$M^{(1)}(\mathbf{k}) = -\frac{e^2k_F}{\pi}\left[1 + \frac{k_F^2-k^2}{2kk_F}\ln\left|\frac{k_F+k}{k_F-k}\right|\right]. \tag{26.14}$$

Up to this point, we have been able to say that we can, under certain conditions, interpret the full Green's function as a quasi-particle propagator.

The example of the Hartree–Fock electron showed that such quasi-particles can indeed appear. The question now arises if such quasi-particles can appear in any system, or if they are very singular phenomena. The answer is:

> **In any many-particle system for which perturbation theory converges, there are quasi-particles in the vicinity of the chemical potential μ.**

To prove this statement, we use the following fact:

$$\lim_{\omega \to \mu} \mathrm{Im}[M(\mathbf{k},\omega)] = \mathrm{sgn}(\mu - \omega) c(\mathbf{k})(\omega - \mu)^2 \tag{26.15}$$

where $c(\mathbf{k}) \geq 0$; $c(\mathbf{k}) \in \mathcal{R}$. We will now outline the proof (for details, see [21]). In the first step of the proof, one shows that

(1) $\lim_{\omega \to \mu} \mathrm{Im}[M^{(2)}_{g_c^{(2)}}] = \mathrm{sgn}(\mu - \omega)(\omega - \mu)^2$.

In the next step, one shows that the contribution from the corresponding dressed diagram behaves in the same way:

(2) $\lim_{\omega \to \mu} \mathrm{Im}[M_{\tilde{g}_c^{(2)}}] = \mathrm{sgn}(\mu - \omega)(\omega - \mu)^2$.

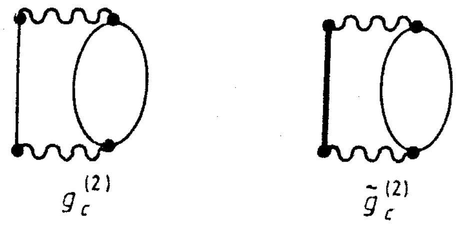


Figure 26.5 *The lowest-order contribution to the life-time of a quasi-particle comes from the skeleton diagram $g_c^{(2)}$. The corresponding diagram with the dressed Green's function is $\tilde{g}_c^{(2)}$.*

To do this, one uses the representation equation (15.29) for the Green's function:

$$G(\mathbf{k},\omega) = \lim_{\xi \to 0^+} \int_0^\infty d\epsilon \left[\frac{A(\mathbf{k},\epsilon)}{\omega - \mu - \epsilon + i\xi} + \frac{B(\mathbf{k},\epsilon)}{\omega - \mu + \epsilon - i\xi} \right].$$

The dependence of the integrand on ω corresponds to the frequency dependence of $G^{(0)}(\mathbf{k},\omega)$, which allows for using the estimate (1) in (2).

Finally, in the last step one shows that as $\omega \to \mu$, the imaginary part of an arbitrary dressed skeleton either behaves as (2) or vanishes faster than $(\omega-\mu)^2$. According to equation (25.1) the irreducible self-energy is obtained from the sum of all dressed skeletons, from which equation (26.14) follows for any system for which perturbation theory converges.

The poles

$$\omega(\mathbf{k}) = \epsilon(\mathbf{k}) - i\Gamma(\mathbf{k})$$

of the Green's function are determined by the equation

$$\omega - \epsilon_k^{(0)} - \mathrm{Re}[M(\mathbf{k},\omega)] - i\mathrm{Im}[M(\mathbf{k},\omega)] = 0. \qquad (26.16)$$

On the basis of equation (26.15), we will now show that for excitation energies close to the Fermi surface (*i.e.*, for $\epsilon(\mathbf{k}) \approx \mu$), the existence condition for quasi-particles, $\Gamma(\mathbf{k}) \ll \epsilon(\mathbf{k}) - \mu$, must be satisfied.

To obtain an estimate for $\Gamma(\mathbf{k})$ (for the case $\epsilon(\mathbf{k}) \approx \mu$), we expand equation (26.16) about the exact real part of $\epsilon(\mathbf{k})$:

$$\begin{aligned} 0 &= \omega - \epsilon_k^{(0)} - M(\mathbf{k},\omega) \\ &\approx \epsilon(\mathbf{k}) - \epsilon_k^{(0)} - \mathrm{Re}\left\{M(\mathbf{k},\epsilon(\mathbf{k}))\right\} - i\,\mathrm{Im}\left\{M(\mathbf{k},\epsilon(\mathbf{k}))\right\} \\ &\quad + \left[1 - \frac{\partial}{\partial\omega'}\,\mathrm{Re}\left\{M(\mathbf{k},\omega')\right\}\Big|_{\omega'=\epsilon(\mathbf{k})}\right][\omega - \epsilon(\mathbf{k})]. \end{aligned}$$

In the expansion of the imagainary part of M, only the lowest-order contributions will be considered, since the imaginary part is in any case very small in the vicinity of $\omega \approx \mu \approx \epsilon(\mathbf{k})$. We obtain the following estimate for $\Gamma(\mathbf{k})$:

$$\begin{aligned} \Gamma(\mathbf{k}) &\approx -\frac{\mathrm{Im}\left\{M(\mathbf{k},\epsilon(\mathbf{k}))\right\}}{1 - \frac{\partial}{\partial\omega'}\mathrm{Re}\left\{M(\mathbf{k},\omega')\right\}\Big|_{\omega'=\epsilon(\mathbf{k})}} \\ &\approx -\frac{\mathrm{sgn}\,[\mu - \epsilon(\mathbf{k})]\,c(\mathbf{k})\,[\epsilon(\mathbf{k}) - \mu]^2}{1 - \frac{\partial}{\partial\omega'}\mathrm{Re}\left\{M(\mathbf{k},\omega')\right\}\Big|_{\omega'=\epsilon(\mathbf{k})}}. \end{aligned}$$

For quasi-particles, *i.e.*, for $\epsilon(\mathbf{k}) > \mu$, Γ is positive and is near the Fermi surface negligibly small compared to $\epsilon(\mathbf{k}) - \mu$, due to the factor $(\epsilon(\mathbf{k}) - \mu)^2$. This is precisely what we wanted to show.

For quasi-holes, Γ is negative, which in view of the form $e^{-\Gamma(\mathbf{k})t}$ for $t < 0$ is quite sensible. Thus, we conclude that $\Gamma(\mathbf{k})$ changes sign at the Fermi surface $\epsilon(\mathbf{k}) = \mu$. Near the Fermi surface we also have for $\epsilon(\mathbf{k}) < \mu$:

$$|\Gamma(\mathbf{k})| \ll |\epsilon(\mathbf{k}) - \mu|.$$

For calculations and to gain physical insight, it is often useful to assign an *effective mass* to quasi-particles (and quasi-holes). To do so, essentially two different possible definitions are used:

(1) For non-interacting systems, we have

$$\epsilon_k^{(0)} = \frac{k^2}{2m} \quad \text{so} \quad \partial_{k_i}\partial_{k_j}\epsilon_k^{(0)} = \frac{1}{m}\delta_{ij}.$$

It is then natural to define an effective-mass tensor at a wavevector $\mathbf{k}_0$ for an arbitrary dispersion relation $\epsilon(\mathbf{k})$ by

$$\left[\frac{1}{m^*}\right]_{ij} \equiv \partial_{k_i}\partial_{k_j}\epsilon(\mathbf{k})\Big|_{\mathbf{k}=\mathbf{k}_0}. \tag{26.17}$$

(2) If we are interested in a dispersion relation $\epsilon(\mathbf{k})$ in the neighborhood of a particular point $\mathbf{k}_0$ (for example a 'band edge' in solid state physics), we can expand $\epsilon(\mathbf{k})$ about $\mathbf{k}_0$ to first order

$$\epsilon(\mathbf{k}) \approx \epsilon(\mathbf{k}_0) + [\nabla\epsilon(\mathbf{k})]_{\mathbf{k}_0}\cdot(\mathbf{k}-\mathbf{k}_0)$$

and compare this with the corresponding expansion for a free particle

$$\epsilon_k^{(0)}(\mathbf{k}) = \frac{k^2}{2m} \approx \frac{k_0^2}{2m} + \frac{1}{m}\mathbf{k}_0\cdot(\mathbf{k}-\mathbf{k}_0) = \epsilon_{k_0}^{(0)} + \frac{1}{m}\mathbf{k}_0\cdot(\mathbf{k}-\mathbf{k}_0)$$

and demand that

$$\sum_{j=1}^{3}\left[\frac{1}{m^{**}}\right]_{ij} k_0^j \equiv (\nabla\epsilon(\mathbf{k}))^i_{\mathbf{k}=\mathbf{k}_0}.$$

The simplest choice is

$$\left[\frac{1}{m^{**}}\right]_{ij} = \frac{(\nabla\epsilon(\mathbf{k}))^i_{\mathbf{k}=\mathbf{k}_0}}{k_0^i}\delta_{ij}. \tag{26.18}$$

For the quasi-particles and quasi-holes discussed here, the effective mass is closely related to the irreducible self-energy. This relation is worth remembering.

We have now come to an application of the quasi-particle concept: The definition of the effective mass $\frac{1}{m^*}$ gives us the possibility of considering an 'effective Newton's equation of motion' for the quasi-particles. To this end, we construct a wavepacket of quasi-particles, which moves with a group velocity $\mathbf{v}_{\text{gr}} = \nabla_{\mathbf{k}}\epsilon(\mathbf{k})$. The work $\Delta\epsilon$ done by an external force $\mathbf{F}$ on the quasi-particle in a time Δt is $\Delta\epsilon = \mathbf{F}\cdot\mathbf{v}_{\text{gr}}\Delta t$. We also have $\Delta\epsilon = \nabla_{\mathbf{k}}\epsilon(\mathbf{k})\cdot\Delta\mathbf{k} = \mathbf{v}_{\text{gr}}\cdot\Delta\mathbf{k}$. By combining these expression we obtain (as $\Delta t \to 0$):

$$\lim_{\Delta t\to 0}\mathbf{v}_{\text{gr}}\cdot\frac{\Delta\mathbf{k}}{\Delta t} = \mathbf{v}_{\text{gr}}\cdot\frac{d\mathbf{k}}{dt} = \mathbf{v}_{\text{gr}}\cdot\mathbf{F}. \tag{26.19}$$

This is a 'quasi-Newtonian equation': if $\mathbf{v}_{\mathrm{gr}}$ could be canceled out, we would obtain $\mathrm{d}\mathbf{k}/\mathrm{d}t = \mathbf{F}$.

We obtain for the ith component of the acceleration of the quasi-particles:

$$\begin{aligned} a_i &\equiv \frac{\mathrm{d}}{\mathrm{d}t}\left[\mathbf{v}_{\mathrm{gr}}\right]_i = \partial_{k_i}\frac{\mathrm{d}}{\mathrm{d}t}\epsilon(\mathbf{k}) = \partial_{k_i}\left[\frac{\mathrm{d}\mathbf{k}}{\mathrm{d}t}\cdot\nabla_{\mathbf{k}}\epsilon(\mathbf{k})\right] \\ &= \partial_{k_i}\left[\mathbf{F}\cdot\nabla_{\mathbf{k}}\epsilon(\mathbf{k})\right] = \partial_{k_i}\sum_j\left[\partial_{k_j}\epsilon(\mathbf{k})\right]F_j \\ &= \sum_j\left[\partial_{k_i}\partial_{k_j}\epsilon(\mathbf{k})\right]F_j = \sum_j\left[\frac{1}{m^*}\right]_{ij}F_j. \end{aligned}$$

With this expression, the motion of quasi-particles can in principle be calculated. This is particularly instructive for the case of so-called crystal-electrons, the dispersion relation of which contains the interaction with the crystal lattice. This dispersion relation has roughly the structure shown in figure 26.6: At the edge of the Brillouin zone, the curvature and hence the effective mass for several bands are negative. This is a reflection of the fact that the crystal-electrons experience Bragg-reflections at this point.

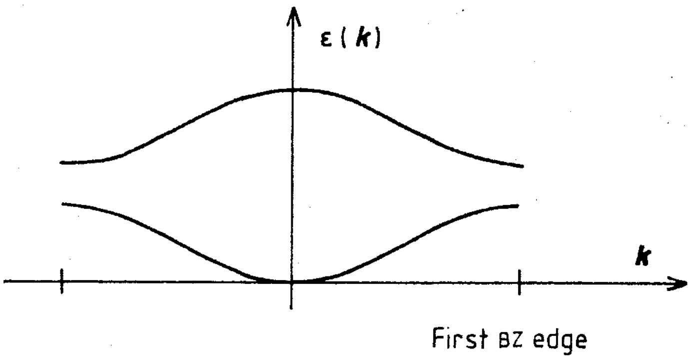


Figure 26.6 *Schematic graph of the electron energies in a crystal. The electron states at the edge of the Brillouin zone undergo Bragg scattering, which opens up an energy gap.*

We obtain another interesting application if we also derive the 'Newton's equation for quasi-particles' for the case of a (velocity-dependent) Lorentz force. The cyclotron resonance frequency

$$\omega_c = \frac{eB}{m^*}$$

can be determined very accurately experimentally. In this way, one obtains information about the dispersion relation $\epsilon(\mathbf{k})$ close to the Fermi surface, since only crystal-electrons near the Fermi surface take part in cyclotron resonance.

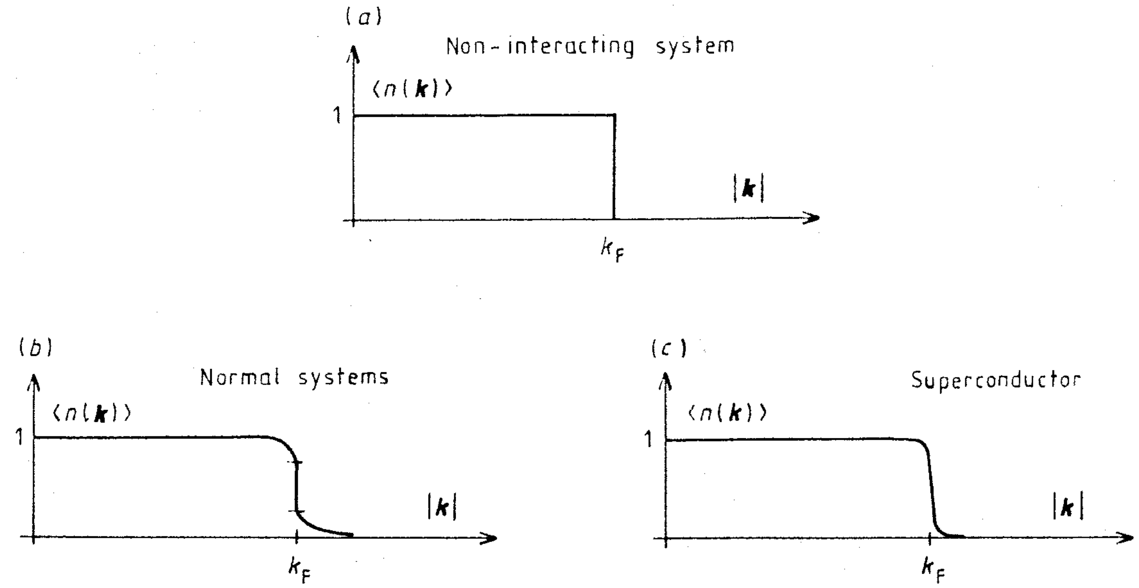


Figure 26.7 *In the non-interacting system (*a*), the momentum distribution function drops discontinuously to zero at the Fermi surface. A finite amount of this discontinuity remains in the interacting system (*b*). For a superconductor (*c*), for which conventional perturbation theory does* not *converge, the momentum distribution function goes continuously to zero.*

In the discussions above, we have termed the surface $\epsilon(\mathbf{k}) = \mu$ the *Fermi surface of interacting systems,* and have learnt of a few properties, for example the change of sign of Γ, of this surface. In the remaining part of this chapter, we will show that this surface also possesses the property which is primarily connected with the concept 'Fermi edge', namely, a sharp drop in the distribution function. In non-interacting systems the momentum distribution function

$$\langle n(\mathbf{k})\rangle = \langle \Phi_0 \mid c^{\dagger}_{\mathbf{k}} c_{\mathbf{k}} \mid \Phi_0\rangle$$

has a sharp edge, as shown in figure 26.7(a). Since the exact interacting ground state can be represented as superpositions of non-interacting configurations, we expect that the distribution function will be somewhat smeared out for interacting systems. We will show that for 'normal' systems, for which usual perturbation theory converges (in contrast to, for example, superconductors), this distribution exhibits a finite, non-zero discontinuity as depicted in figure 26.7(b). To prove this, we insert the expression equation (26.10) for $t < 0$

$$G(\mathbf{k}, t) = iz(\mathbf{k})\theta(\mu - \epsilon(\mathbf{k}))\mathrm{e}^{-i\epsilon(\mathbf{k})t}\mathrm{e}^{-\Gamma(\mathbf{k})t} + I(\mathbf{k}, t)$$

derived previously, into equation (15.34):

$$\langle n(\mathbf{k})\rangle = -i \lim_{\substack{t\to 0\\ t<0}} G(\mathbf{k}, t)$$

and consider two sequences $(\mathbf{k}^+)_\nu$ and $(\mathbf{k}^-)_\nu$ of vectors which converge to a vector $\mathbf{k}_0$ on the Fermi surface from the outside and the inside, respectively, *i.e.*, we have

$$\epsilon(\mathbf{k}_\nu^-) < \mu = \epsilon(\mathbf{k}_0) < \epsilon(\mathbf{k}_\nu^+).$$

It follows that

$$\begin{aligned}
G(\mathbf{k}_\nu^-, t) &= iz(\mathbf{k}_\nu^-)\mathrm{e}^{-i\epsilon(\mathbf{k}_\nu^-)t}\mathrm{e}^{-\Gamma(\mathbf{k}_\nu^-)} + I(\mathbf{k}_\nu^-, t) \ \ (\text{for } t < 0), \\
\lim_{t\to 0^-} G(\mathbf{k}_\nu^-, t) &= iz(\mathbf{k}_\nu^-) + I(\mathbf{k}_\nu^-, 0^-) \\
G(\mathbf{k}_\nu^+, t) &= I(\mathbf{k}_\nu^+, t) \ \ (\text{for } t < 0) \\
\lim_{t\to 0^-} G(\mathbf{k}_\nu^+, t) &= I(\mathbf{k}_\nu^+, 0^-).
\end{aligned}$$

We make the plausible assumption that I is continuous as a function of $\mathbf{k}$, at least near the Fermi surface . (If this assumption is incorrect, there will be an additional contribution $\left[I(\mathbf{k}^+ \to \mathbf{k}_0, 0^-) - I(\mathbf{k}^- \to \mathbf{k}_0, 0^-)\right] i$ in the result below. Since I is small, this would be a small correction to $z(\mathbf{k}_0) \approx 1$ and only slightly affects the size of the discontinuity.)

Altogether, we obtain

$$\lim_{\substack{\mathbf{k}_\nu^+ \to \mathbf{k}_0 \\ \mathbf{k}_\nu^- \to \mathbf{k}_0}} \left[\langle n(\mathbf{k}_\nu^+)\rangle - \langle n(\mathbf{k}_\nu^-)\rangle\right] = z(\mathbf{k}_0).$$

We have then shown that the momentum distribution has a discontinuity of (approximate) magnitude $z(\mathbf{k}_0)$ at each point $\mathbf{k}_0$ on the Fermi surface, and in fact it then looks approximately as we sketched in figure 26.7.

Chapter 27

Diagrammatic calculation of the two-particle Green's function and the polarization propagator

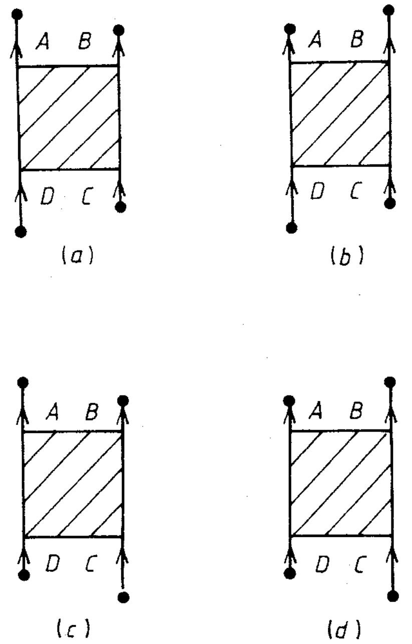
Let us begin by reminding ourselves of the definition of the two-particle Green's function:

$$
\begin{aligned}
& i^2 G(\mathbf{r}_A t_A, \mathbf{r}_B t_B, \mathbf{r}_C t_C, \mathbf{r}_D t_D) \\
&\quad \equiv \frac{\langle \Psi_0 \mid T\left[\psi(\mathbf{r}_A t_A)_H \psi(\mathbf{r}_B t_B)_H \psi^\dagger(\mathbf{r}_C t_C)_H \psi^\dagger(\mathbf{r}_D t_D)_H\right] \mid \Psi_0\rangle}{\langle \Psi_0 \mid \Psi_0\rangle}.
\end{aligned}
$$

(We will in this chapter omit the spin indices for ease of notation.) The first step in the diagrammatic calculation is again the adiabatic switching procedure. Analogously to the case of the single-particle Green's function, it can be shown that (*cf.* equation (18.11)

$$
\begin{aligned}
& i^2 G(\mathbf{r}_A t_A, \mathbf{r}_B t_B, \mathbf{r}_C t_C, \mathbf{r}_D t_D) = \lim_{\epsilon \to 0} \frac{1}{\langle \Phi_0 \mid U_\epsilon(-\infty, \infty) \mid \Phi_0\rangle} \\
& \times \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \int \mathrm{d}t_1 \ldots \int \mathrm{d}t_n \, \mathrm{e}^{-\epsilon(|t_1| + \ldots + |t_n|)} \\
& \times \langle \Phi_0 \mid T\left[V(t_1)_I \ldots V(t_n)_I \psi(\mathbf{r}_A t_A)_I \psi(\mathbf{r}_B t_B)_I \psi^\dagger(\mathbf{r}_C t_C)_I \psi^\dagger(\mathbf{r}_D t_D)_I\right] \mid \Phi_0\rangle.
\end{aligned}
$$

This representation allows for a diagrammatic analysis with essentially the same Feynman-rules as those we derived in Chapter 20. We draw the full two-particle Green's function as a structure with four legs. The external endpoints correspond to the four arguments of the Green's function. Thus, as the single-particle Green's function $G(\mathbf{r}_A t_A, \mathbf{r}_B t_B)$ for each possible time-ordering represented either particle-propagation ($t_A > t_B$) or hole-propagation ($t_B > t_A$), there are three possibilities with the two-particle Green's function: particle-pair propagation, hole-pair propagation and particle–hole propagation. These may be represented as shown in figure 27.1. Again, Feynman rule (1) with the imagined time-axis is used when the end-points are drawn. We also agree to put arrows pointing away from the endpoint if the endpoint corresponds to a creation operator, whereas the arrow points toward the endpoint if it corresponds to an annihilation operator. Accordingly, we obtain the diagrams in figure 27.2(a) and (b) for hole-pair propagation and particle–hole propagation, respectively. As an example, we consider the first few terms in the numerator of the particle-pair propagator. The corresponding diagrams are shown in figure 27.3. The corresponding diagrams for the hole-pair propagator are obtained simply by reversing the directions of all arrows, as shown in figure 27.4. On the other hand, new diagrams appear in the particle–hole propagator, for example the diagrams in figure 27.5.



(a) (b) (c) (d)

Figure 27.1 *Possible diagrammatic representations for particle-pair propagation. In* (a)*,* $t_A > t_B > t_C > t_D$*, in* (b) $t_B > t_A > t_C > t_D$*, in* (c) $t_A > t_B > t_D > t_C$*, and in* (d) $t_B > t_A > t_B > t_C$.

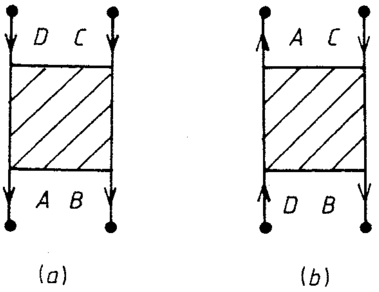


Figure 27.2 *In (a), a diagram for hole-pair propagation for* $t_C, t_D > t_A, t_B$ *is shown. There are three more such diagrams, corresponding to three other possible time-orderings for hole-pair propagation. In (b), a diagram for particle–hole propagation corresponding to* $t_A, t_C > t_B, t_D$ *is drawn. There are three more such diagrams. In addition, there are four more diagrams each for particle–hole propagation for the time-orderings* $t_B, t_C > t_A, t_D$, $t_A, t_D > t_B, t_C$, *and* $t_B, t_D > t_A, t_C$, *respectively.*

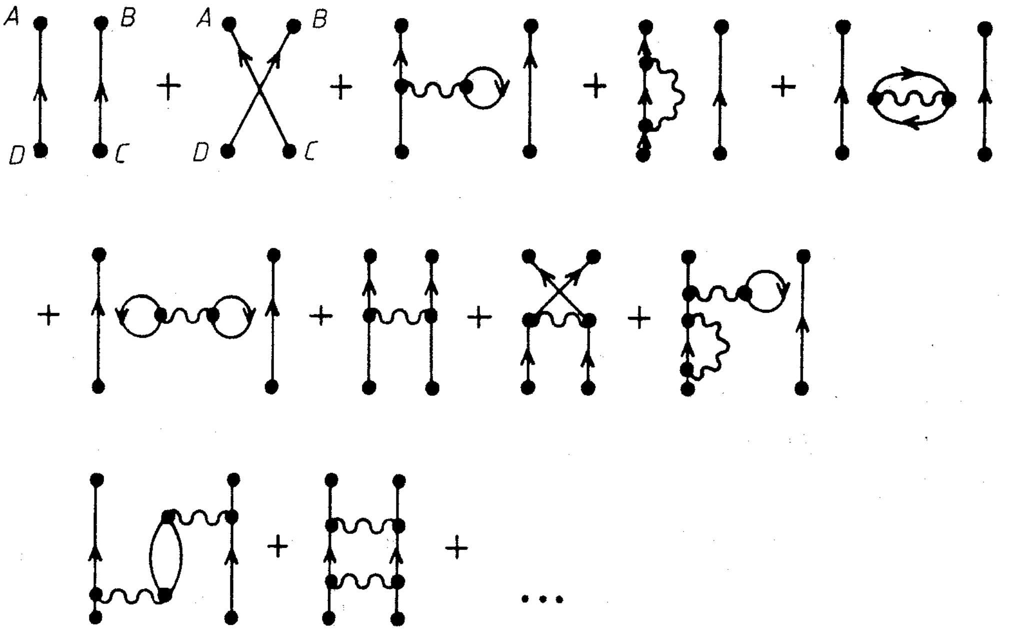


Figure 27.3 *The first few diagrams from the numerator of the particle-pair propagator.*

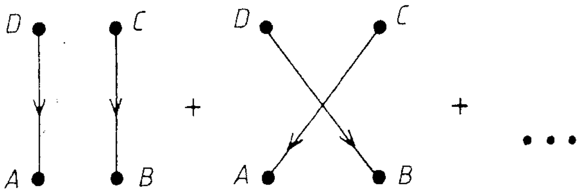


Figure 27.4 *The diagrams of the numerator of the hole-pair propagator are obtained from the diagrams in figure 27.3 simply by changing the directions of all arrows.*

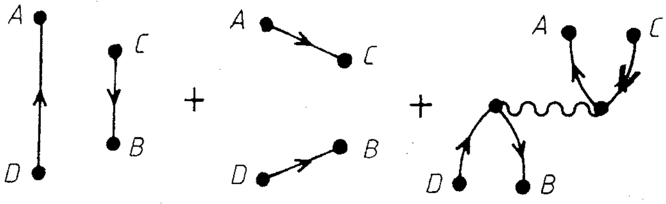


Figure 27.5 *A few particle–hole diagrams.*

The next step is the linked-cluster theorem, which says, just as for the single-particle Green's function, that the disconnected sub-diagrams of the vacuum amplitude are canceled with the denominator:

$$i^2 G(\mathbf{r}_A t_A, \mathbf{r}_B t_B, \mathbf{r}_C t_C, \mathbf{r}_D t_D) = \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \int \mathrm{d}t_1 \ldots \int \mathrm{d}t_n \, \mathrm{e}^{-\epsilon(|t_1|+\ldots+|t_n|)}$$

$$\times \langle \Phi_0 | T \left[V(t_1)_I \ldots V(t_n)_I \psi(\mathbf{r}_A t_A)_I \psi(\mathbf{r}_B t_B)_I \psi^\dagger(\mathbf{r}_C t_C)_I \psi^\dagger(\mathbf{r}_D t_D)_I \right] | \Phi_0 \rangle_L .$$

It should be emphasized that only diagrams which contain pieces that are not connected to any external point are omitted. Thus, diagrams such as those shown in figure 27.6 are 'linked clusters', in this sense, and are to be included.

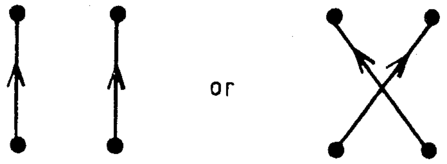


Figure 27.6 *These lowest-order diagrams are to be treated as connected diagrams.*

Before we start to evaluate the perturbation series, we must add a supplement to the Feynman rules for the two-particle Green's function: The translation of $G^{(0)}(A,B,C,D)$, represented by the diagrams in figure 27.7(a), is surely *not*

$$i^0(-)^0\left[G^{(0)}(A,D)G^{(0)}(B,C)+G^{(0)}(A,C)G^{(0)}(B,D)\right] \qquad (27.1)$$

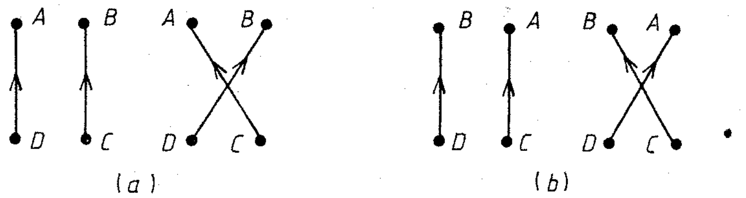
since we can read directly from the definition of the two-particle Green's function that

$$-G^{(0)}(A,B,C,D)=G^{(0)}(B,A,C,D)$$

(see figure 27.7 (b)) which is

$$i^0(-)^0\left[G^{(0)}(A,C)G^{(0)}(B,D)+G^{(0)}(B,C)G^{(0)}(A,D)\right]$$

i.e., the same expression which we already attempted to write as



(a) (b)

Figure 27.7 *The two diagram in* (a) *contribute to* $G^{(0)}(A,B,C,D)$, *whereas the two diagrams in* (b) *contribute to* $G^{(0)}(B,A,C,D)$.

$+G^{(0)}(A,B,C,D)$. This uncertainty of sign can easily be clarified if we go back to the Wick-expansion:

$$\begin{aligned}
&i^2G^{(0)}(A,B,C,D)\\
&= \langle\Phi_0\mid T\left[\psi(A)\psi(B)\psi^\dagger(C)\psi^\dagger(D)\right]\mid\Phi_0\rangle\\
&= \wick{\c1\psi(A)\,\c2\psi(B)\c2\psi^\dagger(C)\c1\psi^\dagger(D)}+\wick{\c1\psi(A)\,\c2\psi(B)\c1\psi^\dagger(C)\c2\psi^\dagger(D)}\\
&= \wick{\c\psi(A)\c\psi^\dagger(D)}\,\wick{\c\psi(B)\c\psi^\dagger(C)}-\wick{\c\psi(A)\c\psi^\dagger(C)}\,\wick{\c\psi(B)\c\psi^\dagger(D)}\\
&= \left[iG^{(0)}(A,D)\right]\left[iG^{(0)}(B,C)\right]-\left[iG^{(0)}(A,C)\right]\left[iG^{(0)}(B,D)\right].
\end{aligned}$$

The minus-sign in the last line of this equation must then replace the plus-sign in equation (27.1). (The factors i^2 on both sides of the equation cancel out.) Thus, the paradox is resolved. We see that we must add a Feynamn rule concerning the overall sign of the diagram. This rule must, for example, correctly give the sign of the diagrams in figure 27.8. We state Feynman rule (6)A:

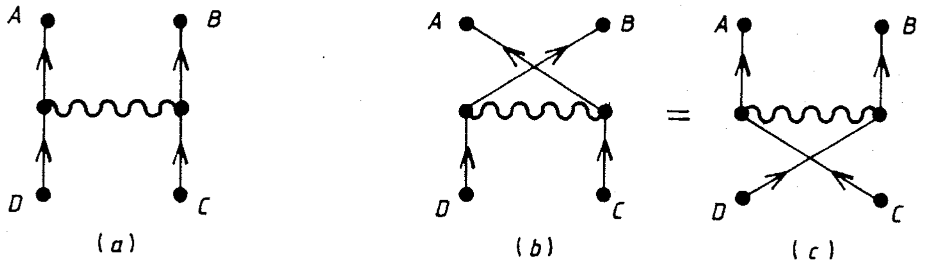


Figure 27.8 *If the reference diagram* (a) *has a plus-sign, then the two diagrams* (b) *and* (c) *must have a minus sign.*

> Two diagrams, which differ by the interchange of two incoming or outgoing fermion lines, differ by a minus sign.

Diagrams which contribute to $G(A, B, C, D)$ and which have fermion lines running from D to A (and thus also from C to B), then have a plus sign (in addition to all other pre-factors according to the other Feynman rules). The notation 'rule (6)A' is to emphasize the close relationship with the loop-theorem, which we will now treat briefly. The diagrams in figure 27.9 can be interpreted as the contributions to the single-particle Green's function $G(A, D)$ shown in figure 27.10. These two diagrams differ by a minus sign, according to the loop-theorem (rule (6)). However, they can also be

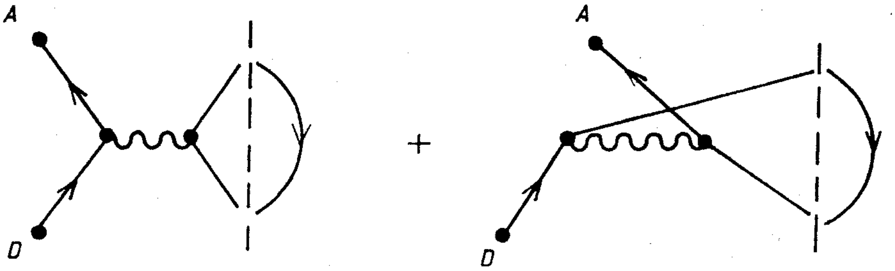


Figure 27.9 *These two diagrams of the two-particle Green's functions can be interpreted as single-particle Green's function diagrams by closing the propagator lines at the dashed lines.*

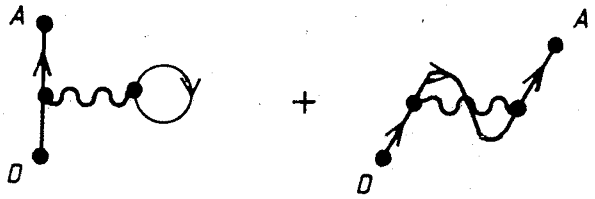


Figure 27.10 *Single-particle Green's function diagrams corresponding to the two-particle Green's function diagrams in figure 27.9.*

interpreted as contributions to

$$\int\int G(A,B,C,D)G(C,B)\,\mathrm{d}C\,\mathrm{d}B$$

(see figure 27.11). As such, they acquire a relative minus sign, according to the complementary rule (6)A.

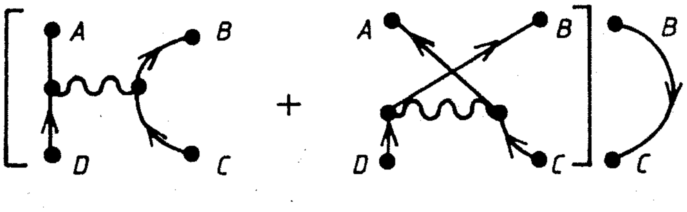
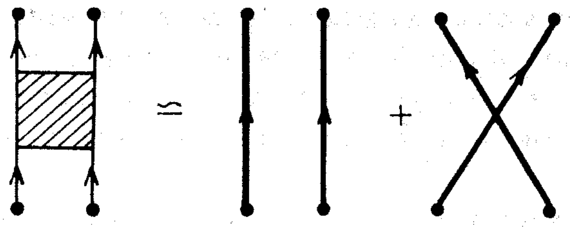


Figure 27.11 *The endpoints B and C of the diagrams in figure 27.9 can be closed with a single-particle Green's function to yield diagrams for the Green's function G(A, D).*

One particular possible way of summing up the perturbation series is again by 'dressing the skeletons' by successively inserting self-energy insertions. We will now show that the approximation to the two-particle Green's function consisting of the sum of the two lowest-order dressed skeletons



(27.2)

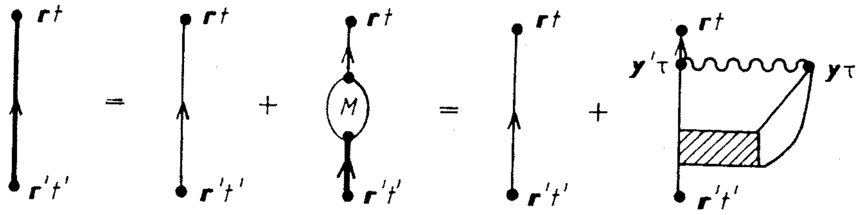
corresponds precisely to the Hartree–Fock approximation. With the machinery that we have at our disposal at this point, the proof is quite simple. We use the relation discussed earlier between the irreducible self-energy and the two-particle Green's function:

$$\begin{aligned}\int \mathrm{d}\tau \int \mathrm{d}^3y\, M(\mathbf{r}t,\mathbf{y}\tau)G(\mathbf{y}\tau,\mathbf{r}'t') \\ = \quad -i\int \mathrm{d}^3y\, v(\mathbf{r},\mathbf{y})\, G_2(\mathbf{r}t,\mathbf{y}t,\mathbf{y}t^+,\mathbf{r}'t').\end{aligned}$$

If this relation is inserted in Dyson's equation, we obtain an integral equation which corresponds to the differential equation of motion, equation (16.7):

$$\begin{aligned}G(\mathbf{r}t,\mathbf{r}'t') \quad = \quad & G^{(0)}(\mathbf{r}t,\mathbf{r}'t') - i\int \mathrm{d}^3y' \int \mathrm{d}^3y \int \mathrm{d}\tau \\ & \times G^{(0)}(\mathbf{r}t,\mathbf{y}'\tau)v(\mathbf{y},\mathbf{y}')G_2(\mathbf{y}'\tau,\mathbf{y},\tau,\mathbf{y}\tau^+,\mathbf{r}'t') \quad (27.3)\end{aligned}$$

with the diagrammatical representation



(27.4)

In the interpretation of the diagrammatic representation in equation (27.4), it should be borne in mind that each interaction line in a diagram of the single-particle Green's function leaves a factor of i, according to Feynman rule (7) (disregarding additional degeneracy factors, which are in any case omitted in non-indexed diagrams, *i.e.*, sums over degenerate diagrams). Consequently, the single interaction line in equation (27.4) must also contribute a factor of i. Furthermore, a factor (-1) must be added in the translation. This factor takes into account that for each diagram of the two-particle Green's function, which acquires a plus-sign according to the rule (6)A, becomes a loop, which must have a factor of (-1), by connecting the two legs on the right-hand side. No loop, which acquires a minus sign according to rule (6)A and compensates the minus sign, is contained in the other diagrams. The two following illustrations will demonstrate this process for the lowest-order diagrams. These statements are easily verified using the formulation of rule (6)A. This rule demands a plus sign precisely when the two legs on the right-hand side within the two-particle Green's function are connected with fermion lines; by connecting these legs a loop thus emerges.

If we insert the approximation equation (27.2) in equation (27.4), we obtain figure 27.12. This is precisely Dyson's equation shown in figure 27.13. This approximation for M corresponds precisely to the Hartree–Fock approximation, as we showed in Chapter 25.

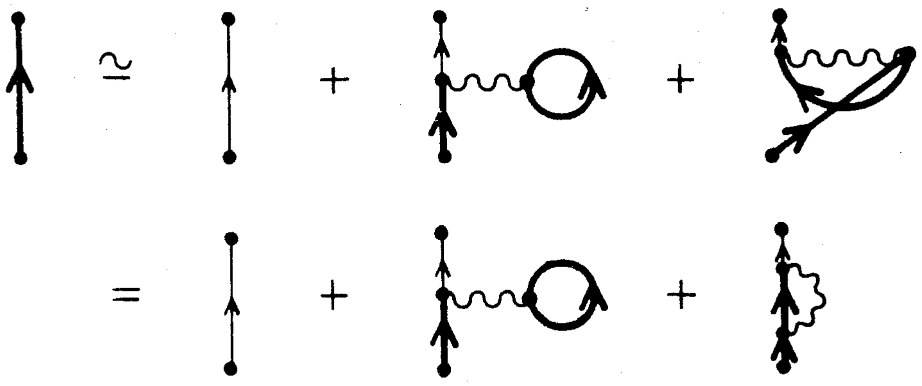
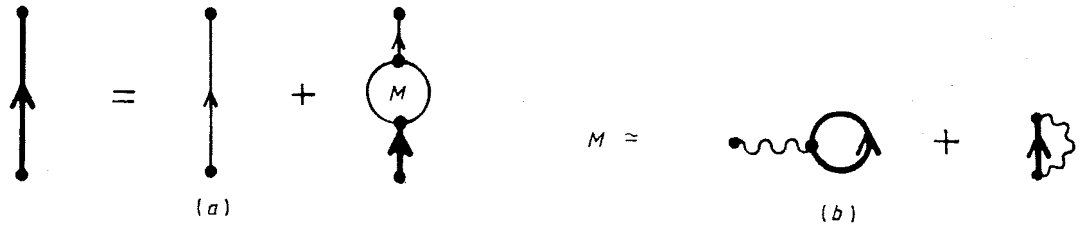


Figure 27.12 *Approximation for the dressed Green's function.*



(a) (b)

Figure 27.13 *The diagrams in figure 27.12 are Dyson's equation* (a) *with the self-energy* M *approximated by* (b).

We will not here further pursue the diagrammatic analysis of the general two-particle Green's function. Instead, we consider a special case, which in practice is extremely important, namely, the already earlier introduced polarization propagator. It is defined as

$$i\Pi(\mathbf{r}t,\mathbf{r}'t') \equiv \frac{1}{\langle\Psi_0 \mid \Psi_0\rangle}\langle\Psi_0 \mid T\left[\widetilde{\rho}(\mathbf{r}t)_H\widetilde{\rho}(\mathbf{r}'t')_H\right] \mid \Psi_0\rangle$$

where

$$\widetilde{\rho}(\mathbf{r})_S = \psi^\dagger(\mathbf{r})\psi(\mathbf{r}) - \frac{\langle\Psi_0 \mid \psi^\dagger(\mathbf{r})\psi(\mathbf{r}) \mid \Psi_0\rangle}{\langle\Psi_0 \mid \Psi_0\rangle} \equiv \rho(\mathbf{r}) - \langle\rho(\mathbf{r})\rangle. \qquad (27.5)$$

Apparently, we have

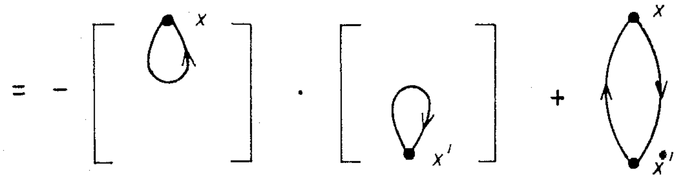
$$\begin{aligned} &i\Pi(\mathbf{r}t,\mathbf{r}'t') \\ &= \frac{1}{\langle\Psi_0 \mid \Psi_0\rangle}\left\{\begin{array}{ll} \langle\Psi_0 \mid \psi^\dagger(\mathbf{r}t)_H\psi(\mathbf{r}t)_H\psi^\dagger(\mathbf{r}'t')_H\psi(\mathbf{r}'t')_H \mid \Psi_0\rangle & \text{for } t > t' \\ \langle\Psi_0 \mid \psi^\dagger(\mathbf{r}'t')_H\psi(\mathbf{r}'t')_H\psi^\dagger(\mathbf{r}t)_H\psi(\mathbf{r}t)_H \mid \Psi_0\rangle & \text{for } t' > t \end{array}\right\} \\ &\quad -\langle\rho(\mathbf{r})\rangle\langle\rho(\mathbf{r}')\rangle \\ &= +G(\mathbf{r}t,\mathbf{r}'t',\mathbf{r}t^+,\mathbf{r}'(t')^+) - \langle\rho(\mathbf{r})\rangle\langle\rho(\mathbf{r}')\rangle, \end{aligned}$$

where the correct order of the field operators is ensured by the infinitesimally larger times $t^+ > t$ and $(t')^+ > t'$.

The polarization propagator describes, as the name implies, the spreading of a particle–hole pair. We will now see which diagrams contribute to it. In zeroth order, we obtain for the perturbation expansion of the first term with the help of Wick's theorem (x stands for $(\mathbf{r}t)$):

$$\begin{aligned}
&G^{(0)}(x,x',x,x') \\
&\quad= \langle\Phi_0 \mid T\left[\psi^\dagger(x)_I\psi(x)_I\psi^\dagger(x')_I\psi(x')_I\right] \mid \Phi_0\rangle \\
&\quad= \overbracket{\psi^\dagger(x)\psi(x)}\,\overbracket{\psi^\dagger(x')\psi^\dagger(x')} + \overbracket{\psi^\dagger(x)\,\overbracket{\psi(x)\psi^\dagger(x)}\psi(x')} \\
&\quad= \overbracket{\psi(x)\psi^\dagger(x)}\,\overbracket{\psi(x')\psi^\dagger(x')} - \overbracket{\psi(x')\psi^\dagger(x)}\,\overbracket{\psi(x)\psi^\dagger(x')} \\
&\quad= \left[iG^{(0)}(x,x)\right]\left[iG^{(0)}(x',x')\right] - \left[iG^{(0)}(x',x)\right]\left[iG^{(0)}(x,x')\right] \\
&\quad= -G^{(0)}(x,x)G^{(0)}(x',x') + G^{(0)}(x',x)G^{(0)}(x,x').
\end{aligned}$$

These two terms have the diagrammatical representation

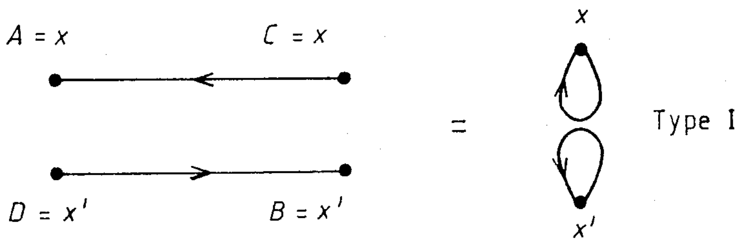


(27.6)

With the help of the relation which we proved in Chapter 15 between density and the single-particle Green's function, we have

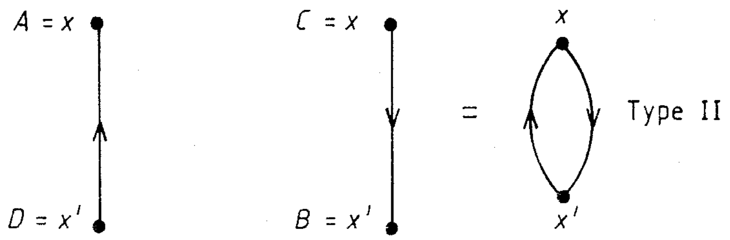
$$G^{(0)}(x,x',x,x') = +\langle\rho^{(0)}(\mathbf{r})\rangle\langle\rho^{(0)}(\mathbf{r}')\rangle + G^{(0)}(x',x)G^{(0)}(x,x').$$

We have derived the diagrams (27.6) by hand, *i.e.*, with Wick's theorem, to emphasize an important point which can easily lead to translation errors. The two-particle Green's function considered always has two (fixed) equal arguments and, accordingly, two legs with identical indices. These legs are terminated at the same points in the diagrams. Hence, to zeroth order, we obtain this special two-particle Green's function from the diagrams:



(27.7)

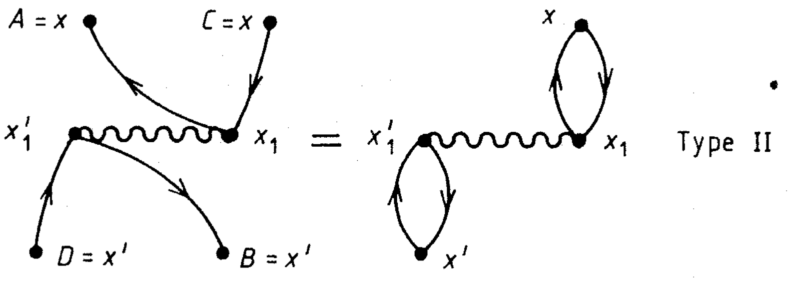
and



(27.8)

So long as no interaction lines end on the external endpoints, these are *not vertices;* in particular, there are then no loops which have been closed in the sense of the loop theorem. Instead, the rule (6)A must be used for the diagrams of this special two-particle Green's function. Consequently, the upper graph, (27.7), acquires a minus sign (note that the endpoints A–C and D–B are connected), in agreement with the result equation (27.6) obtained by hand. The following *point of view,* which is easily verified for the diagrams above and also for the general diagrams below, is equivalent. The two endpoints with the same index close one or two loops, and, in particular, precisely one loop if and only if rule (6)A requires a plus sign for the corresponding two-particle Green's function diagram. *Between interaction lines,* the diagrams for $i\Pi$ yield, according to the loop theorem, the factor $-i\Pi$.

We now consider an additional example: the diagram



(27.9)

acquires a minus sign as a diagram of the two-particle Green's function, according to rule (6)A. As a sub-diagram between two interaction lines, it acquires a plus sign, according to the loop theorem. It is clear that the entire expansion of $G(x, x', x, x')$ can be divided into two types of diagrams, those in which the line starting at x is connected in any way (including by interaction lines) to the line starting at x' (type II), and those for which this is not the case (type I). It is also clear, that line starting at x in the diagrams of type I must come back to x. Hence, all these diagrams acquire a minus sign according to rule (6)A. Thus, if we interpret all the parts which are attached to x and x', respectively, as diagrams of the full single-particle Green's functions $G(x, x)$ and $G(x', x')$, we must insert by hand an overall minus sign in front of the corresponding product, as illustrated in figure 27.16. The first term in figure 27.14

$$[-iG(x,x)]\,[-iG(x',x')] = \langle\rho(\mathbf{r})\rangle\langle\rho(\mathbf{r}')\rangle$$

cancels out according to the definition of $i\Pi$, so that we obtain

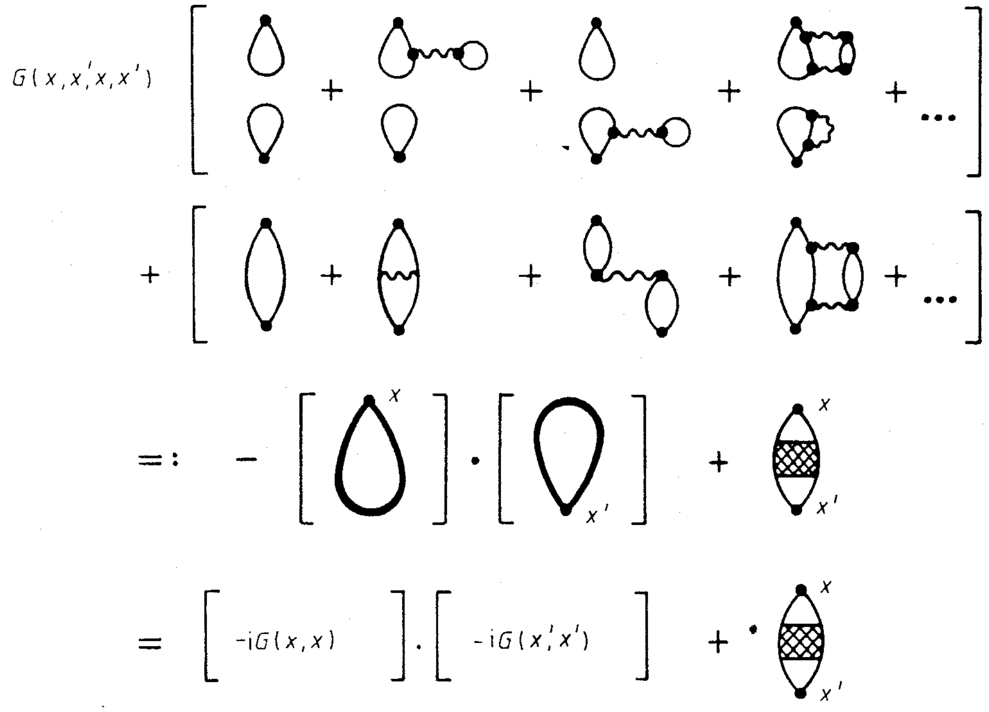
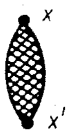


Figure 27.14 *The two-particle Green's function $G(x, x', x, x')$ can be expanded as a sum of type I and type II diagrams.*

$$i\Pi(x,x') =$$  $\equiv$ the sum of all type II diagrams in $G(x, x', x, x')$. (27.10)

Hereafter, we denote $i\Pi(x, x')$ by  .

The contributions to the polarization propagator are then in zeroth order

$$i\Pi^{(0)}(x,x') = G^{(0)}(x,x')G^{(0)}(x',x) =$$ 

in first order, we obtain the diagrams in figure 27.15, and in second order we have, for example the diagrams in figure 27.16. Just as we did with the self-energy, we now define the so-called *irreducible polarization insertions* as those diagrams which cannot be separated into polarization insertions of lower order by cutting a single interaction line. Of the diagrams of second order depicted in figure 27.16, for example, the first three are reducible, whereas the rest are irreducible.

$i\Pi^{(1)}(x,x') =$

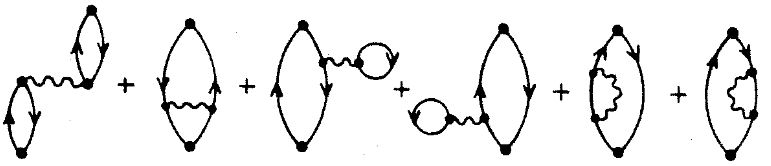


Figure 27.15 *First-order diagrams for the polarization propagator.*

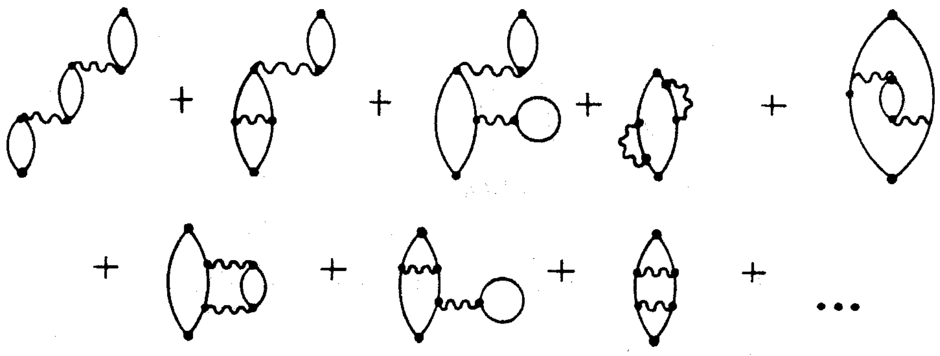


Figure 27.16 *Some second-order diagrams for the polarization propagator.*

If we define

$iQ(x,x') \equiv$

$\equiv$ the sum of all irreducible polarization insertions

the polarization propagator can be represented as shown in figure 27.18. This is Dyson's equation for the polarization propagator. When we translate the diagrams into mathematical expressions, we note that by cutting the interaction lines for all terms except for the second loop they become identically indexed legs of a two-particle Green's function. The question of the sign associated with this is easily answered if we, as discussed in detail above, consider $-i\Pi$ and correspondingly $-iQ$ as insertions in an interaction

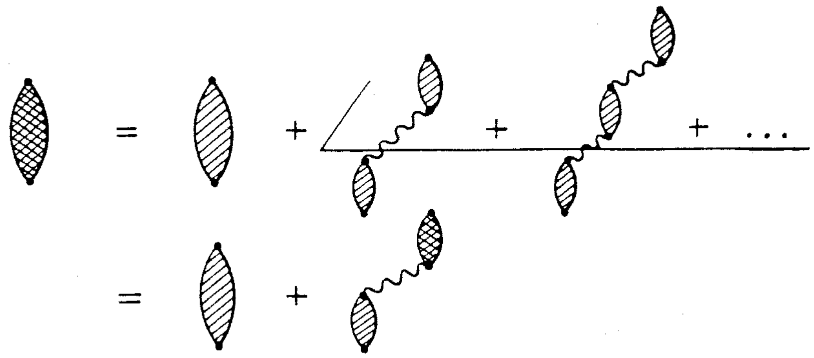


Figure 27.17 *Dyson's equation for the polarization propagator.*

line. The number of loops is not changed if we cut the interaction line, so that rule (6)A does not come into effect from this point of view. We can then write

$$\begin{aligned}&[-i\Pi(x,x')]\\ =\ &[-iQ(x,x')]+i^1\int \mathrm{d}^4y\int \mathrm{d}^4y'\,[-iQ(x,y)]\,u(y,y')\,[-i\Pi(y',x')]\,.\end{aligned}$$

We cancel out the factor $(-i)$ and obtain

$$\Pi(x,x')=Q(x,x')+\int \mathrm{d}^4y\int \mathrm{d}^4y'\,Q(x,y)u(y,y')\Pi(y',x'). \tag{27.11}$$

For translationally invariant systems with instantaneous spin-independent interactions, this equation becomes particularly simple:

$$\Pi(\mathbf{q},\omega)=Q(\mathbf{q},\omega)+Q(\mathbf{q},\omega)u(\mathbf{q})\Pi(\mathbf{q},\omega) \tag{27.12}$$

with the solution

$$\Pi(\mathbf{q},\omega)=\frac{Q(\mathbf{q},\omega)}{1-u(\mathbf{q})Q(\mathbf{q},\omega)}. \tag{27.13}$$

The use of the polarization propagator has an important application in the theory of linear response. To see this, we consider an interacting system, which for $t\le 0$ is in the ground state $|\,\Psi_0\rangle$ of the Hamiltonian $H=H_0+V$. At $t=0$ we apply a perturbation

$$H_{\mathrm{ext}}(t)=\int \mathrm{d}^3r\,v_{\mathrm{ext}}(\mathbf{r}t)\psi^\dagger(\mathbf{r})\psi(\mathbf{r}). \tag{27.14}$$

We want the linear response for an arbitrary observable

$$A=\int \mathrm{d}^3r\,a(\mathbf{r})\psi^\dagger(\mathbf{r})\psi(\mathbf{r}) \tag{27.15}$$

of the system, *i.e.*, the part of the deviation of the expectation value

$$\delta\langle A\rangle(t) = \langle \Psi(t) \mid A \mid \Psi(t)\rangle - \langle \Psi_0 \mid A \mid \Psi_0\rangle \tag{27.16}$$

that is linear in the perturbation H_{ext}. Here, $\mid \Psi(t)\rangle$ is the solution of the full time-dependent Schrödinger equation

$$i\partial_t \mid \Psi(t)\rangle = [H + H_{\text{ext}}(t)] \mid \Psi(t)\rangle.$$

To calculate the linear response, we go over to the interaction picture relative to $(H + H_{\text{ext}}(t))$, *i.e.*, to the Heisenberg picture relative to H (thus, we use the subscript H). In this picture, the wavefunction is

$$\mid \Psi(t)\rangle_H = \mathrm{e}^{+iHt} \mid \Psi(t)\rangle \tag{27.17}$$

and it satisfies the equation of motion (*cf.* (14.12))

$$i\frac{\partial}{\partial t} \mid \Psi(t)\rangle_H = H_{\text{ext}}(t)_H \mid \Psi(t)\rangle_H \tag{27.18}$$

with

$$H_{\text{ext}}(t)_H = \mathrm{e}^{iHt} H_{\text{ext}}(t) \mathrm{e}^{-iHt}.$$

The solution up to terms linear in H_{ext} of equation (27.18) is

$$\mid \Psi(t)\rangle_H = \mid \Psi_0\rangle - i\int_0^t \mathrm{d}t'\, H_{\text{ext}}(t')_H \mid \Psi_0\rangle$$

so that, together with equation (27.17), we obtain

$$\mid \Psi(t)\rangle = \mathrm{e}^{-iHt}\left[1 - i\int_0^t \mathrm{d}t'\, H_{\text{ext}}(t')_H\right] \mid \Psi_0\rangle + \mathrm{O}(H_{\text{ext}}^2).$$

From this, it follows that

$$\begin{aligned}
&\langle \Psi(t) \mid A \mid \Psi(t)\rangle \\
&= \langle \Psi_0 \mid \left[1 + \int_0^t \mathrm{d}t'\, H_{\text{ext}}(t')_H\right] \underbrace{\mathrm{e}^{+iHt} A \mathrm{e}^{-iHt}}_{=A(t)_H} \\
&\quad \times \left[1 - i\int_0^t \mathrm{d}t'\, H_{\text{ext}}(t')_H\right] \mid \Psi_0\rangle + \mathrm{O}(H_{\text{ext}}^2) \\
&= \langle \Psi_0 \mid A(t)_H \mid \Psi_0\rangle - i\int_0^t \mathrm{d}t'\, \langle \Psi_0 \mid [A(t)_H, H_{\text{ext}}(t')_H] \mid \Psi_0\rangle \\
&\quad + \mathrm{O}(H_{\text{ext}}^2).
\end{aligned}$$

The linear response equation (27.16) for the observable A is then:

$$\delta\langle A\rangle(t) = -i\int_0^t \mathrm{d}t'\, \langle \Psi_0 \mid [A(t)_H, H_{\text{ext}}(t')_H] \mid \Psi_0\rangle. \tag{27.19}$$

We then insert equations (27.14), (27.15) and the definition of the density-fluctuation operator, equation (27.5), to obtain

$$\begin{aligned}\delta\langle A\rangle(t) &= -i\int_0^t \mathrm{d}t'\int \mathrm{d}^3r\int \mathrm{d}^3r'\, a(\mathbf{r})v_{\text{ext}}(\mathbf{r}'t')\\ &\quad\times\langle\Psi_0 \mid [\widetilde{\rho}(\mathbf{r}t)_H,\widetilde{\rho}(\mathbf{r}'t')_H] \mid \Psi_0\rangle\end{aligned}$$

If we introduce a retarded polarization propagator (analogous to the retarder Green's function, *cf.* equation (26.1))

$$i\Pi^R(\mathbf{r}t,\mathbf{r}'t') = \theta(t-t')\frac{\langle\Psi_0 \mid [\widetilde{\rho}(\mathbf{r}t)_H,\widetilde{\rho}(\mathbf{r}'t')_H] \mid \Psi_0\rangle}{\langle\Psi_0 \mid \Psi_0\rangle} \tag{27.20}$$

we have

$$\delta\langle A\rangle(t) = \int_0^\infty \mathrm{d}t'\int \mathrm{d}^3r\int \mathrm{d}^3r'\, a(\mathbf{r})v_{\text{ext}}(\mathbf{r}'t')\Pi^R(\mathbf{r}t,\mathbf{r}'t'). \tag{27.21}$$

In particular, we obtain for the linear response of the density:

$$\delta\langle\rho(\mathbf{r})\rangle(t) = \int_0^\infty \mathrm{d}t'\int \mathrm{d}^3r'\, v_{\text{ext}}(\mathbf{r}'t')\Pi^R(\mathbf{r}t,\mathbf{r}'t'). \tag{27.22}$$

Hence, the retarded polarization propagator is identical to the so-called 'density-density response function', *i.e.*, the function which describes the linear response of the density to a perturbation which couples to the density (*cf.* (27.14)). For initially homogeneous systems (systems which are homogeneous for $t \le 0$), we obtain by Fourier transforming

$$\delta\rho(\mathbf{q},\omega) = \Pi^R(\mathbf{q},\omega)v_{\text{ext}}(\mathbf{q},\omega). \tag{27.23}$$

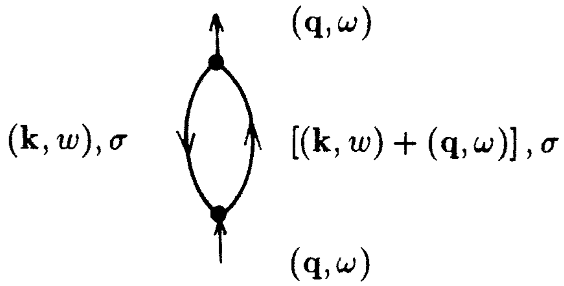
A direct diagrammatic analysis of Π^R is not possible, since Wick's theorem can only be applied to time-ordered products. Fortunately, one can, as with the retarded Green's function (see equation (26.4), as well as equations (26.5) and (26.3)), by using the corresponding Lehmann representation, derive a relation between Π and Π^R. We have

$$\text{for } \omega\in\mathcal{R}:\quad \begin{aligned}\mathrm{Re}[\Pi^R(\mathbf{q},\omega)] &= \mathrm{Re}[\Pi(\mathbf{q},\omega)]\\ \mathrm{Im}[\Pi^R(\mathbf{q},\omega)] &= \mathrm{sgn}(\omega)\mathrm{Im}[\Pi(\mathbf{q},\omega)].\end{aligned} \tag{27.24}$$

We close this chapter by stating the response function for an, in practice, particularly important example of a response function: the so-called Lindhard function. This is the response function of a homogeneous system of non-interacting particles. It is obtained from the polarization propagator with $u(x,x') = 0$, *i.e.*, from the zeroth-order diagram

$$i\Pi^{(0)}(\mathbf{q},\omega)$$

$$=$$



$$= 2\int\frac{\mathrm{d}^3k}{(2\pi)^3}\int\frac{\mathrm{d}w}{2\pi}G^{(0)}(\mathbf{k},w)G^{(0)}(\mathbf{k}+\mathbf{q},w+\omega).$$

The evaluation of this four-dimensional integral is possible, but tedious, using elementary methods (see, for example, Fetter and Walecka [22]. The results are, with the abbreviations

$$q \equiv |\mathbf{q}|/k_F$$

and

$$\nu \equiv \frac{\omega}{(k_F^2/m)}$$

$$\begin{aligned}&\mathrm{Re}[\Pi^{(0)}(q,\omega)]\\ &= \frac{mk_F}{2\pi^2}\left\{-1+\frac{1}{2q}\left[1-\left(\frac{\nu}{q}-\frac{q}{2}\right)^2\right]\ln\left|\frac{1+(\nu/q-q/2)}{1-(\nu/q-q/2)}\right|\right.\\ &\left.-\frac{1}{2q}\left[1-\left(\frac{\nu}{q}+\frac{q}{2}\right)^2\right]\ln\left|\frac{1+\left(\frac{\nu}{q}+\frac{q}{2}\right)}{1-\left(\frac{\nu}{q}+\frac{q}{2}\right)}\right|\right\}\end{aligned} \qquad (27.25)$$

$$\mathrm{Im}[\Pi^{(0)}(q,\omega)]$$

$$= \frac{mk_F}{2\pi}\begin{cases} 0 & \text{for} \quad \nu > \frac{q^2}{2}+q \\ -\frac{1}{2q}\left[1-\left(\frac{\nu}{q}-\frac{q}{2}\right)^2\right] & \text{for} \quad \left|\frac{q^2}{2}-q\right| < \nu < \left|\frac{q^2}{2}+q\right| \\ -\frac{\nu}{q} & \text{for} \quad \nu < \left|\frac{q^2}{2}-q\right| \text{ and } q < 2 \\ 0 & \text{for} \quad \nu < \left|\frac{q^2}{2}-q\right| \text{ and } q > 2. \end{cases} \qquad (27.26)$$

We will learn an application of this result in the next chapter when we discuss the effective interaction in the electron gas.

Chapter 28

Effective interaction and dressed vertices, an advanced perspective on plasmons

The polarization propagator has an important application in the calculation of the so-called effective, or dressed, interaction. One automatically comes to this definition if one tries to partially sum the perturbation expansion for the Green's function by successive insertions of polarization insertions in the interaction lines (see figure 28.1). The summation of *all* polarization insertions gives, by definition, the full polarization propagator, so the effective interaction is given by

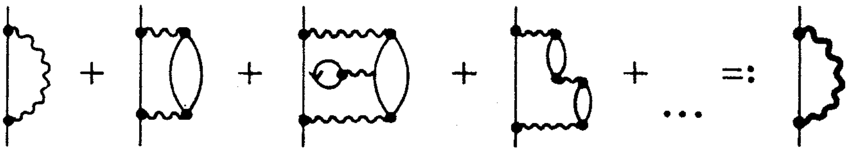


Figure 28.1 *Summation of all polarization insertions yields an effective interaction.*

$$i\,u_{\text{eff}}(x,x') = i\,u(x,x') + i^2 \int \mathrm{d}^4y \int \mathrm{d}^4y'\, u(x,y)\left[-i\Pi(y,y')\right] u(y',x')$$

as illustrated in figure 28.2. In this definition, a dressed interaction line, as well as a usual bare one, contribute a factor i in the translation to formal language. We obtain

$$u_{\text{eff}}(x,x') = u(x,x') + \int \mathrm{d}^4y \int \mathrm{d}^4y'\, u(x,y)\Pi(y,y')u(y',x'). \qquad (28.1)$$

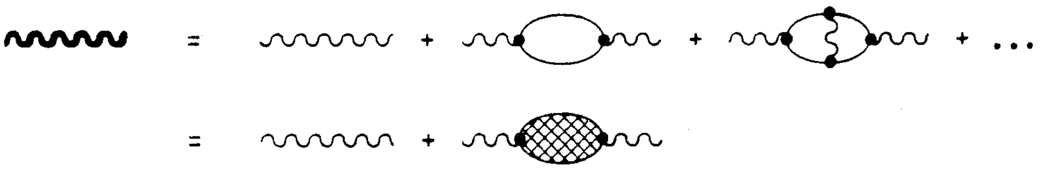


Figure 28.2 *Diagrammatic representation of the effective interaction.*

With the definition of the irreducible polarization propagator Q, we can derive Dyson's equation for the effective interaction:

$$u_{\text{eff}}(x,x') = u(x,x') + \int \mathrm{d}^4y \int \mathrm{d}^4y'\, u(x,y)Q(y,y')u_{\text{eff}}(y',x'). \qquad (28.2)$$

as illustrated in figure 28.3. This equation too is particularly simple for

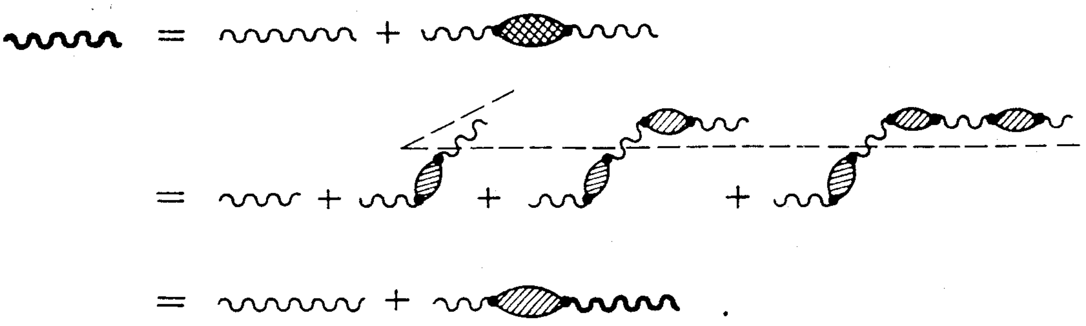


Figure 28.3 *Dyson's equation for the effective interaction.*

translationally invariant systems with spin-independent instantaneous interactions:

$$u_{\text{eff}}(\mathbf{q},\omega) = u(\mathbf{q}) + u(\mathbf{q})Q(\mathbf{q},\omega)u_{\text{eff}}(\mathbf{q},\omega). \qquad (28.3)$$

We solve this equation for the effective interaction and define the (in general frequency and momentum-dependent) dielectric function $\epsilon(\mathbf{q},\omega)$:

$$u_{\text{eff}}(\mathbf{q},\omega) = \frac{u(\mathbf{q})}{1-u(\mathbf{q})Q(\mathbf{q},\omega)} \equiv \frac{u(\mathbf{q})}{\epsilon(\mathbf{q},\omega)}. \qquad (28.4)$$

Thus, in contrast to the bare particle-particle interaction, the effective interaction takes into account the polarization of the medium in the sense of a linear response theory. The frequency dependence means, after Fourier back-transforming, that we now have a time-dependent interaction. This can clearly be understood as a certain inertia of the polarization cloud.

From equation (28.4), we obtain the following equation:

$$\epsilon(\mathbf{q},\omega) = 1 - u(\mathbf{q})Q(\mathbf{q},\omega) \tag{28.5}$$

which together with equation (27.13) yields a relation between the full polarization propagator and the dielectric function

$$\frac{1}{\epsilon(\mathbf{q},\omega)} = 1 + u(\mathbf{q})\Pi(\mathbf{q},\omega). \tag{28.6}$$

We will now discuss an example for Coulomb systems ($u(q) = 4\pi e^2/q^2$): the so-called *random-phase approximation* (RPA). This is basically nothing but the summation of ring diagrams just as in the Gell-Mann–Brueckner theory. We approximate the Green's function by the diagrams shown in figure 28.4. As a consequence, the approximation for the effective interaction is as shown in figure 28.5. We can interpret this approximation in the following way. In the perturbation expansion of the effective interaction, the zeroth-order polarization propagator is inserted instead of the full irreducible polarization:

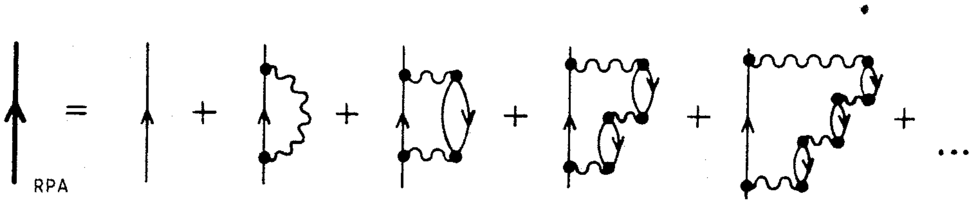


Figure 28.4 *Random-phase approximation for the Green's function.*

RPA: $Q \approx \Pi^{(0)}$, *i.e.*,

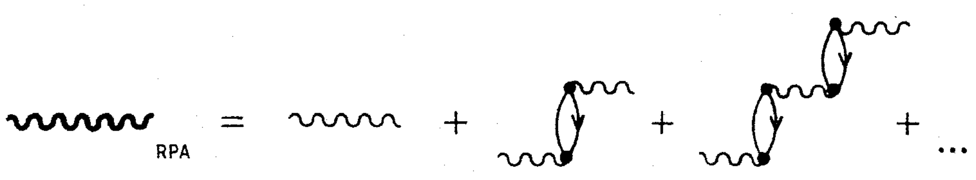


Figure 28.5 *Random-phase approximation for the effective interaction.*

This yields

$$u_{\text{eff}}^{(\text{RPA})}(\mathbf{q},\omega) = \frac{u(\mathbf{q})}{1 - u(\mathbf{q})\Pi^{(0)}(\mathbf{q},\omega)} \tag{28.7}$$

and

$$\epsilon^{(\text{RPA})}(\mathbf{q},\omega) = 1 - u(\mathbf{q})\Pi^{(0)}(\mathbf{q},\omega) \tag{28.8}$$

respectively. The name RPA was originally coined within the framework of plasmon theory, where, under the assumption of randomly distributed phase-factors, one can neglect a part of the electron–electron interaction. As we have seen, the plasmon theory gives a result similar to the ring-diagram approximation by Gell-Mann and Brueckner. Thus, the term RPA has come to be applied also for the latter theory. In this context, the physical reason for the name is however not quite clear, nor is the ring-diagram approximation in its original sense identical to the RPA.

From the explicit representation, equations (27.25) and (27.26), of the Lindhard function, we obtain following limits:

$$\begin{aligned} &\lim_{q\to 0} \epsilon^{(\text{RPA})}(\mathbf{q},\omega) \\ &= \lim_{q\to 0} \left\{ 1 + \frac{2me^2k_F}{\pi}\frac{1}{q^2}\left\{ 1 + \frac{k_F}{q}\left[1 - \frac{1}{4}\left(\frac{q}{k_F}\right)^2\right] \ln\left|\frac{k_F + q/2}{k_F - q/2}\right| \right\}\right\} \\ &= 1 + \frac{4me^2k_F}{\pi}\frac{1}{q^2} \end{aligned} \tag{28.9}$$

and

$$\epsilon^{(\text{RPA})}(0,\omega) = 1 - \frac{\omega_p^2}{\omega^2}. \tag{28.10}$$

Equation (28.9) yields the following result for the effective interaction in the limit of $q/k_F \ll 1$

$$u_{\text{eff}}^{(\text{RPA})}(q,\omega = 0) \approx \frac{4\pi e^2}{q^2 + \lambda^2} \quad \text{where } \lambda^2 = \frac{6\pi(N/\Omega)e^2}{\epsilon_F} \tag{28.11}$$

which, after Fourier back-transforming, gives the following form for the static effective interaction for $rk_F \gg 1$:

$$u_{\text{eff}}^{(\text{RPA})}(r) \approx \frac{e^2}{r}e^{-\lambda r}. \tag{28.12}$$

Equation (28.12) is a screened Coulomb potential. This is in accordance with the physical picture that we have already made: the bare electron repels other electrons because of the Coulomb repulsion and the exchange interaction, which reduces the probability of finding other electrons in its immediate vicinity. Thus, the electron drags a 'hole cloud' with it and hence becomes a quasi-electron with an altered dispersion relation. This can of course be calculated from the corresponding RPA for the self-energy M. Due to the screening, the full Coulomb interaction between the bare electrons becomes an effective interaction between quasi-electrons, which here is obtained approximately as a Yukawa-potential. (For a closer loook at the idea that the effective interaction is an interaction between quasi-particles, see Falicov [23].)

Equation (28.10) implies that the dielectric function $\epsilon^{(\mathrm{RPA})}(0,\omega)$ vanishes as ω approaches the plasma frequency ω_p. Consequently, it follows from equation (28.6) that the response function $\Pi^{(\mathrm{RPA})}$ of the electron gas in this case becomes infinite in this limit. This means that an infinitesimal perturbation will result in a finite change in the electron density. This concept is connected with an eigenmode of the system, in this case a plasma oscillation. At this point, we have the opportunity to elegantly calculate the dispersion relation $\omega(\mathbf{q})$ of the plasmons. We set

$$\epsilon^{(\mathrm{RPA})}(\mathbf{q},\omega(\mathbf{q}))=0.$$

This yields, for small q,

$$\lim_{q\to 0}\omega(q)^2\approx\omega_p^2\left[1+\frac{3}{5}\frac{(k_F/m)^2q^2}{\omega_p^2}\right]^2. \tag{28.13}$$

We close this chapter with a discussion of yet another way of partially summing the perturbation expansion: the dressing of vertices. We discussed in Chapter 25 how the $G^{(0)}$-line can be dressed by successive insertions of self-energy insertions. The corresponding approximations for the self-energy, for example the one shown in figure 28.6, then yields an equation to be solved self-consistently. We can use this idea to *simultaneously* dress the interaction lines with polarization insertions; for example, from figure 28.6, we obtain figure 28.7. Note that dressing the interaction line in the direct term would be incorrect, since it would lead to double-counting. Since the effective interaction in general is time-dependent, this results in a time-dependent equation to be solved self-consistently.

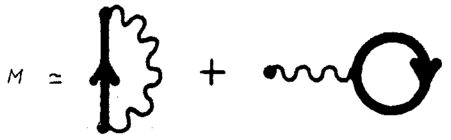


Figure 28.6 *Self-consistent Hartree–Fock approximation for the self-energy M.*

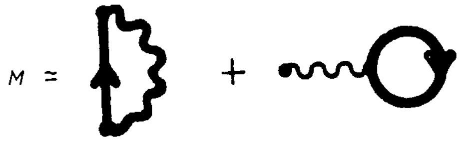


Figure 28.7 *In the Hartree–Fock approximation for M, the interaction line of the exchange term can also be dressed, in addition to the Green's functions.*

It is easy to erroneously believe that the approximation for M depicted in figure 28.7 yields the exact self-energy if all possible self-energy insertions and all possible polarization insertions on the interaction line are included. However, the diagrams in figure 28.8, for example, are not obtained in this way. Such diagrams can also by summed formally. We first define the so-called *vertex insertion* as a diagram with two $G^{(0)}$-legs and on interaction leg. Such diagrams can clearly be placed at a normal vertex and in this way 'dress the vertex'. Examples are shown in figure 28.9. It is clear that, for example, the diagram figure 28.8(a) can be obtained by the following replacement shown in figure 28.10. We now define an irreducible vertex insertion as a vertex insertion which has no self-energy insertions on the incoming and outgoing $G^{(0)}$-lines and no polarization insertion on the incoming and outgoing interaction lines. Correspondingly (written for translationally invariant systems)

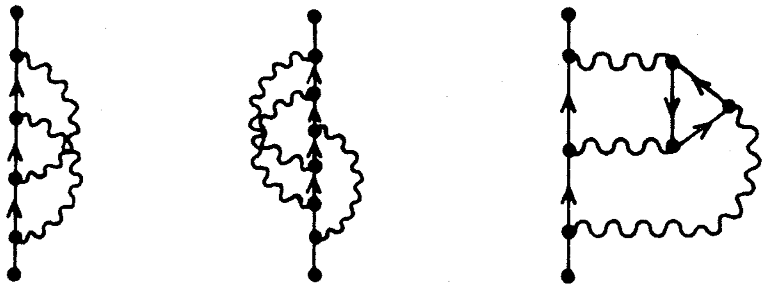

(a) (b) (c)

Figure 28.8 *Diagrams* (a), (b) *and* (c) *cannot be obtained only by dressing interaction lines and Green's functions.*

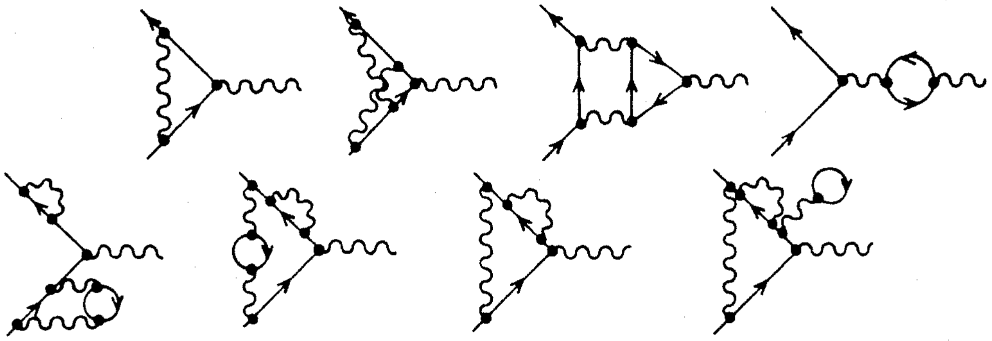


Figure 28.9 *Examples of diagrams which can be included in the dressed vertex.*

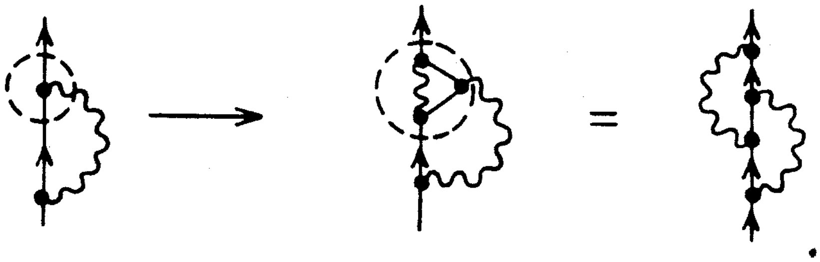


Figure 28.10 *The diagram figure 28.8(*a*) can be constructed by a vertex-insertion into a first-order Green's function diagram.*

irreducible vertex function $\equiv$ $\Lambda(\mathbf{k}, \mathbf{q})$

$\equiv$ the sum of all irreducible vertex insertions with the corresponding indices on the external legs

(see figure 28.11). Since each vertex insertion has two $G^{(0)}$-legs and one interaction leg, we can sometimes combine all vertex insertions which differ only in the self-energy and polarization insertions, respectively, on the external lines by dressing the Green's functions and the interaction lines:

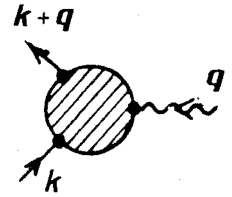
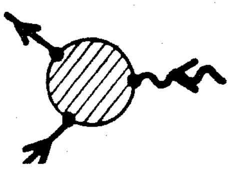
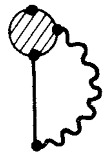


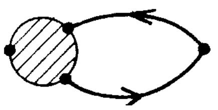
Figure 28.11 *The irreducible vertex function* $\Lambda(\mathbf{k}, \mathbf{q})$.

sum over all vertex insertions = 

In particular, we have the exact equations

$M =$  +  (28.14)

and

$Q =$  (28.15)

Even though these two equations look unappealingly asymmetric, it is clear from their derivations that the vertex function Λ can only be at one end; otherwise, some diagrams will be counted twice (see figures 28.12 and 28.13).

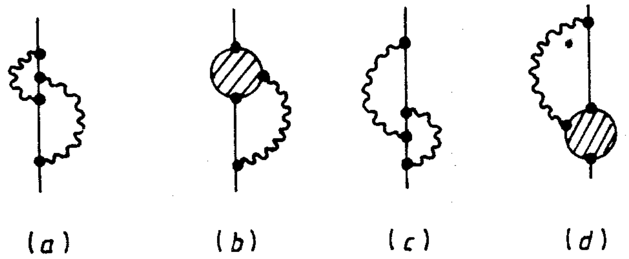


Figure 28.12 *The diagram* (a) *is included in the diagram* (b), *but also in diagram* (c) *in the form shown in* (d).

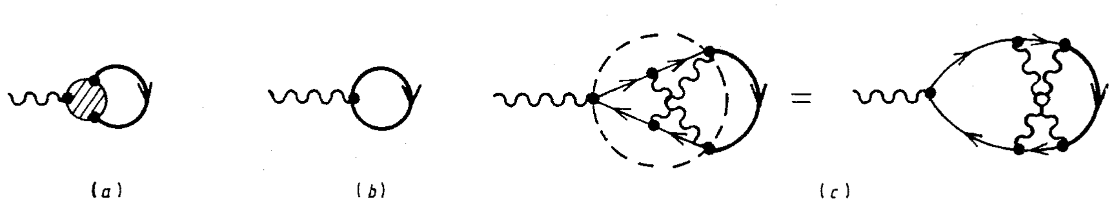


Figure 28.13 *The diagram* (a) *must not be included in the direct term* (b), *since vertex diagrams are included, as shown in* (c).

Of course, the irreducible vertex diagrams can also be reduced to a few skeleton diagrams; examples are shown in figure 28.14. Again, self-consistent approximation can be derived through approximations such as the one shown in figure 28.15.We realize what an enormous number of diagrams we obtain if we on the right-hand side insert only the lowest-order approximations for u_{eff}, G and Λ.

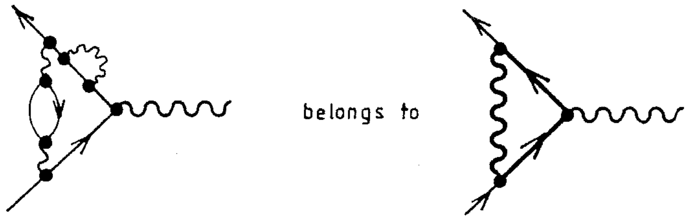


Figure 28.14 *Examples of skeleton diagrams of the irreducible diagram.*

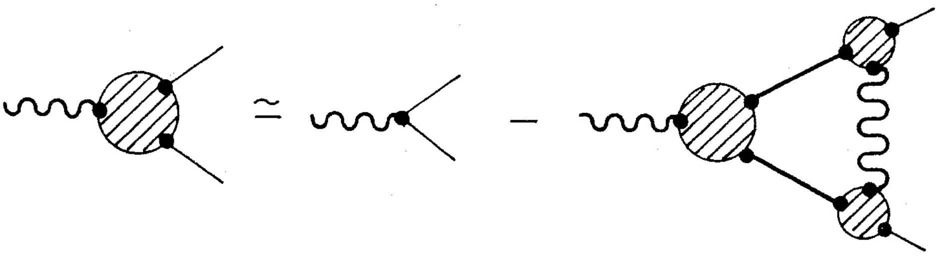


Figure 28.15 *Self-consistent approximation for the irreducible vertex*

In many problems, the so-called ladder diagrams (see figure 28.16) give the dominant contribution. These diagrams can then be summed.

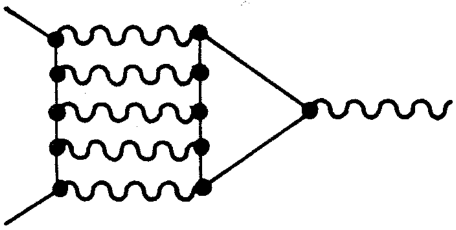


Figure 28.16 *A vertex ladder diagram.*

We have now learnt several different ways of partial summation. Which way is best depends on the particular problem, especially on the nature of the interaction.

Chapter 29

Perturbation theory at finite temperatures

We will in this final chapter of Part III briefly indicate how the formalism discussed up to this point has to be generalized in order to be applied to temperature-dependent systems. The starting point is the so-called *ensemble average* to calculate equilibrium expectation values of observables of the system under consideration. Let $\mid \Psi_i\rangle$ be the exact states of the system, with energies E_i

$$H \mid \psi_i\rangle = E_i \mid \Psi_i\rangle$$

and particle numbers N_i

$$N \mid \Psi_i\rangle = N_i \mid \Psi_i\rangle.$$

Let P_i be the probability of finding the system in the state $\mid \Psi_i\rangle$. The expectation value of an arbitrary operator A is then obtained from the ensemble average

$$\langle A\rangle \equiv \sum_i P_i\langle\Psi_i \mid A \mid \Psi_i\rangle.$$

If the system under consideration can exchange energy in the form of heat as well as particles with its environment, one uses the grand canonical ensemble. In this case, the probability P_i depends on the temperature T and the chemical potential μ of the system, and is obtained from the following well-known expression:

$$P_i = P_i(T,\mu) = \frac{\mathrm{e}^{-\beta(E_i-\mu N_i)}}{\sum_n \mathrm{e}^{-\beta(E_n-\mu N_n)}} \qquad \beta = \frac{1}{k_B T}$$

where k_B is Boltzmann's constant.

We now define the so-called Bloch density operator as

$$\rho_G \equiv \mathrm{e}^{-\beta(H-\mu N)}. \tag{29.1}$$

The index G stands for 'grand canonical'. We have

$$\langle A\rangle = \frac{\sum_i \mathrm{e}^{-\beta(E_i-\mu N_i)}\langle\Psi_i \mid A \mid \Psi_i\rangle}{\sum_n \mathrm{e}^{-\beta(E_n-\mu N_n)}}$$

hence

$$\langle A\rangle = \frac{\sum_i\langle\Psi_i \mid \rho_G A \mid \Psi_i\rangle}{\sum_n\langle\Psi_n \mid \rho_G \mid \Psi_n\rangle} = \frac{\mathrm{Tr}\,[\rho_G A]}{\mathrm{Tr}\,[\rho_G]} \tag{29.2}$$

with the trace taken over any complete basis. The denominator has a special name; it is called the grand canonical partition function:

$$Z_G \equiv \mathrm{Tr}\,[\rho_G]\,. \tag{29.3}$$

We denote ensemble average of the non-interacting system with the Hamiltonian $H = H_0$ by the subscript 0:

$$\langle A\rangle_0 \equiv \frac{\mathrm{Tr}\left[\rho_G^{(0)} A\right]}{\mathrm{Tr}\left[\rho_G^{(0)}\right]} = \frac{\mathrm{Tr}\left[\mathrm{e}^{-\beta(H_0-\mu N)}A\right]}{\mathrm{Tr}\left[\mathrm{e}^{-\beta(H_0-\mu N)}\right]}. \tag{29.4}$$

As an example, we calculate the number of particles with momentum $\mathbf{k}$, *i.e.*, the momentum distribution function, for a system of non-interacting free fermions. The eigenfunctions of H_0 are Slater determinants $\mid \Phi_i\rangle$ of plane waves with

$$\begin{aligned} n(\mathbf{k}) \mid \Phi_i\rangle &\equiv n_i(\mathbf{k}) \\ &= \begin{cases} 0 & \text{if the momentum state } \mathbf{k} \text{ is unoccupied in } \mid \Phi_i\rangle \\ 1 & \text{if the momentum state } \mathbf{k} \text{ is occupied in } \mid \Phi_i\rangle. \end{cases} \end{aligned}$$

We have

$$\langle n(\mathbf{k})\rangle_0 = \frac{\sum_i\langle\Phi_i \mid \rho_G^{(0)} n(\mathbf{k}) \mid \Phi_i\rangle}{\sum_i\langle\Phi_i \mid \rho_G^{(0)} \mid \Phi_i\rangle} = \frac{\sum_i n_i(\mathbf{k})\langle\Phi_i \mid \rho_G^{(0)} \mid \Phi_i\rangle}{\sum_i\langle\Phi_i \mid \rho_G^{(0)} \mid \Phi_i\rangle}. \tag{29.5}$$

We calculate the individual terms in this expression:

$$\begin{aligned} \langle\Phi_i \mid \rho_G^{(0)} \mid \Phi_i\rangle &= \langle\Phi_i \mid \mathrm{e}^{-\beta(H_0-\mu N)} \mid \Phi_i\rangle \\ &= \langle\Phi_i \mid \exp\left[-\beta\sum_{\mathbf{q}}\left(\frac{q^2}{2m}-\mu\right)c_{\mathbf{q}}^\dagger c_{\mathbf{q}}\right] \mid \Phi_i\rangle \\ &= \langle\Phi_i \mid \exp\left[-\beta\sum_{\mathbf{q}}\left(\frac{q^2}{2m}-\mu\right)n_i(\mathbf{q})\right] \mid \Phi_i\rangle \\ &= \exp\left[-\beta\sum_{\mathbf{q}}\left(\epsilon_q^{(0)}-\mu\right)n_i(\mathbf{q})\right] \\ &= \prod_{\mathbf{q}}\exp\left[-\beta\left(\epsilon_q^{(0)}-\mu\right)n_i(\mathbf{q})\right]. \end{aligned}$$

The sum over all configurations $| \Phi_i\rangle$ can, by an arbitrary but fixed renumeration of the momentum, be written as

$$\sum_{|\Phi_i\rangle = |n_i(1), n_i(2), \dots\rangle} = \sum_{n_i(1)=0}^{1} \sum_{n_i(2)=0}^{1} \sum_{\cdots} \cdots .$$

We then obtain for the denominator of equation (29.5)

$$\begin{aligned} Z_G^{(0)} &= \sum_i \prod_{\mathbf{q}} \mathrm{e}^{-\beta(\epsilon_q^{(0)}-\mu)n_i(\mathbf{q})} \\ &= \sum_{n_i(1)=0}^{1} \sum_{n_i(2)=0}^{1} \dots \mathrm{e}^{-\beta(\epsilon_1^{(0)}-\mu)n_i(1)} \mathrm{e}^{-\beta(\epsilon_2^{(0)}-\mu)n_i(2)} \dots \\ &= \prod_{\mathbf{q}} \left[1+\mathrm{e}^{-\beta(\epsilon_q^{(0)}-\mu)}\right]. \end{aligned}$$

The numerator of equation (29.5) becomes

$$\begin{aligned} \sum_i n_i(\mathbf{k}) \langle \Phi_i \mid \rho_G^{(0)} \mid \Phi_i\rangle &= \sum_i n_i(\mathbf{k}) \prod_{\mathbf{q}} \exp\left[-\beta\left(\epsilon_q^{(0)}-\mu\right) n_i(\mathbf{q})\right] \\ &= \sum_i n_i(\mathbf{k}) \mathrm{e}^{-\beta(\epsilon_k^{(0)}-\mu)n_i(\mathbf{k})} \prod_{\mathbf{q}\neq\mathbf{k}} \mathrm{e}^{-\beta(\epsilon_q^{(0)}-\mu)n_i(\mathbf{q})} \\ &= \sum_{n_i(1)=0}^{1} \sum_{n_i(2)=1}^{1} \cdots \\ &= \mathrm{e}^{-\beta(\epsilon_k^{(0)}-\mu)} \prod_{\mathbf{k}\neq\mathbf{q}} \left[1+\mathrm{e}^{-\beta(\epsilon_q^{(0)}-\mu)}\right]. \end{aligned}$$

We combine these two expressions to arrive at

$$\begin{aligned} \langle n(\mathbf{k})\rangle_0 &= \frac{\mathrm{e}^{-\beta(\epsilon_k^{(0)}-\mu)} \left[\prod_{\mathbf{q}\neq\mathbf{k}} \left(1+\mathrm{e}^{-\beta(\epsilon_q^{(0)}-\mu)}\right)\right]}{\left[\prod_{\mathbf{q}} \left(1+\mathrm{e}^{-\beta(\epsilon_q^{(0)}-\mu)}\right)\right]} \\ &= \frac{\mathrm{e}^{-\beta(\epsilon_k^{(0)}-\mu)}}{1+\mathrm{e}^{-\beta(\epsilon_k^{(0)}-\mu)}} \\ &= \frac{1}{1+\mathrm{e}^{\beta(\epsilon_k^{(0)}-\mu)}}. \end{aligned} \tag{29.6}$$

This is the well-known Fermi distribution function. We will hereafter abbreviate it as

$$\langle n(\mathbf{k})\rangle_0 \equiv f_{\mathbf{k}}.$$

The decisive observation for the perturbation expansion at finite temperatures, which we will arrive at later, is that ρ_G satisfies a Schrödinger-type of equation, namely the *Bloch equation*

$$-\frac{\partial}{\partial\beta}\rho_G = (H - \mu N)\,\rho_G. \tag{29.7}$$

If we make the substitutions

$$\begin{array}{rcl} \rho_G & \leftrightarrow & \Psi \\ H-\mu N & \leftrightarrow & H \\ \beta & \leftrightarrow & it \end{array}$$

we obtain the usual Schrödinger equation. This similarity makes the construction of the formalism possible in parallel with the zero-temperature theory. First, we define a 'Heisenberg picture' by

$$O(\tau)_H \equiv \mathrm{e}^{(H-\mu N)\tau} O_S \mathrm{e}^{-(H-\mu N)\tau} \text{ for } t \in \mathcal{R}. \tag{29.8}$$

The two operators transformed in this way are in general not unitary. They are, however, each others' inverse, so that the transformation of a product is the product of transformations. The fact that the transformation operators in general are not unitary has as a consequence that a transformed creation operator

$$\psi^\dagger_\alpha(\mathbf{r}\tau)_H \equiv \mathrm{e}^{(H-\mu N)\tau}\psi^\dagger_\alpha(\mathbf{r})\mathrm{e}^{-(H-\mu N)\tau}$$

in general is *not* the adjoint of the transformed annihilation operator

$$\psi_\alpha(\mathbf{r}\tau)_H \equiv \mathrm{e}^{(H-\mu N)\tau}\psi_\alpha(\mathbf{r})\mathrm{e}^{-(H-\mu N)\tau}.$$

It is important to keep in mind that $(\psi^\dagger)_H$ and not $(\psi_H)^\dagger$ satisfies the canonical anti-commutation relation with the annihilation operator ψ_H.

We now define the temperature-dependent single-particle Green's function for fermions through the ensemble-average:

$$\begin{aligned} G_{\alpha\gamma}(\mathbf{r}\tau,\mathbf{r}'\tau') &\equiv -\langle T\left[\psi_\alpha(\mathbf{r}\tau)_H\psi^\dagger_\gamma(\mathbf{r}'\tau')_H\right]\rangle \\ &= -\frac{\mathrm{Tr}\left\{\rho_G T\left[\psi_\alpha(\mathbf{r}\tau)_H\psi^\dagger_\gamma(\mathbf{r}'\tau')_H\right]\right\}}{\mathrm{Tr}\left\{\rho_G\right\}}. \end{aligned} \tag{29.9}$$

The operator T is defined as before; it orders the field operators according to increasing τ and multiplies with the sign of the necessary permutation. In this definition, as also in the Bloch-equation, no factor of i appears.

From the Green's function defined in this way, we can calculate

(1) the (ensemble) expectation value of any single-particle operator, and

(2) the internal energy $E(T,\mu) = \langle H \rangle$ of the system, and thus also the expectation value of the two-particle interaction.

An interaction picture can also be introduced by separating $H_0 - \mu N$ from $H - \mu N$:

$$K \equiv H - \mu N = (H_0 - \mu N) + V \equiv K_0 + V \tag{29.10}$$

and defining

$$O(\tau)_I \equiv \mathrm{e}^{K_0 \tau} O_S \mathrm{e}^{-K_{tau}}. \tag{29.11}$$

The Heisenberg picture and the interaction picture are related by

$$\begin{aligned} O(\tau)_H &= \mathrm{e}^{K\tau} O_S \mathrm{e}^{-K\tau} = \mathrm{e}^{K\tau} \mathrm{e}^{-K_0\tau} O(\tau)_I \mathrm{e}^{+K_0\tau} \mathrm{e}^{-K\tau} \\ &= U(0,\tau) O(\tau)_I U(\tau,0) \end{aligned}$$

where

$$U(\tau_1,\tau_2) \equiv \mathrm{e}^{+K_0\tau_1} \mathrm{e}^{-K(\tau_1-\tau_2)} \mathrm{e}^{-K_0\tau_2}. \tag{29.12}$$

The operator U defined in equation (29.12) is not in general unitary, but we have as before

$$\begin{aligned} U(\tau_1,\tau_2)U(\tau_2,\tau_3) &= U(\tau_1,\tau_3) \\ U(\tau_1,\tau_1) &= 1. \end{aligned}$$

One can easily show that U satisfies the following equation of motion (we will not perform the details of this calculation; it runs entirely parallel with the discussions in Chapters 14 and 15):

$$\frac{\partial}{\partial \tau} U(\tau,\tau') = -V(\tau)_I U(\tau,\tau') \tag{29.13}$$

with the formal solution

$$U(\tau,\tau') = \sum_{n=0}^{\infty} \frac{(-)^n}{n!} \int_{\tau'}^{\tau} \mathrm{d}\tau_1 \ldots \int_{\tau'}^{\tau} \mathrm{d}\tau_n \, T\left[V(\tau_1)_I \ldots V(\tau_n)_I\right]. \tag{29.14}$$

The representation given by equation (29.14) is the basis for the perturbation expansion for temperatures $T > 0$. For example, from this equation we obtain for the partition function

$$\begin{aligned} Z_G &= \mathrm{Tr}\left\{\mathrm{e}^{-\beta(H-\mu N)}\right\} = \mathrm{Tr}\left\{\mathrm{e}^{-\beta K_0} U(\beta,0)\right\} \\ &= \sum_{n=0}^{\infty} \frac{(-)^n}{n!} \int_0^{\beta} \mathrm{d}\tau_1 \ldots \int_0^{\beta} \mathrm{d}\tau_n \, \mathrm{Tr}\left\{\mathrm{e}^{-\beta(H_0-\mu N)} T\left[V(\tau_1)_I \ldots V(\tau_n)_I\right]\right\}. \end{aligned} \tag{29.15}$$

The trace can be elegantly evaluated in the complete basis of eigenfunctions of the unperturbed system with the result

$$\begin{aligned} Z_G &= \sum_{n=0}^{\infty} \frac{(-)^n}{n!} \int_0^\beta \mathrm{d}\tau_1 \ldots \int_0^\beta \mathrm{d}\tau_n \\ &\quad \times \sum_i \mathrm{e}^{-\beta(E_i^{(0)}-\mu N_i)} \langle \Phi_i \mid T\left[V(\tau_1)_I \ldots V(\tau_n)_I\right] \mid \Phi_i \rangle . \end{aligned} \tag{29.16}$$

Thus, the partition function Z_G corresponds to the vacuum amplitude of the $T = 0$–formalism; just as the vacuum amplitude, Z_G stands in the denominator of the Green's function, and gives rise to disconnected diagrams which cancel out with the disconnected parts of the diagrams in the numerator. A direct evaluation of the numerator of the Green's function yields

$$\begin{aligned} &G_{\alpha\gamma}(\mathbf{r}\tau, \mathbf{r}'\tau') \\ &= -\frac{1}{Z_G} \sum_{n=0}^{\infty} \frac{(-)^n}{n!} \int_0^\beta \mathrm{d}\tau_1 \ldots \int_0^\beta \mathrm{d}\tau_n \\ &\qquad \times \mathrm{Tr}\left\{ \mathrm{e}^{-\beta(H_0-\mu N)} T\left[V(\tau_1)_I \ldots V(\tau_n)_I \psi_\alpha(\mathbf{r}\tau)_I \psi_\gamma^\dagger(\mathbf{r}'\tau')_I \right] \right\} . \end{aligned}$$

We note that the integration intervals here, as well as in equation (29.16), are $[0, \beta]$.

In contrast to the usual (temperature-independent) Green's function, we have to determine *not* a matrix element of 'time'-ordered products in each term, but, as we see in the representation equation (29.16) of the denominator, we have to determine a trace, *i.e.*, an infinite sum of such matrix elements. Wick's theorem in the form that we know it will not help us in the evaluation of these matrix elements, since the normal-order products only vanish when they act on the ground state $\mid \Phi_0 \rangle$; in the trace, all states $\mid \Phi_i \rangle$ appear. We can, however, find a generalization of Wick's theorem, which will help us. The idea is to interpret Z_G and the numerator and denominator of the of the Green's function individually as ensemble-averages with respect to $\rho_G^{(0)} = \exp[-\beta(H_0 - \mu N)]$. To do this, we expand $1/Z_G^{(0)}$ and obtain

$$\begin{aligned} &G_{\alpha\gamma}(\mathbf{r}\tau, \mathbf{r}'\tau') \\ &= \frac{\sum_{n=0}^{\infty} \frac{(-)^n}{n!} \int_0^\beta \mathrm{d}\tau_1 \ldots \int_0^\beta \mathrm{d}\tau_n \langle T\left[V(\tau_1)_I \ldots V(\tau_n)_I \psi_\alpha(\mathbf{r}\tau)_I \psi_\gamma^\dagger(\mathbf{r}'\tau')_I \right] \rangle_0}{\sum_{n=0}^{\infty} \frac{(-)^n}{n!} \int_0^\beta \mathrm{d}\tau_1 \ldots \int_0^\beta \mathrm{d}\tau_n \langle T\left[V(\tau_1)_I \ldots V(\tau_n)_I\right] \rangle_0} . \end{aligned} \tag{29.17}$$

In Chapter 19, the normal-order and contraction of operators were introduced to evaluate the matrix elements. The contractions became c-numbers; in particular we had that the expectation value of normal-ordered products vanishes (here written for translationally invariant systems):

$$\begin{aligned}\overbracket{c_{\mathbf{k}}(t)c_{\mathbf{k}'}}(t') &= \langle\Phi_0 \mid T\left[c_{\mathbf{k}}(t)c_{\mathbf{k}'}(t')\right] - N\left[c_{\mathbf{k}}(t)c_{\mathbf{k}'}(t')\right] \mid \Phi_0\rangle \\ &= \langle\Phi_0 \mid T\left[c_{\mathbf{k}}(t)c_{\mathbf{k}'}(t')\right] \mid \Phi_0\rangle = G^{(0)}(\mathbf{k}t, \mathbf{k}'t').\end{aligned}$$

We use this property as a model for defining the contraction in the finite-temperature theory:

$$\begin{aligned}\overbracket{c_{\mathbf{k}}(\tau)_I c^{\dagger}_{\mathbf{k}'}}(\tau')_I &= \langle T\left[c_{\mathbf{k}}(\tau)_I c^{\dagger}_{\mathbf{k}'}(\tau')\right]\rangle_0 \\ &= G^{(0)}(\mathbf{k}\tau, \mathbf{k}'\tau') \qquad (29.18)\\ \overbracket{c_{\mathbf{k}}(\tau)_I c_{\mathbf{k}'}}(\tau')_I &= 0 \qquad (29.19)\\ \overbracket{c^{\dagger}_{\mathbf{k}}(\tau)_I c^{\dagger}_{\mathbf{k}'}}(\tau')_I &= 0. \qquad (29.20)\end{aligned}$$

These definitions are extended linearly. For example, we set

$$\overbracket{c_{\mathbf{k}'}(\ldots)_I \sum_{\nu} \alpha_{\nu} c^{\dagger}_{\mathbf{k}_{\nu}}}(\ldots)_I = \sum_{\nu} \alpha_{\nu}\, \overbracket{c_{\mathbf{k}'}(\ldots)_I c^{\dagger}_{\mathbf{k}_{\nu}}}(\ldots)_I.$$

Furthermore, we have

$$\begin{aligned}\overbracket{c_{\mathbf{k}}(0^{+})_I c^{\dagger}_{\mathbf{k}'}}(0)_I &= \langle c_{\mathbf{k}} c^{\dagger}_{\mathbf{k}'}\rangle_0 = \delta_{\mathbf{k},\mathbf{k}'}(1 - f_{\mathbf{k}}) \qquad (29.21)\\ \overbracket{c_{\mathbf{k}}(0)_I c^{\dagger}_{\mathbf{k}'}}(0)_I &= \langle -c^{\dagger}_{\mathbf{k}'} c_{\mathbf{k}}\rangle_0 = -\delta_{\mathbf{k},\mathbf{k}'} f_{\mathbf{k}}. \qquad (29.22)\end{aligned}$$

These ensemble averages are obtained, as was the example of the momentum distribution function, directly from the definition equation (29.4) of $\langle\;\rangle_0$ as weighted averages of expectation values relative to Slater determinants.

As in Chapter 14, we find that

$$\begin{aligned}c_{\mathbf{k}}(\tau)_I &= \mathrm{e}^{-(\epsilon^{(0)}_k-\mu)\tau} c_{\mathbf{k}}(0) &&= \mathrm{e}^{-(\epsilon^{(0)}_k-\mu)} c_{\mathbf{k}} \qquad (29.23)\\ c^{\dagger}_{\mathbf{k}}(\tau)_I &= \mathrm{e}^{+(\epsilon^{(0)}-\mu)\tau} c^{\dagger}_{\mathbf{k}}(0) &&= \mathrm{e}^{+(\epsilon^{(0)}_k-\mu)\tau} c^{\dagger}_{\mathbf{k}}. \qquad (29.24)\end{aligned}$$

We can then calculate the contraction defined in equation (29.18):

$$\begin{aligned}
&\overbracket{c_{\mathbf{k}}(\tau)_I c^{\dagger}_{\mathbf{k}'}(\tau')_I} \\
&= \theta(\tau-\tau')\langle c_{\mathbf{k}}(\tau)_I c^{\dagger}_{\mathbf{k}'}(\tau')_I\rangle_0 - \theta(\tau'-\tau)\langle c^{\dagger}_{\mathbf{k}'}(\tau')_I c_{\mathbf{k}}(\tau)_I\rangle_0 \\
&= \mathrm{e}^{-(\epsilon^{(0)}_k-\mu)(\tau-\tau')}\left[\theta(\tau-\tau')\langle c_{\mathbf{k}} c^{\dagger}_{\mathbf{k}'}\rangle_0 - \theta(\tau'-\tau)\langle c^{\dagger}_{\mathbf{k}'} c_{\mathbf{k}}\rangle_0\right],
\end{aligned}$$

and from equations (29.21) and (29.22) it finally follows that

$$\begin{aligned}
&\overbracket{c_{\mathbf{k}}(\tau)_I c^{\dagger}_{\mathbf{k}'}(\tau')_I} \\
&= G^{(0)}(\mathbf{k}\tau,\mathbf{k}'\tau') \\
&= \delta_{\mathbf{k},\mathbf{k}'}\mathrm{e}^{-(\epsilon^{(0)}_k-\mu)(\tau-\tau')}\left[\theta(\tau-\tau')(1-f_{\mathbf{k}}) - \theta(\tau'-\tau)f_{\mathbf{k}}\right].
\end{aligned} \tag{29.25}$$

This is the temperature-dependent analog of the momentum Green's function equation (15.23). Correspondingly, we have for the space-dependent Green's function

$$\begin{aligned}
G^{(0)}_{\alpha\gamma}(\mathbf{r}\tau,\mathbf{r}'\tau') &= \langle T\left[\psi_\alpha(\mathbf{r}\tau)_I\psi^{\dagger}_{\gamma}(\mathbf{r}'\tau')_I\right]\rangle_0 \\
&= \overbracket{\psi_\alpha(\mathbf{r}\tau)_I\psi^{\dagger}_{\gamma}(\mathbf{r}'\tau')_I}.
\end{aligned} \tag{29.26}$$

We cannot prove a Wick's theorem as an operator identity for temperature-dependent systems with these results, but we have nevertheless the following statement for the ensemble average [24, 25]:

$$\langle T\left[\ldots c_{\mathbf{k}}(.)\ldots c^{\dagger}_{\mathbf{k}'}(.)\ldots\right]\rangle_0 \quad = \quad \text{sum of all completely contracted terms.}$$

This statement is sufficient to construct a diagrammatic perturbation expansion with the same diagrams and almost the same translation rules as before. Only the prefactors change, since no factors of i appear.

We find an interesting difference in the evaluation of the diagrams: For temperatures $T > 0$ each state $\mid \mathbf{k}\rangle$ is occupied with a certain probability $f_{\mathbf{k}}$ and unoccupied with a certain probability $(1 - f_{\mathbf{k}})$. A principal division in particle and hole states is no longer possible, since each state to a certain extent is both. For this reason diagrams which vanish at zero temperatures (in translationally invariant systems) give non-zero contributions; see, for example, figure 29.1. Such diagrams are frequently called *anomalous diagrams*.

All questions that were discussed in the zero-temperature formalism can also be investigated for systems at finite temperatures. Additional interesting applications include

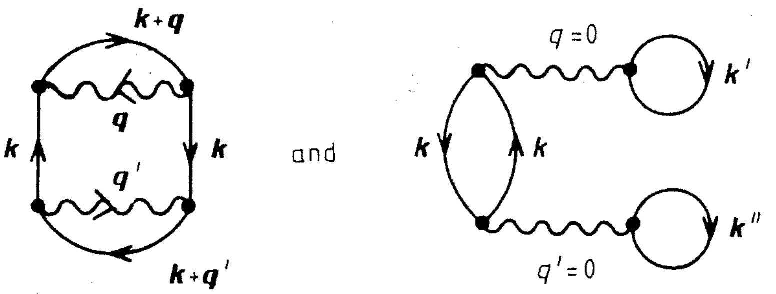


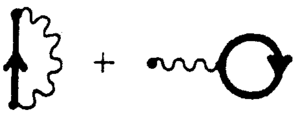
Figure 29.1 *The following diagrams do not contribute to the ground state energy, but they do contribute to the grand canonical potential at non-zero temperatures.*

- the summation of the ring-diagram contribution to $Z_G = Z_G(T, \mu)$. One obtains an (approximately valid) equation of state

$$\frac{p\Omega}{k_B T} = \ln Z_G$$

  for a dense electron gas;

- the derivation of the Hartree–Fock equations for systems at finite temperatures through the approximation

$M(T,\mu) \approx$  ;

- calculation of transition temperatures, such as the temperature of the phase transition into a superconducting state;

- the general question of finite-temperature corrections to the zero-temperature results.

We will not here further pursue the possible uses of the finite-temperature formalism, but only address one remarkable point, which puts the usual perturbation theory for $T = 0$ in a somewhat different light. In many cases, the contributions of the anomalous diagrams do not go to zero, as one would expect, in the limit $T \to 0$. The question then arises of which result gives the correct result for the ground state energy of the system: the earlier zero-temperature result or the limit $T \to 0$ of a finite-temperature calculation. The answer is relatively simple. The original zero-temperature theory is marred by a particular uncertainty. In the proof of the Gell-Mann–Low theorem, we could not show that the adiabatically generated state is the

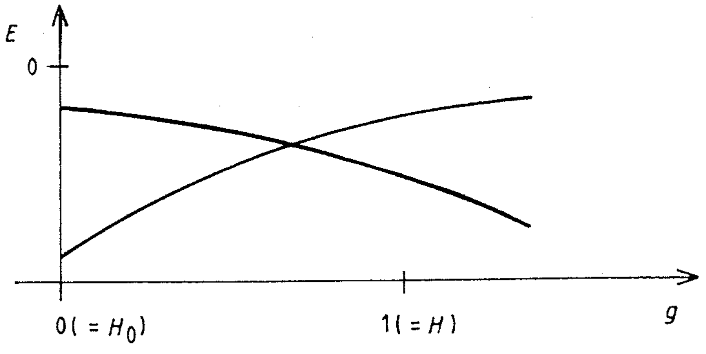


Figure 29.2 *The ground state energy at zero temperature may not evolve adiabatically to the* ground *state of the interacting system.*

ground state of the full Hamiltonian; it was only guaranteed, that it is an eigenstate. Hence, if the spectrum of eigenvalues is exhibited as a function of the coupling constant, one cannot expect that the ground state of the full problem is obtained by turning on the interactions adiabatically; instead, one may end up in an excited state (see figure 29.2). With the help of examples (see for example [26]) one can show that in such cases the $T \longrightarrow 0$ limit of the temperature-dependent theory gives a state with lower energy. Thus, the temperature-dependent theory is really the correct one, since it does not involve any adiabatic turning-on. The integrals that appear in this theory have the structure of $\exp(-\ldots)$, *i.e.*, they are, in contrast to the earlier integrals with the structure $\exp(-i\ldots)$, convergent without any additional convergence factors. However, in quite a few cases, for example in systems with spherical Fermi surfaces, the results from the two different theories do not differ.

Part IV

Fermi Liquid Theory

Chapter 30

Introduction

The ground state of a homogeneous, translationally invariant system of fermions has a well-defined Fermi surface at chemical potential μ. It is useful to define a Fermi temperature T_F by

$$T_F = \frac{1}{k_B} \lim_{T \to 0} \mu. \qquad (30.1)$$

This temperature sets a scale for the excitations in the system. For a homogeneous non-interacting system of density n in three dimensions, the Fermi temperature is given by

$$T_F = \epsilon_F / k_B = \frac{\left(3\pi^2 n\right)^{2/3}}{2mk_B} \qquad (30.2)$$

where ϵ_F is the Fermi energy, $\epsilon_F = k_F^2/(2m)$. Some physical systems consist of fermions at temperatures much lower than the Fermi temperature. Such systems are said to be degenerate. One example of such a system is ^{3}He at temperatures well below its condensation temperature, but well above the temperature at which ^{3}He becomes a superfluid. Another example is given by the conduction electrons in a metal at room temperature. These form a degenerate fermion system because the Fermi temperature is very high, of the order of 10^4 K.

The physical properties of a degenerate non-interacting Fermi system are usually treated in graduate-level textbooks in statistical mechanics. These properties are essentially determined by the statistics of the particles – the Pauli exclusion principle prohibits occupation of any single-particle state by more than one particle.

In real degenerate fermion systems, there are very strong particle interactions, frequently of the order of $k_B T_F$. Therefore, one may expect that the properties of a real degenerate fermion system will differ considerably from those of an ideal non-interacting degenerate fermion system. It is, however, a remarkable fact that the properties of real degenerate systems are qualitatively very similar to those of non-interacting ones. The reason for this is that in both interacting and non-interacting systems, the physical properties are determined by low-lying excitations, and at low temperatures there are only a few such excitations present. This is due to the severe restrictions imposed by the Pauli exclusion principle on the available phase-space for low-lying excitations. Hence, there is a strong correspondence between the nature of the low-lying excitations in interacting and non-interacting degenerate fermion systems. In the interacting system, however, many properties of low-lying single-particle excitations, such as mass, are typically different from those of the non-interacting system. This effect, which is due to the strength of the interactions, is called renormalization. There is also a residual interaction between these excitations in an interacting system, but this residual interaction only quantitatively modifies the values of macroscopic properties even though it may in fact be very strong.

Degenerate Fermi systems are well understood in terms of a theory put forward by Landau in 1950 [27]. This theory applies to normal Fermi liquids. These are interacting translationally invariant isotropic fermion systems, such as liquid ^{3}He in the temperature range discussed above. The theory may also be applied with minor modifications to the conduction electrons in a metal. The modifications account for the fact that the conduction electrons in a metal do not constitute an isotropic translationally invariant system, due to the crystal lattice of discrete ions. The theory is a semi-phenomenological one, in the sense that all properties are determined in terms of a few parameters. These parameters can be determined from a few experiments and then used to make new independent predictions. This is the course followed by Landau when he introduced the theory and shortly thereafter used it to predict the existence of zero sound in ^{3}He. The theoretical basis for the Landau Fermi liquid theory was rigorously demonstrated by Luttinger and Nozières in 1962 [28, 29], when they verified the theory using infinite order perturbation theory. In other words, the theory is valid in any system where perturbation theory converges. The microscopic derivation by Luttinger and Nozières also showed how the parameters in the theory can be calculated directly from first principles. Such calculations have been performed for, for example, simple metals. One of the most extensive calculations to this date of Fermi liquid parameters for various metals was performed by Rice in 1965 [30] .

Through the years since the introduction of Landau's Fermi liquid theory, the fundamental concepts of the theory, such as the existence of a Fermi surface and quasi-particles, have become cornerstones in condensed matter physics for the understanding of Fermi systems. Recent developments in condensed matter physics have again shown the importance of these concepts. One such development is the so-called Kondo effect, in which a minimum in the resistivity of metals with a small concentration of magnetic impurities is observed at low temperatures. A complete theoretical understanding of the Kondo effect did not emerge until after the development of renormalization group theory. Nevertheless, the low temperature behavior of the Kondo effect could be understood by the application of Fermi liquid theory [31]. We will discuss the application of Fermi liquid theory to the Kondo problem in a later chapter.

Another more recent area is the physics of high-T_c superconductors. The materials that exhibit high-T_c superconductivity all contain planes of copper oxide, and these planes are separated by, for example, rare earth atoms. At the present, the consensus has emerged that all the interesting physics happens in the essentially two-dimensional layers of copper oxide. The model that is frequently used to describe this system is the so-called Hubbard Hamiltonian. Not even the normal properties of this Hamiltonian are completely understood at the present time. However, there have been some very interesting developments in the theory of the normal properties of these materials, which may be a first steps towards a complete theory of high-T_c superconductivity. In these developments, attempts are made to investigate to what extent the normal state of the system can be described as a Fermi liquid. It is argued by some researchers that this state of the Hubbard Hamiltonian is a somewhat exotic variation of a Fermi liquid, termed a marginal Fermi liquid. The essential point for our illustrative purposes here, however, is that it is the concepts from the Landau Fermi liquid theory that play a major role in these developments [32].

Chapter 31

Equilibrium properties

We consider first a translationally invariant system of N non-interacting fermions in a unit volume. For a translationally invariant system, momentum $\mathbf{k}$ and spin $\sigma = \pm\frac{1}{2}$ are good quantum numbers. The many-body wavefunction of the system is a Slater-determinant of single-particle states $\varphi_{\mathbf{k},\sigma}$ with energies $\epsilon_k^{(0)} = k^2/2m$, where m is the mass of the particles. Any eigenstate of the system may then be completely described by a distribution function $n_{\mathbf{k},\sigma}$, which gives the occupancies of the single-particle states. In the ground state, this distribution function is $n_k^{(0)}$, given by

$$n_k^{(0)} = \begin{cases} 1 & \text{if } \epsilon_k^{(0)} < \epsilon_F \\ 0 & \text{if } \epsilon_k^{(0)} > \epsilon_F \end{cases}$$

and the ground state energy of this N-particle system is

$$E_0^{(N)} = \sum_{k<k_F,\sigma} \epsilon_k^{(0)}.$$

Let us add one particle to the system. The ground state of this $(N+1)$-particle system is obtained by placing the additional particle in a momentum state of momentum $|\mathbf{k}| = k_F$. The difference between the ground state energy $E_0^{(N+1)}$ and $E_0^{(N)}$ is

$$E_0^{(N+1)} - E_0^{(N)} = \frac{\partial E_0^{(N)}}{\partial N} = \mu$$

where μ is the chemical potential of the system. Since the additional particle was added on the Fermi surface, we have

$$\mu = \epsilon_F.$$

The value of μ depends on the temperature, but for degenerate systems the deviation of μ from ϵ_F is of order $(T/T_F)^2$, which we will ignore.

The elementary excitations of the non-interacting system are particles and holes. These excitations are obtained by adding a particle with $k > k_F$ or removing a particle with $k < k_F$. The thermodynamic properties of the system are determined by these elementary excitations, so it is convenient to have a measure of the departure of a state of the system from its ground state. Such a measure is given by the quantity $\delta n_{\mathbf{k},\sigma}$, defined by

$$\delta n_{\mathbf{k},\sigma} \equiv n_{\mathbf{k},\sigma} - n_k^{(0)}.$$

This quantity measures the difference in the occupation numbers of the single-particle states from their values in the ground state and thus describes the excited states of the system. For example, $\delta n_{\mathbf{k},\sigma} = \delta_{\mathbf{k},\mathbf{k}'}\delta_{\sigma,\sigma'}$ with $k > k_F$ corresponds to the excitation of a particle, and $\delta n_{\mathbf{k},\sigma} = -\delta_{\mathbf{k},\mathbf{k}'}\delta_{\sigma,\sigma'}$ with $k < k_F$ corresponds to the excitation of a hole. The internal energy of an excitation is then readily expressed in terms of $\delta n_{\mathbf{k}\sigma}$ and is

$$E - E_0 = \sum_{\mathbf{k},\sigma} \epsilon_k^{(0)} \delta n_{\mathbf{k},\sigma}.$$

It is clear that at non-zero but low enough temperatures, such that $k_B T \ll \mu$, only particles and holes near the Fermi energy will be excited thermally, so $\delta n_{\mathbf{k},\sigma}$ is of order unity only in a narrow region with thickness of order $k_B T/\mu$ near the Fermi surface and zero otherwise. It is then convenient to measure the energies relative to the chemical potential, which can be done by using the free energy F. This is the appropriate thermodynamic potential of a system in contact with a particle reservoir, so that the number of particles is allowed to fluctuate, but with the restriction that the average number of particles be fixed at N. This free energy is defined as

$$F = E - \mu N$$

and the free energy of an excitation is thus

$$F - F_0 = \sum_{\mathbf{k},\sigma} \left(\epsilon_k^{(0)} - \mu\right) \delta n_{\mathbf{k},\sigma}.$$

We now turn to a real, interacting system. We assume that the system is isotropic and translationally invariant. These assumptions are made for convenience – the theory can be formulated for anisotropic and non-translationally invariant systems (see [33, 34]). As a consequence of the first assumption, the Fermi surface of the interacting system is spherical for reasons of symmetry. By a theorem due to Luttinger [35], the Fermi surface of the interacting system must enclose the same volume as a corresponding non-interacting system with the same particle density so that the values of k_F and μ do not change as the interactions are turned on. As a consequence of the second assumption, momentum $\mathbf{k}$ and spin σ are good quantum numbers and can be used to label excited states of the interacting system, precisely as was the case with the non-interacting system. This enables us to generate quasi-particle states of the interacting system from those of the non-interacting system. The mechanism that allows us to do so is the adiabatic generation of the interacting eigenstates $\psi_{\mathbf{k}\sigma}$ from the non-interacting ones. We imagine that the coupling constant for the particle–particle interactions can be tuned continuously from zero to its final, real strength. We then assume that there is a one-to-one correspondence between the excited states of the non-interacting system and those of the interacting system in the following way. We start with a particular quasi-particle state $n_{\mathbf{k},\sigma}$ of the non-interacting system. We then slowly (in a sense which will be made more precise later) turn on the interactions. In this way we will then generate a quasi-particle state of the interacting system. For example, a non-interacting state with a single-particle excitation $n_{\mathbf{k},\sigma} = n_k^{(0)} + \delta_{\mathbf{k}\mathbf{k}'}\delta_{\sigma,\sigma'}$ will in this way generate a single quasi-particle excitation of momentum $\mathbf{k}'$ and spin σ' of the interacting state. In this way, we have a one-to-one correspondence between the excited states of non-interacting and of the interacting systems, and from a state of the non-interacting system containing $\delta n_{\mathbf{k},\sigma}$ quasi-particles we generate a state of the interacting system containing $\delta n_{\mathbf{k},\sigma}$ quasi-particles. These are precisely the quasi-particles discussed in Chapter 26.

For this adiabatic generation of the excited states to be valid, we must assume that all eigenstates of elementary excitations of the interacting system can be reached in this way. This holds for the ground state of the interacting system, provided the requirements of the Gell-Mann–Low theorem in Chapter 18 are satisfied and if, for example, the Fermi surface is spherical. An example of when all eigenstates of the interacting system may not be generated adiabatically is provided by a system with attractive interactions. In this case the interacting ground state can be a superfluid liquid. Also, the adiabatic generation of excited states can only be valid for low-lying excitations near the Fermi-surface. The reason for this is that the adiabatic procedure must obviously take place in a time shorter than the life-time of the excitations – otherwise we would not end up in a well-defined excited state. But we have already seen that the life-time of an excited state of momentum $\mathbf{k}$ goes as $[(k - k_F)/k_F]^{-2}$, so if the momentum of the excitation in the non-interacting is too far from the Fermi surface, we may not be able to generate the corresponding interacting excited state adiabatically. This limits the validity of the Fermi liquid theory to excitations in the immediate vicinity of the Fermi surface.

The free energy of the interacting system can be expressed in terms of $n_{\mathbf{k},\sigma}$. In particular, it can be expressed in the deviation $\delta n_{\mathbf{k},\sigma}$ from the ground state quasi-particle distribution function $n_k^{(0)}$:

$$F = F[\delta n_{\mathbf{k},\sigma}].$$

If the deviation is small, in a sense which will be made more precise shortly, we can expand the free energy in a power series in $\delta n_{\mathbf{k},\sigma}$. To second order in the deviation, we obtain

$$F - F_0 = \sum_{\mathbf{k},\sigma}(\epsilon_k - \mu)\delta n_{\mathbf{k},\sigma} + \frac{1}{2}\sum_{\mathbf{k}\sigma,\mathbf{k}'\sigma'} f_{\mathbf{k}\sigma,\mathbf{k}'\sigma'}\delta n_{\mathbf{k},\sigma}\delta n_{\mathbf{k}',\sigma'} \tag{31.1}$$

In the first summation on the right-hand side of equation (31.1), $\epsilon_k - \mu$ is the free energy of a single quasi-particle of momentum $\mathbf{k}$ and spin σ. In the presence of other quasi-particles the interactions between quasi-particles change this free energy to

$$\tilde{\epsilon}_k - \mu = \epsilon_k + \sum_{\mathbf{k}'\sigma'} f_{\mathbf{k}\sigma,\mathbf{k}'\sigma'}\delta n_{\mathbf{k}',\sigma'} - \mu. \tag{31.2}$$

It follows immediately from the adiabatic generation that only one quasi-particle can occupy each available quasi-particle state. By applying statistical mechanics to a gas of quasi-particles, we can then calculate the probability $f(\epsilon)$ that there is a quasi-particle with energy ϵ in the system. This probability is

$$f(\epsilon) = \frac{1}{e^{\beta(\epsilon-\mu)} + 1},$$

where $\beta = 1/k_B T$. As $T \to 0$, this expression tends to a step function at $\epsilon = \mu$. At finite temperatures, the energy ϵ will depend on the temperature since thermally excited quasi-particles will affect the energy ϵ through equation (31.2), and $f(\epsilon)$ becomes a very complicated function. Note that, as a consequence of the fact that each quasi-particle state can be occupied by only one quasi-particle, the quasi-particles are distributed according to the Fermi–Dirac distribution function, and we can treat them as fermions. It is not at all trivial to actually prove that the quasi-particles *are* fermions and this may not even be the case. However, for our purposes here, it suffices to know that we can *treat* them as fermions.

The quasi-particles are close to the Fermi surface because of the restriction on $k - k_F$. We may then expand the energies ϵ_k about the Fermi surface. To lowest order in $(k - k_F)$, the expansion can be written

$$\epsilon_k - \mu = \frac{k_F}{m^*}(k - k_F) \tag{31.3}$$

where the *effective mass* m^* of a quasi-particle is defined as

$$\frac{1}{m^*} \equiv \frac{|\nabla_{\mathbf{k}}\epsilon_k|}{k_F}, \tag{31.4}$$

with the gradient evaluated at the Fermi surface. This definition is the same as equation (26.18) for m^{**}. We will here follow convention and use the notation m^*.

The free energy given in equation (31.1) has the form of the free energy of a gas of interacting particles, the quasi-particles, where the particle interaction is given by the function $f_{\mathbf{k}\sigma,\mathbf{k}'\sigma'}$, usually called the Landau f-function. The expansion of the free energy is an expansion in the ratio of the number $\delta n_{\mathbf{k},\sigma}$ of these particles to the total number N of particles in the system. Thus, the expansion is valid for $\sum_{\mathbf{k},\sigma} |\delta n_{\mathbf{k},\sigma}| \ll N$. This condition holds for temperatures T much less than the chemical potential of the system. Note that there is no particular restriction on the strength of the quasi-particle interactions.

For systems invariant under space inversion and time-reversal (which is the case in the absence of magnetic fields) the Landau f-function must satisfy

$$\begin{aligned} f_{\mathbf{k}\sigma,\mathbf{k}'\sigma'} &= f_{-\mathbf{k}-\sigma,-\mathbf{k}'-\sigma'} \\ f_{\mathbf{k}\sigma,\mathbf{k}'\sigma'} &= f_{\mathbf{k}-\sigma,\mathbf{k}'-\sigma'}. \end{aligned}$$

Furthermore, we will always take $|\mathbf{k}| = k_F$ since the excitations are very close to the Fermi surface. The f-function is then a function only of the relative orientations of $\mathbf{k}$ and $\mathbf{k}'$ and of σ and σ'. Thus, the spin-component depends only on if σ and σ' are parallel or anti-parallel. It is convenient to separate these two independent spin-components $f^{\uparrow\uparrow}_{\mathbf{k}\mathbf{k}'}$ and $f^{\uparrow\downarrow}_{\mathbf{k}\mathbf{k}'}$ into spin-symmetric and anti-symmetric parts:

$$\begin{aligned} f^{\uparrow\uparrow}_{\mathbf{k}\mathbf{k}'} &= f^{s}_{\mathbf{k}\mathbf{k}'} + f^{a}_{\mathbf{k}\mathbf{k}'} \\ f^{\uparrow\downarrow}_{\mathbf{k}\mathbf{k}'} &= f^{s}_{\mathbf{k}\mathbf{k}'} - f^{a}_{\mathbf{k}\mathbf{k}'}. \end{aligned}$$

Because of the isotropy, the spin-symmetric and anti-symmetric parts only depend on the angle ξ between $\mathbf{k}$ and $\mathbf{k}'$, so we can expand these components in a series of Legendre polynomials

$$f^{s(a)}_{\mathbf{k}\mathbf{k}'} = \sum_{\ell=0}^{\infty} f^{s(a)}_{\ell} P_\ell(\cos\xi).$$

Usually, the coefficients $f^{s(a)}_\ell$ are expressed in a dimensionless form $F^{s(a)}_\ell$ by multiplying them by the density-of-states at the Fermi surface, $\nu(0)$ (see below), so that

$$\nu(0) f^{s(a)}_\ell = \frac{m^* k_F}{\pi^2} f^{s(a)}_\ell \equiv F^{s(a)}_\ell. \tag{31.5}$$

The coefficients $F^{s(a)}_\ell$ then measure the interaction strength relative to the kinetic energy of the quasi-particles and completely determine the interaction between them. The great usefulness of the theory lies in the fact that in practical applications, only a few of the parameters $F_\ell^{s(a)}$ and m^* need to be included. They can then be determined from a few experiments, and new *independent* predictions can then be made using these values of the parameters.

As we have argued before, the physical properties at low energies depend crucially on the number of states available for low-energy excitations. This number is given by the density-of-states at the Fermi surface, $\nu(0)$. Let us calculate $\nu(0)$ for a Fermi liquid. We know how to convert a sum over quasi-particle states $\mathbf{k}, \sigma$ to an integral:

$$\sum_{\mathbf{k},\sigma} g(k) = \sum_{\sigma} \frac{1}{(2\pi)^3} \int g(k) \mathrm{d}^3k = \frac{2}{(2\pi)^3} \int g(k) \mathrm{d}^3k$$

where $g(k)$ is some function of $|\mathbf{k}|$ only. (Remember that the system has unit volume.) Instead of summing over particle states $(\mathbf{k}, \sigma)$, we can sum over energy levels. To do so, we introduce the density-of-states $\nu(\epsilon)$, which is the number of states per unit volume and unit energy. Thus,

$$\sum_{\mathbf{k},\sigma} g(k) = \frac{2 \cdot 4\pi}{(2\pi)^3} \int_0^\infty g(k) k^2 \mathrm{d}k = \int g(\epsilon) \nu(\epsilon) \mathrm{d}\epsilon.$$

For quasi-particles, $\epsilon_{\mathbf{k},\sigma} = k^2/(2m^*)$, so that $\mathrm{d}k = m^* \mathrm{d}\epsilon/k = m^* \mathrm{d}\epsilon/\sqrt{2m^*\epsilon}$. By changing integration variable, we obtain

$$\frac{1}{\pi^2} \int_0^\infty k^2 g(k)\, \mathrm{d}k = \int g(\epsilon) m^* \sqrt{2m^*\epsilon}\, \mathrm{d}\epsilon.$$

Hence,

$$\nu(\epsilon) = m^* \sqrt{2m^*\epsilon}.$$

With $\epsilon_F = k^2/(2m^*)$, we obtain for the density-of-states at the Fermi surface:

$$\nu(0) = \frac{m^* k_F}{\pi^2}. \tag{31.6}$$

We will now calculate the specific heat of a Fermi liquid. The specific heat is given by the increase in internal energy due to an infinitesimal increase δT in temperature:

$$\delta E = C_v \delta T.$$

To lowest order in (T/T_F), the increase in internal energy is given by

$$\delta E = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k},\sigma} \delta n_{\mathbf{k},\sigma}$$

increasing the temperature leads to an increase in the number of quasi-particles, $\delta n_{\mathbf{k},\sigma}$. There is also an increase in the internal energy due to the quasi-particle interactions, but this term is of order $(T/T_F)^3$ and can be ignored here. Hence, the specific heat is that of a non-interacting gas of quasi-particles. The increase in internal energy is then given by the the number of quasi-particles within an energy k_BT of the Fermi surface. This number is given by the product of the number of the density-of-states at the Fermi surface, $\nu(0)$, and k_BT. The energy of excitation is of the order of k_BT, which gives the standard result that $C_v \propto \nu(0)k_B^2T$. An exact calculation is straightforward and completely analogous to the calculation of C_v for a free elctron gas. The result is

$$C_v = \frac{\pi^2}{3}\nu(0)k_B^2T.$$

The only change in C_v in the interacting Fermi liquid from that of the non-interacting Fermi liquid is due to the change in the density-of-states at the Fermi surface. With the density-of-states given by equation (31.6), we obtain

$$C_v = \frac{m^* k_F}{3}k_B^2T. \tag{31.7}$$

The effective mass m^* can thus be obtained directly from measurements of the heat capacity of the Fermi liquid.

Next, we turn to the propagation of ordinary sound in a Fermi liquid, for example the propagation of sound in liquid ^{3}He. These sound waves are due to vibrations of the quasi-particles, where the restoring force is provided by frequent collisions between them. The speed of sound v_s is obtained from thermodynamics and is given by

$$v_s^2 = \frac{1}{m}\frac{\partial P}{\partial n}$$

where P is the pressure. Using thermodynamic Maxwell relations, it is easy to show that

$$\frac{\partial P}{\partial n} = N\frac{\partial \mu}{\partial N}$$

so that

$$v_s^2 = \frac{N}{m}\frac{\partial \mu}{\partial N}. \tag{31.8}$$

We will evaluate equation (31.8) by calculating the inverse $\frac{\partial N}{\partial \mu}$ of $\frac{\partial \mu}{\partial N}$ using Fermi liquid theory. We begin by considering the change $\mathrm{d}N$ in N due to a change $\mathrm{d}\mu$ in the chemical potential. If the chemical potential increases an amount $\mathrm{d}\mu$, the Fermi wavenumber increases an amount

$$\mathrm{d}k_F = \frac{\partial k_F}{\partial \mu}\mathrm{d}\mu.$$

Quasiparticles on the new Fermi surface must have an energy $\epsilon(\mu + \mathrm{d}\mu)$ which satisfies

$$\epsilon(\mu + \mathrm{d}\mu) - \epsilon(\mu) = \mathrm{d}\mu.$$

This increase in quasi-particle energy to $\epsilon(\mu + \mathrm{d}\mu)$ has two contributions. The first one comes from the fact that k_F increases due to the increase in N, and this contribution is $v_F \mathrm{d}k_F$. As a result of increasing the Fermi surface, new quasi-particles are added at $k_F + \mathrm{d}k_F$. The second contribution comes from the interactions involving these new quasi-particles and is $\sum_{\mathbf{k}'\sigma'} f_{\mathbf{k}\sigma,\mathbf{k}'\sigma'}\delta n_{\mathbf{k}'\sigma'}$. Collecting these two terms we obtain

$$v_F \mathrm{d}k_F + \sum_{\mathbf{k}'\sigma'} f_{\mathbf{k}\sigma,\mathbf{k}'\sigma'}\delta n_{\mathbf{k}'\sigma'} = \mathrm{d}\mu.$$

Since the quasi-particles are on the Fermi surface, we can write

$$\delta n_{\mathbf{k},\sigma} = -\frac{\mathrm{d}n_k^{(0)}}{\mathrm{d}\epsilon_k}\frac{\partial \epsilon_k}{\partial k}\mathrm{d}k_F = \delta(\epsilon_k - \epsilon_F) v_{\mathbf{k}} \mathrm{d}k_F$$

so

$$v_k \frac{\partial k_F}{\partial \mu} + \sum_{\mathbf{k}'\sigma'} f_{\mathbf{k}\sigma,\mathbf{k}'\sigma'} v_{\mathbf{k}'} \frac{\partial k'_F}{\partial \mu}\delta(\epsilon_{k'} - \mu) = 1. \tag{31.9}$$

This equation then gives the change in k_F if the chemical potential increases. The increase $\mathrm{d}N$ in the number of particles within the expanded Fermi surface is just

$$\mathrm{d}N = \sum_{\mathbf{k}\sigma} \delta n_{\mathbf{k},\sigma} = \sum_{\mathbf{k}\sigma} \delta(\epsilon_k - \mu) v_{\mathbf{k}} \mathrm{d}k_F$$

so that

$$\frac{N}{m v_s^2} = \frac{\partial N}{\partial \mu} = \sum_{\mathbf{k}\sigma} \delta(\epsilon_k - \mu)\frac{\partial k_F}{\partial \mu} v_{\mathbf{k}}. \tag{31.10}$$

In an isotropic system, the Fermi surface is spherical and so $\frac{\partial k_F}{\partial \mu}$ is independent of direction. We perform the integral over $\mathbf{k}'$ in equation (31.9) over the Fermi surface:

$$\begin{aligned}
&\sum_{\mathbf{k}',\sigma'} f_{\mathbf{k}\sigma,\mathbf{k}'\sigma'} v_{\mathbf{k}'} \frac{\partial k'_F}{\partial \mu}\delta(\epsilon_{k'} - \mu) \\
&= \frac{1}{(2\pi)^3}\sum_{\sigma'}\int f_{\mathbf{k}\sigma,\mathbf{k}'\sigma'} v_{k'} \frac{\partial k'_F}{\partial \mu}\delta(\epsilon_{k'} - \mu) k'^2 \cos\xi \, \mathrm{d}k' \mathrm{d}\xi \mathrm{d}\varphi' \\
&= \frac{2\pi}{(2\pi)^3}\sum_{\sigma'}\int f_{\mathbf{k}\sigma,\mathbf{k}'\sigma'} v_{k'} \frac{\partial k'_F}{\partial \mu}\delta(k' - k_F)\frac{m^*}{k_F} k'^2 \cos\xi \, \mathrm{d}k' \mathrm{d}\xi
\end{aligned}$$

$$\begin{aligned}
&= \frac{1}{4\pi^2} m^* k_F v_k \frac{\partial k_F}{\partial \mu} \sum_{\sigma'} \int f_{\mathbf{k}\sigma,\mathbf{k}'\sigma'} \cos\xi \, d\xi \\
&= \frac{m^* k_F}{4\pi^2} v_k \frac{\partial k_F}{\partial \mu} \int \left[f^{\uparrow\uparrow}_{\mathbf{k}\mathbf{k}'} + f^{\uparrow\downarrow}_{\mathbf{k}\mathbf{k}'} \right] \cos\xi \, d\xi \\
&= \frac{m^* k_F}{4\pi^2} v_k \frac{\partial k_F}{\partial \mu} 2 \int f^s_{\mathbf{k}\mathbf{k}'} \cos\xi \, d\xi \\
&= \frac{m^* k_F}{2\pi^2} v_k \frac{\partial k_F}{\partial \mu} \int \sum_{\ell=0}^{\infty} f^s_\ell P_\ell(\cos\xi) \cos\xi \, d\xi \\
&= \frac{m^* k_F}{2\pi^2} v_k \frac{\partial k_F}{\partial \mu} 2 f^s_0 = v_k \frac{\partial k_F}{\partial \mu} F^s_0 .
\end{aligned}$$

Here, we used the fact that **k** also is on the Fermi surface, and in the last line we used equation (31.5). The result of this integration in equation (31.9) yields

$$v_k \frac{\partial k_F}{\partial \mu} = \frac{1}{1 + F^s_0}.$$

With this result inserted in equation (31.10) we obtain

$$\frac{N}{m v_s^2} = \frac{\partial N}{\partial \mu} = \sum_{\mathbf{k}\sigma} \delta(\epsilon_k - \mu) \frac{1}{1 + F^s_0}.$$

Integrating over **k** and summing over σ, we obtain

$$\frac{N}{m v_s^2} = \frac{\nu(0)}{1 + F^s_0}$$

or

$$v_s^2 = \frac{N}{m\nu(0)} [1 + F^s_0] .$$

If we insert the expression equation (31.6) for $\nu(0)$, and also use the relation between the density N (remember that the system has unit volume) and k_F, $N = k_F^3/(3\pi^2)$, we finally obtain

$$v_s^2 = \frac{k_F^2}{3mm^*} [1 + F^s_0] . \tag{31.11}$$

The interactions thus enter into the speed of sound in two places. First, the density-of-states at the Fermi surface, $\nu(0)$, is modified by the effective mass m^*, and second, the interactions enter in the parameter F^s_0. For example, if the quasi-particle interaction is repulsive, the speed of sound increases due to the positive F^s_0.

The parameter m^* can be obtained from specific heat measurements, so measurement of the speed of sound will yield F^s_0. For example, for liquid

^{3}He at temperatures where the Fermi liquid theory applies, $F_0^s = 10.8$ at a pressure of 0.28 atm.

Note that if $F_0^s < -1$, the system is unstable, because density fluctuations will build up exponentially.

Finally, we will calculate the Pauli spin susceptibility χ_P of a Fermi liquid. In the presence of a uniform external magnetic field $\mathbf{H}$, the quasi-particles acquire an additional energy $-g\mu_B\sigma H$, where g is the Landé factor, which we take to be 2, μ_B is the Bohr magneton and $\sigma = \pm\frac{1}{2}$. In equilibrium the system must have a single chemical potential μ. As a consequence, the quasi-particles with spin $-\frac{1}{2}$ (which have their energies increased) must have their Fermi surface reduced by an amount δk_F, whereas the Fermi surface of the spin $+\frac{1}{2}$ quasi-particles must increase an amount δk_F. This will modify the distribution $n_{\mathbf{k},\sigma}$of the quasi-particles. The change $\delta n_{\mathbf{k},\sigma}$ in the quasi-particle distribution function is

$$\begin{aligned} \delta n_{\mathbf{k},\sigma} &= +1 \quad \text{for } \sigma = +\tfrac{1}{2} \text{ and } k_F \leq k \leq k_F + \delta k_F \\ \delta n_{\mathbf{k},\sigma} &= -1 \quad \text{for } \sigma = -\tfrac{1}{2} \text{ and } k_F - \delta k_F \leq k \leq k_F \end{aligned} \tag{31.12}$$

In turn, these changes in the quasi-particle distribution will modify the quasi-particle energies through the quasi-particle interactions. The relation between $\delta n_{\mathbf{k},\sigma}$ and the change $\delta\epsilon_{\mathbf{k}\sigma}$ of the quasi-particles is

$$\delta\epsilon_{\mathbf{k}\sigma} = -g\mu_B\sigma H + \sum_{\mathbf{k}\sigma,\mathbf{k}'\sigma'} f_{\mathbf{k}\sigma,\mathbf{k}'\sigma'}\delta n_{\mathbf{k}'\sigma'}. \tag{31.13}$$

We look for a solution for $\delta\epsilon_{\mathbf{k},\sigma}$ of the form

$$\delta\epsilon_{\mathbf{k}\sigma} = -\eta\sigma H. \tag{31.14}$$

With this *ansatz*, the change δk_F in the Fermi surface is

$$\delta k_F = \left|\frac{\partial k_F}{\partial \epsilon_k}\right| |\delta\epsilon_k| = \left|\frac{\partial \epsilon_k}{\partial k_F}\right|^{-1} |\delta\epsilon_k| = \frac{m^*}{k_F}\frac{\eta H}{2}. \tag{31.15}$$

Using equation (31.12), we can write equation (31.13) as

$$\begin{aligned} \delta\epsilon_{\mathbf{k}\sigma} &= -g\mu_B\sigma H + \sum_{\mathbf{k}'} f_{\mathbf{k}\sigma,\mathbf{k}'\sigma}\delta n_{\mathbf{k}',\sigma} + \sum_{\mathbf{k}'} f_{\mathbf{k}\sigma,\mathbf{k}'-\sigma}\delta n_{\mathbf{k}'-\sigma} \\ &= -g\mu_B\sigma H + \frac{1}{(2\pi)^3}k_F^2\delta k_F(2\sigma)\int \mathrm{d}\gamma' \left[f_{\mathbf{k}\sigma,\mathbf{k}'\sigma} - f_{\mathbf{k}\sigma,\mathbf{k}'-\sigma}\right] \end{aligned} \tag{31.16}$$

where $\mathbf{k}$ and $\mathbf{k}'$ are on the Fermi surface k_F and $d\gamma'$ is the element of solid angle. If we now insert equation (31.15) and also use equation (31.5), we obtain

$$\begin{aligned}
\delta\epsilon_{\mathbf{k}\sigma} &= -g\mu_B\sigma H + \frac{1}{(2\pi)^3}k_F^2\delta k_F 4\sigma \int \mathrm{d}\gamma'\, f^a_{\mathbf{k}\mathbf{k}'} \\
&= -g\mu_B\sigma H + \frac{4\sigma\cdot 2\pi}{(2\pi)^3}k_F^2\delta k_F \int \sum_{\ell=0}^{\infty} f^a_\ell P_\ell(\cos\xi)\cos\xi\,\mathrm{d}\xi \\
&= -g\mu_B\sigma H + \frac{2\sigma}{\pi^2}k_F^2\delta k_F f^a_0 \\
&= -g\mu_B\sigma H + \sigma H F^a_0 \eta.
\end{aligned} \tag{31.17}$$

Inserting the *ansatz* equation (31.14) in equation (31.17) yields for η

$$-\eta\sigma H = -g\mu_B\sigma H + \sigma H F^a_0\eta,$$

or

$$\eta = \frac{g\mu_B}{1+F^a_0}. \tag{31.18}$$

The magnetization M of the system is

$$M = \chi_P H = \sum_{\mathbf{k}\sigma} g\mu_B\sigma\delta n_{\mathbf{k},\sigma} = g\mu_B\frac{m^* k_F}{4\pi^2}\eta H. \tag{31.19}$$

The Pauli spin susceptibility χ_P is then

$$\chi_P = \frac{M}{H} = \frac{m^* k_F}{4\pi^2}\frac{(g\mu_B)^2}{1+F^a_0} = \frac{m^* k_F}{\pi^2}\frac{\mu_B^2}{1+F^a_0}. \tag{31.20}$$

The effect of the interactions is again a renormalization of the response of the system, here by a factor $(1+F^a_0)^{-1}$ (apart from the change in the density-of-states at the Fermi surface). Moreover, we note that if $F^a_0 < -1$ the susceptibility becomes infinite, which signals an instability of the spin system; for example, the system may become ferromagnetic.

Chapter 32

Transport equation and collective modes

We will now turn our attention to the case where the system is non-uniform. This would be the case, for example, if an external field which varies in space is applied or if there are internal long-range fluctuations. We restrict ourselves to the case where the system is only weakly non-uniform. The idea is then to imagine that the system is divided into small sub-units, each of which is in local equilibrium. In each sub-unit, we can then define a quasi-particle distribution function $n_{\mathbf{k},\sigma}(\mathbf{r},t)$, where $\mathbf{r}$ is the position vector of the sub-unit. Of course, for this to make sense, the spatial variation of the system must be on a length scale much larger than the size of each sub-unit. We are only interested in linear response and write

$$n_{\mathbf{k},\sigma}(\mathbf{r},t) = n_k^{(0)} + \delta n_{\mathbf{k},\sigma}(\mathbf{r},t).$$

We can simplify further by Fourier transforming. Since we are only interested in linear response, we can then study the response of each Fourier component $\mathbf{q}$ separately, and write

$$n_{\mathbf{k},\sigma}(\mathbf{r},t) = n_k^{(0)} + \delta n_{\mathbf{k},\sigma}(\mathbf{q},\omega)\mathrm{e}^{i(\mathbf{q}\cdot\mathbf{r}-\omega t)}.$$

It is tempting to interpret the quantity $\delta n_{\mathbf{k},\sigma}(\mathbf{r},t)$ as the probability of finding a quasi-particle $(\mathbf{k},\sigma)$ at position $\mathbf{r}$ at time t. However, this interpretation is not quite correct. Indeed, attempts to interpret the quasi-particle distribution function in terms of localized wave-packets of quasi-particles will lead to unexpected effects (see [36]). We shall find later that $\delta n_{\mathbf{k},\sigma}(\mathbf{q},\omega)$ can be interpreted as the probability *amplitude* of finding a quasi-particle–quasi-hole *pair* of total momentum $\mathbf{q}$. This will become apparent when we derive the Landau theory from infinite-order perturbation theory. We shall then also find that the precise limits of validity on the theory are

$$qv_F \ll \mu$$

$$\omega \ll \mu. \tag{32.1}$$

These conditions then say what one would intuitively expect – that the wavelengths of the disturbances of the system must be much larger than the Fermi wavelength, and that their energies must be much smaller than the Fermi energy. These conditions will ensure that only quasi-particles in the immediate vicinity of the Fermi surface will be involved in the excitations.

With these preliminaries behind us, we can then proceed to expand the total free energy of the system. This expansion now has the form

$$\begin{aligned} F &= F_0 + \sum_{\mathbf{k},\sigma} \int \mathrm{d}^3 r \, [\epsilon_k(\mathbf{r}) - \mu] \, \delta n_{\mathbf{k},\sigma}(\mathbf{r}) \\ &\quad + \frac{1}{2} \sum_{\mathbf{k}\sigma,\mathbf{k}'\sigma'} \int\!\!\int \mathrm{d}^3 r \, \mathrm{d}^3 r' \, f_{\mathbf{k}\sigma,\mathbf{k}'\sigma'}(\mathbf{r},\mathbf{r}') \delta n_{\mathbf{k}\sigma}(\mathbf{r}) \delta n_{\mathbf{k}'\sigma'}(\mathbf{r}'). \end{aligned}$$

Again, we will restrict ourselves to translationally invariant systems. In this case, the quasi-particle energy does not depend on $\mathbf{r}$ and is simply ϵ_k, and the interaction function $f_{\mathbf{k}\sigma,\mathbf{k}'\sigma'}(\mathbf{r},\mathbf{r}')$ depends on $\mathbf{r}$ and $\mathbf{r}'$ only through $(\mathbf{r}-\mathbf{r}')$. Moreover, the interaction function represents the short-range forces between the quasi-particles. If we are considering neutral systems, this is obviously true. It is not clear if we are considering charged systems, such as the conduction electrons in a solid. However, in such systems, the trick is to separate out the long-range part of the Coulomb interaction between the quasi-particles, which leads to a term in the energy, which is treated separately . This part is the direct Hartree interaction (not shown here). The remainder of the Coulomb interaction are then short-ranged exchange-correlation interactions, which are described by an interaction function $f_{\mathbf{k}\sigma,\mathbf{k}'\sigma'}$. So in either case, $f_{\mathbf{k}\sigma,\mathbf{k}'\sigma'}(\mathbf{r}-\mathbf{r}')$ is short-ranged, with a range of the order of an atomic length. We can then replace this by $f_{\mathbf{k}\sigma,\mathbf{k}'\sigma'}\delta(\mathbf{r}-\mathbf{r}')$ inside the integral. With all these simplifications, the total free energy is then

$$\begin{aligned} F &= F_0 + \sum_{\mathbf{k},\sigma} \int \mathrm{d}^3 r \, (\epsilon_k - \mu) \delta n_{\mathbf{k}\sigma}(\mathbf{r}) \\ &\quad + \frac{1}{2} \sum_{\mathbf{k}\sigma,\mathbf{k}'\sigma'} \int \mathrm{d}^3 r \, f_{\mathbf{k}\sigma,\mathbf{k}'\sigma'} \delta n_{\mathbf{k}\sigma}(\mathbf{r}) \delta n_{\mathbf{k}'\sigma'}(\mathbf{r}). \end{aligned}$$

From this we see that a quasi-particle $(\mathbf{k},\sigma)$ at a point $\mathbf{r}$ has an energy

$$\epsilon_{\mathbf{k}\sigma}(\mathbf{r}) = \epsilon_k + \sum_{\mathbf{k}'\sigma'} f_{\mathbf{k}\sigma,\mathbf{k}'\sigma'} \delta n_{\mathbf{k}'\sigma'}(\mathbf{r}).$$

This energy now varies both with momentum $\mathbf{k}$ and with respect to position $\mathbf{r}$, so $\nabla_{\mathbf{k}}\epsilon_{\mathbf{k}\sigma}(\mathbf{r})$ and $\nabla_{\mathbf{r}}\epsilon_{\mathbf{k}\sigma}(\mathbf{r})$ are both non-zero. The first of these gradients,

$\nabla_{\mathbf{k}}\epsilon_{\mathbf{k}\sigma}(\mathbf{r})$ is just the local velocity of the quasi-particle. The spatial gradient, however, represents a diffusion force, which tends to push the quasi-particle to a region of low energy.

Landau derived the transport equation for quasi-particles by treating them as independent particles described by a classical Hamiltonian $\epsilon_{\mathbf{k}\sigma}(\mathbf{r})$. The time-development of the distribution function is then given by the explicit time-derivative plus the Poisson bracket of the distribution function with the classical Hamiltonian:

$$\frac{\partial n_{\mathbf{k}\sigma}(\mathbf{r},t)}{\partial t}+\sum_{\alpha}\left\{\frac{\partial n_{\mathbf{k},\sigma}(\mathbf{r},t)}{\partial r_{\alpha}}\frac{\partial\epsilon_{\mathbf{k}\sigma}(\mathbf{r})}{\partial k_{\alpha}}-\frac{\partial n_{\mathbf{k},\sigma}(\mathbf{r},t)}{\partial k_{\alpha}}\frac{\partial\epsilon_{\mathbf{k}\sigma}(\mathbf{r})}{\partial r_{\alpha}}\right\}=0 \quad (32.2)$$

where $\alpha = x, y, z$ denotes Cartesian components. In this expression, however, we have ignored the rate of change of $n_{\mathbf{k},\sigma}(\mathbf{r},t)$ due to collisions between the quasi-particles. By a procedure which is well-known in the theory of the Boltzmann equation (see, for example [37]), we can insert such a term by hand, so equation (32.2) becomes

$$\frac{\partial n_{\mathbf{k}\sigma}(\mathbf{r},t)}{\partial t}+\sum_{\alpha}\left\{\frac{\partial n_{\mathbf{k},\sigma}(\mathbf{r},t)}{\partial r_{\alpha}}\frac{\partial\epsilon_{\mathbf{k}\sigma}(\mathbf{r})}{\partial k_{\alpha}}-\frac{\partial n_{\mathbf{k},\sigma}(\mathbf{r},t)}{\partial k_{\alpha}}\frac{\partial\epsilon_{\mathbf{k}\sigma}(\mathbf{r})}{\partial r_{\alpha}}\right\}=I(n). \quad (32.3)$$

Here $I(n)$ is a collision integral, which is a functional of the quasi-particle distribution function. The collision integral measures the rate of change of $n_{\mathbf{k},\sigma}(\mathbf{r},t)$ due to collisions. Quasi-particle collisions are not important for frequencies ω larger than the typical quasi-particle collision frequency ν and $I(n)$ can be dropped in these cases. The collision frequency is proportional to the square of the number of quasi-particles, which is proportional to $(T/T_F)^2$ for low temperatures.

The quasi-particle distribution $n_{\mathbf{k},\sigma}$ is meaningless other than on the Fermi surface. Therefore, we want the transport equation in terms of the physically sensible quantity $\delta n_{\mathbf{k},\sigma}(\mathbf{r},t)$. The assumption that the distribution function deviates very little from its homogeneous equilibrium value $n_k^{(0)}$ allows us to cast the transport equation in terms of the equilibrium value of the distribution function plus corrections linear in the deviation from equilibrium. This gives an equation linear in $\delta n_{\mathbf{k},\sigma}(\mathbf{r},t)$. The result is

$$I(n) = \frac{\partial \delta n_{\mathbf{k},\sigma}(\mathbf{r},t)}{\partial t} + \sum_{\alpha} \left\{ v_{\mathbf{k},\alpha} \frac{\partial \delta n_{\mathbf{k},\sigma}(\mathbf{r},t)}{\partial r_\alpha} + v_{\mathbf{k},\alpha} \delta(\epsilon_k - \mu) \sum_{\mathbf{k}'\sigma'} f_{\mathbf{k}\sigma,\mathbf{k}'\sigma'} \frac{\partial \delta n_{\mathbf{k}'\sigma'}(\mathbf{r},t)}{\partial r_\alpha} \right\}. \tag{32.4}$$

Our first application of the transport equation (32.4) is to calculate the particle current density $\mathbf{j_k}$ in a state containing a quasi-particle $\delta n_{\mathbf{k},\sigma}$. Since the total number of particles is conserved, the continuity equation

$$\frac{\partial n}{\partial t} + \nabla \cdot \mathbf{J} = 0 \tag{32.5}$$

must hold, with $\mathbf{J}$ the total (particle) current density. We can obtain this equation by summing the transport equation (32.4) over $\mathbf{k}$ and σ. The result is

$$\frac{\partial n(\mathbf{r},t)}{\partial t} + \sum_{\mathbf{k}\sigma} \frac{\partial \delta n_{\mathbf{k},\sigma}(\mathbf{r},t)}{\partial r_\alpha} \left\{ v_{\mathbf{k},\alpha} + \sum_{\mathbf{k}'\sigma'} f_{\mathbf{k}\sigma,\mathbf{k}'\sigma'} v_{k'\alpha} \delta(\epsilon_{k'} - \mu) \right\} = 0. \tag{32.6}$$

The right side of equation (32.6) vanishes since the collisions conserve the number of particles. Comparing equation (32.6) with the continuity equation (32.5), we see that

$$\mathbf{j}_{\mathbf{k}\sigma} = \mathbf{v_k} + \sum_{\mathbf{k}'\sigma'} f_{\mathbf{k}\sigma,\mathbf{k}'\sigma'} \delta(\epsilon_{k'} - \mu) \mathbf{v}_{\mathbf{k}'} \tag{32.7}$$

is the current density carried by a system containing a quasi-particle $(\mathbf{k},\sigma)$. Similar expressions can be obtained for the energy current $\mathbf{Q}$ and the momentum current density $\Pi_{\alpha\beta}$ by multiplying equation (32.4) by ϵ_k or $\mathbf{k}$ and integrating while making use of energy or momentum conservation.

The equation (32.7) enables us to derive a relation between the effective mass m^* and the f-function for translationally invariant systems. Consider a non-interacting system in a state containing one quasi-particle with momentum $\mathbf{k}$. The current carried by this state is then

$$\mathbf{j_k} = \frac{\mathbf{k}}{m}. \tag{32.8}$$

Now turn on the interactions adiabatically. This takes the non-interacting state to an interacting state containing one quasi-particle with momentum $\mathbf{k}$. Since the system is translationally invariant, the momentum is conserved. The current carried in the interacting state is then also $\frac{\mathbf{k}}{m}$. Comparing this with equation (32.7) we obtain

$$\frac{\mathbf{k}}{m} = \frac{\mathbf{k}}{m^*} - \sum_{\mathbf{k}'\sigma'} f_{\mathbf{k}\sigma,\mathbf{k}'\sigma'} \frac{\partial n^{(0)}_{k'}}{\partial \epsilon_{k'}} \mathbf{v}_{\mathbf{k}'}. \tag{32.9}$$

We may, without loss of generality, take $\mathbf{k}$ parallel to $\hat{\mathbf{z}}$. It is then simple to carry out the integrations in equation (32.9):

$$\begin{aligned} -\sum_{\mathbf{k}'\sigma'} f_{\mathbf{k}\sigma,\mathbf{k}'\sigma'} \frac{\partial n^{(0)}_{k'}}{\partial \epsilon_{k'}} v_{k',z} &= \sum_{\mathbf{k}'\sigma'} f_{\mathbf{k}\sigma,\mathbf{k}'\sigma'} \delta(\epsilon_{k'} - \mu) v_{k',z} \\ &= \frac{2\pi}{(2\pi)^3} \sum_{\sigma'} \int f_{\mathbf{k}\sigma,\mathbf{k}'\sigma'} \frac{m^*}{k'} \delta(k' - k_F) v_{k'} \cos\xi \cos\xi k'^2 \, \mathrm{d}k' \mathrm{d}\xi \\ &= \frac{2m^* k_F}{4\pi^2} v_k \int f^s_{\mathbf{k}\mathbf{k}'} \cos^2\xi \, \mathrm{d}\xi \\ &= \frac{m^* k_F}{2\pi^2} v_k \int \sum_{\ell=0}^{\infty} f^s_\ell P_\ell(\cos\xi) P_1(\cos\xi) \cos\xi \, \mathrm{d}\xi \\ &= \frac{m^* k_F}{2\pi^2} v_k f^s_1 \frac{2}{3} = v_k \frac{F^s_1}{3}. \end{aligned}$$

This result inserted in equation (32.9) together with $v_k = k/m^*$ yield the relation

$$\frac{m^*}{m} = 1 + \frac{F^s_1}{3}. \tag{32.10}$$

Equation (32.10) give important additional information about the quasi-particle interactions. If the effective mass m^* is known, for example from specific heat measurements, the parameter F^s_1 can be calculated.

The first application of the transport equation (32.4) was made by Landau when he predicted the existence of a new collective mode in liquid ^{3}He. This mode was detected a few years after Landau's prediction. The mode is a collective oscillation of the quasi-particle gas where the restoring force comes from the interaction $f_{\mathbf{k}\sigma,\mathbf{k}'\sigma'}$ between the quasi-particles, and has a dispersion similar to ordinary sound waves in that the energy of the mode is proportional to the wavelength of the mode. Therefore, the mode was named 'zero sound'. In an ordinary sound wave, on the other hand, the restoring force is provided by frequent adiabatic collision between the quasi-particles, and these collisions restore local equilibrium. Hence, for the ordinary sound waves to propagate, the frequency ω of the mode must be much less than the collision frequency ν. In contrast, the collision frequency must be much less than ω for the zero-sound modes, so that collisions do not affect the oscillation. Since the collision frequency goes as $(T/T_F)^2$ at low temperatures, this is always the case for sufficiently low temperatures.

To analyze the transport equation for collective modes, we first set

$$\delta n_{\mathbf{k},\sigma}(\mathbf{r},t) = \delta n_{\mathbf{k},\sigma} e^{i(\mathbf{q}\cdot\mathbf{r}-\omega t)}.$$

With this form of $\delta n_{\mathbf{k},\sigma}(\mathbf{r},t)$, the transport equation (32.4) becomes

$$(\mathbf{q}\cdot\mathbf{v_k} - \omega)\,\delta n_{\mathbf{k}\sigma} - \mathbf{q}\cdot\mathbf{v_k}\frac{\partial n_k^{(0)}}{\partial \epsilon_k}\sum_{\mathbf{k}'\sigma'} f_{\mathbf{k}\sigma,\mathbf{k}'\sigma'}\delta n_{\mathbf{k}'\sigma'} = 0. \tag{32.11}$$

We simplify this equation by introducing polar and azimuthal angles (θ, φ) relative to $\mathbf{q}$ and by introducing a dimensionless quantity s defined by

$$s = \frac{\omega}{qv_F} = \frac{\omega m^*}{qk_F}.$$

The collective mode is an oscillation of the Fermi surface. Hence, we introduce the displacement $u(\mathbf{k}\sigma)$ of the Fermi surface at the point $\mathbf{k}$ on the Fermi surface; in terms of $u(\mathbf{k}\sigma)$, we have $\delta n_{\mathbf{k}\sigma} = \delta(\epsilon_k - \mu)v_F u(\mathbf{k}\sigma)$, so the transport equation then becomes

$$(\cos\theta - s)u(\theta,\varphi,\sigma) + \cos\theta\sum_{\sigma'}\int d\gamma' F(\xi,\sigma,\sigma')u(\theta',\varphi',\sigma') = 0 \tag{32.12}$$

where $d\gamma'$ is the element of solid angle, ξ is the angle between $\mathbf{k}$ and $\mathbf{k}'$, and F is the reduced interaction function

$$F(\mathbf{k}\sigma,\mathbf{k}'\sigma') = \frac{m^* k_F}{\pi^2} f_{\mathbf{k}\sigma,\mathbf{k}'\sigma'} = \nu(0) f_{\mathbf{k}\sigma,\mathbf{k}'\sigma'}.$$

Equation (32.12) is a homogeneous linear integral equation for the displacement $u(\mathbf{k}\sigma)$ of the Fermi surface due to the collective modes. The equation is an eigenvalue equation, and it can be shown that the eigenvalue s may only take discrete values. It follows that the energy $\omega = sqv_F$ of a mode is linear in q. This is a consequence of the short range of the quasi-particle interactions. For long-range interactions, such as the Coulomb interaction, the frequency is 'lifted' and is non-zero at infinite wavelengths. The reason for this is that a local variation in the quasi-particle density, due to the zero-sound mode, will result in a local accumulation of charge and macroscopic electric fields. This is the case for the plasma oscillations of an electron gas, which are precisely the zero-sound mode of the interacting electron gas, discussed in Chapter 11. The frequency of plasma oscillations becomes $\omega_p = 4\pi ne^2/m^*$ as $q \to 0$.

Equation (32.12) has many different solutions. Distinction is usually made between two main categories, those modes for which the different spin orientations oscillate in phase, and those for which the spin orientations are out of phase. The latter are called spin waves. The zero-sound mode is the simplest in-phase mode. In this case, only the symmetric interactions F^s matter. We make a further simplification by assuming that only the constant term F_0^s need be included. With these simplifications, equation (32.12) becomes

$$\left(\frac{s}{\cos\theta} - 1\right) u(\theta,\varphi) = 2F_0^s \int u(\theta',\varphi')d\Omega'. \tag{32.13}$$

The right hand side of equation (32.13) does not depend on the angles (θ,φ), so the solution for $u(\theta,\varphi)$ must be of the form

$$u(\theta,\varphi) \propto \frac{\cos\theta}{s-\cos\theta}. \tag{32.14}$$

Inserting this in (32.13) and integrating over solid angle we obtain the dispersion relation. The result is

$$\frac{s}{2}\ln\frac{s+1}{s-1} - 1 = \frac{1}{F_0^s}. \tag{32.15}$$

From equation (32.14) we see that the Fermi surface has an egg-shaped deformation for a zero-sound mode. The deformation becomes smaller and smaller as F_0^s vanishes. In this so-called weak-coupling limit we have $s = 1$ with $v = v_F$, to be contrasted with the *sound* velocity $v_s = v_F/\sqrt{3}$. On the other hand, as the coupling F_0^s grows, the strong-coupling limit of s is $s = \sqrt{F_0^s/3}$. We also see from equation (32.15) that the solutions for s are purely imaginary for $F_0^s < -1$ — if the interactions are attractive and strong enough, the system is unstable.

The zero-sound modes in liquid He^3 were discovered by Abel, Anderson and Wheatley in 1966 [38]. The technique used in the experiment was to monitor the absorption of sound waves at a fixed temperature, which means that the collision frequency ν is fixed. At high frequencies $\omega \gg \nu$, zero-sound waves can propagate, and the damping due to collisions is proportional to T^2. As the frequency ω is reduced, however, there will eventually be a crossover to normal (first) sound, for which the damping goes as ω^2/T^2 (a fact not proven here). By detecting the cross-over in the damping at fixed temperature from being constant to varying as ω^2 the existence of the zero-sound mode could be established.

Finally, there are, as we have said, many other different modes possible. It is a good exercise to solve the transport equation for transverse waves, for which $u(\theta,\varphi) \propto e^{i\varphi}$. These mode can be supported if the term $F_1 \cos\theta e^{i\varphi}$ is included. Similarly, there are the spin (antisymmetric) waves where $u(\theta,\varphi,\sigma) = u(\theta,\varphi)\sigma$.

Chapter 33

Microscopic derivation of the Landau Fermi liquid theory

In this chapter, we will derive the Landau Fermi liquid theory using ordinary perturbation theory to infinite order. We will thus verify the theory for any system in which the perturbation theory converges. Any such system is then a normal Fermi liquid, but there may of course exist normal Fermi liquids for which the Landau theory holds, but for which perturbation theory does not converge. Moreover, we will exclude systems with attractive interactions between the particles. Attractive interactions may cause a phase-transition to occur, such as the superfluid transition in ^{3}He or the superconducting transition in certain metals, in which case the structure of the ground state changes and the system is not normal. In this case, ordinary perturbation theory, in which we expand about the non-interacting ground state, does not converge. It is possible, however, to construct other perturbation theories for such systems but we will not further discuss that here. We will also restrict the derivation to systems with short-range interactions. It is fairly straightforward to extend the derivation to long-range interactions, such as the Coulomb interaction, but a bit tedious. For a derivation which includes long-range interactions, see Nozières [34]. Finally, we will also assume that the system is isotropic and translationally invariant. These assumptions are not restrictive, but simplify the notation.

Specifically, we will verify the following hypothesis and properties of the Landau Fermi liquid theory.

(1) The elementary excitations of the system are quasi-particles and quasi-holes, separated by a Fermi surface S_F. The energy ϵ_k of a quasi-particle is a continuous function when $\mathbf{k}$ crosses S_F, as is the gradient $\nabla_{\mathbf{k}}\epsilon_k = \mathbf{v}_{\mathbf{k}}$.

(2) The current carried by a quasi-particle is given by equation (32.7),

$$\mathbf{j}_\mathbf{k} = \mathbf{v}_\mathbf{k} - \sum_{\mathbf{k}'\sigma'} f_{\mathbf{k}\sigma,\mathbf{k}'\sigma'} \frac{\partial n_k^{(0)}}{\partial \epsilon_{k'}} \mathbf{v}_{\mathbf{k}'}.$$

(3) When the system is compressed, the distortion $\partial k_F/\partial \mu$ of the Fermi surface is given by equation (31.9):

$$v_k \frac{\partial k_F}{\partial \mu} = 1 - \sum_{\mathbf{k}'\sigma'} f_{\mathbf{k}\sigma,\mathbf{k}'\sigma'} v_{k'} \frac{\partial k_F'}{\partial \mu} \delta(\epsilon_{k'} - \mu).$$

(4) The collisionless transport equation for the quasi-particles is given by equation (32.11):

$$(\mathbf{q} \cdot \mathbf{v}_\mathbf{k} - \omega)\, \delta n_{\mathbf{k}\sigma}(\mathbf{q}, \omega) - \mathbf{q} \cdot \mathbf{v}_{\mathbf{k}\sigma} \frac{\partial n_k^{(0)}}{\partial \epsilon_k} \sum_{\mathbf{k}'\sigma'} f_{\mathbf{k}\sigma,\mathbf{k}'\sigma'} \delta n_{\mathbf{k}'\sigma'}(\mathbf{q}, \omega) = 0.$$

In the course of verifying (1)–(4), we will also obtain a microscopic expressions for the interaction function $f_{\mathbf{k}\sigma,\mathbf{k}'\sigma'}$ and the quasi-particle distribution function $\delta n_{\mathbf{k}\sigma}(\mathbf{q}, \omega)$.

The original derivation was given by Nozières and Luttinger [28, 29], and is also presented in Nozières [34]. This derivation is based on the so-called Ward identities, which are relations between self-energies and vertex functions. Here, we will closely follow the derivation given by Nozières. Rickayzen [39] has given a somewhat shorter derivation of the transport equation. His derivation does not explicitly use the Ward identities.

The verification will proceed in the following way. We will first briefly review the discussion about quasi-particles in Chapter 26, from which the hypothesis (1) follows immediately. Once we have firmly established the existence of the quasi-particles, we will proceed by defining quasi-particle creation and annihilation operators. These operators later be used to form a microscopic expression for the quasi-particle distribution function. Next, we will turn to a rather lengthy and formal discussion of correlation functions, which describe the response of the system to an external perturbation. It is these correlation functions that we will cast in a form from which we can identify the properties (2)–(4) of the Landau Fermi liquid theory. This will be done by examining the correlation functions on the Fermi surface and using the Ward identities.

For simplicity, we will ignore the spin of the particles. This is just to make the notation a little bit more comprehensible.

In Chapter 26, we discussed the form of the Green's function near the Fermi surface. We found that the low-lying excitations of the system, the energies of which are given by the locations of the poles of the Green's function, behave essentially as particles – as we approach the Fermi surface, the lifetime of the excitations diverges and the width of the spectral density at the poles of the Green's function goes to zero. Because of the particle-like properties of the excitations, we call them quasi-particles or quasi-holes, depending on whether the real part of the location of the pole is above or below the Fermi surface. The energy of the excitations, however, is a smooth function of frequency as we pass through the Fermi surface. This establishes the hypothesis (1). We establish this hypothesis formally by examining the Green's function near the Fermi surface. According to Chapter 26, the Green's function $G(\mathbf{k},\omega)$ is

$$G(\mathbf{k},\omega)=\frac{1}{\omega-\epsilon_k^{(0)}-M(\mathbf{k},\omega)} \tag{33.1}$$

where $\epsilon_k^{(0)}=k^2/2m$ and $M(\mathbf{k},\omega)$ is the self-energy. The self-energy is a smooth function at the Fermi surface, where the imaginary part of $M(\mathbf{k},\omega)$ vanishes. The Fermi surface is determined by

$$\mu-\epsilon_F-M(k_F,\mu)=0. \tag{33.2}$$

To examine the low-lying excitations, it is convenient to change frequency variable $\omega-\mu\rightarrow\tilde{\omega}$ and to expand the denominator of $G(\mathbf{k},\tilde{\omega})$ about $\tilde{\omega}=0$ and $k=k_F$ with the result

$$\tilde{\omega}-\left(\epsilon_k^{(0)}+M(\mathbf{k},\tilde{\omega})-\mu\right) \tag{33.3}$$

$$=\tilde{\omega}-\left\{(k-k_F)\left[\frac{k_F}{m}+\left.\frac{\partial M(\mathbf{k},\tilde{\omega})}{\partial k}\right|_{k=k_F}\right]+\tilde{\omega}\left.\frac{\partial M(\mathbf{k},\tilde{\omega})}{\partial\tilde{\omega}}\right|_{\tilde{\omega}=0}+\dots\right\} \tag{33.4}$$

The elementary excitations are at the energies at which the Green's function $G(\mathbf{k},\tilde{\omega})$ has poles. We may separate the contribution to the Green's functions from these poles from contributions due to multi-particle excitations. We have shown in Chapter 26 that the imaginary part of $M(\mathbf{k},\tilde{\omega})$ is quadratic in $(k-k_F)$ and $\tilde{\omega}$. All terms in equation (33.4) to first order in $(k-k_F)$ and $\tilde{\omega}$ are thus real. Neglecting quadratic terms, we can then write

$$G(\mathbf{k},\tilde{\omega})=\frac{z_k}{\tilde{\omega}-(\epsilon_k-\mu)} \tag{33.5}$$

where z_k is the residue of $G(\mathbf{k},\tilde{\omega})$ at k_F and $\tilde{\omega}=0$,

$$z_k=\frac{1}{1-\left.\frac{\partial M(\mathbf{k},\tilde{\omega})}{\partial\tilde{\omega}}\right|_{\tilde{\omega}=0}} \tag{33.6}$$

and

$$\epsilon_k = k_F \frac{(k - k_F)}{m^*} + \mu. \tag{33.7}$$

Here the effective mass m^* is given by

$$m^* = \frac{z_k}{\frac{1}{m} + \frac{1}{k_F} \left. \frac{\partial M(\mathbf{k},\widetilde{\omega})}{\partial k} \right|_{k=k_F}}. \tag{33.8}$$

If we add the quadratic terms to equation (33.5), we can write the Green's function near the Fermi surface as

$$G(\mathbf{k},\widetilde{\omega}) = G_{\text{inc}} + \frac{z_k}{\widetilde{\omega} - (\epsilon_k - \mu)} \tag{33.9}$$

where the pole near the Fermi surface has been separated out. This pole is due to a quasi-particle excitation. The part G_{inc} is a slowly varying function which is regular on the Fermi surface. This part is the incoherent part of the Green's function. It arises from configurations of several elementary excitations and is of order $\widetilde{\omega}^2$ as $\widetilde{\omega} \to 0$.

With this review, which clearly establishes the existence of the quasi-particles and quasi-holes, we may define a quasi-particle annihilation operator $C_{\mathbf{k},H}$ in the Heisenberg picture by (see [29])

$$\begin{aligned} C_{\mathbf{k}}(t=0)_H &= \frac{\eta_k}{\sqrt{z_k}} \int_{-\infty}^{0} \mathrm{e}^{\eta_k t'} c_{\mathbf{k}\alpha}(t')_H \mathrm{e}^{i\epsilon_k t'} \mathrm{d}t' \\ &= \frac{\eta_k}{\sqrt{z_k}} \int_{-\infty}^{0} \mathrm{e}^{iHt' + \eta_k t'} c_{\mathbf{k}\alpha} \mathrm{e}^{-iHt'} \mathrm{e}^{i\epsilon_k t'} \mathrm{d}t'. \end{aligned} \tag{33.10}$$

Here η_k is an infinitesimal frequency such that $\eta_k \ll \mu$ and $\eta_k \gg \Gamma_k$, where Γ_k^{-1} is the lifetime of a quasi-particle $(\mathbf{k},\alpha)$. The operator $C_{\mathbf{k},H}$ and its Hermitian conjugate $C^\dagger_{\mathbf{k},H}$ are quasi-particle annihilation and creation operators. As $|\mathbf{k}|$ approaches the Fermi surface, $C^\dagger_{\mathbf{k}}(t)_H \mid \Psi_0\rangle$ behaves for longer and longer times as an exact normalized eigenstate of the Hamiltonian H with an additional quasi-particle $(\mathbf{k},\alpha)$. Intuitively, this happens because $\exp(-i\epsilon_k t' + \eta_k t') c^\dagger_{\mathbf{k}\alpha}(t')_H$ on $\mid \Psi_0\rangle$ gives a distribution of single-particle states with momentum $\mathbf{k}$. If the excitation energy of such a state is $\widetilde{\epsilon}_k$, the integrand will oscillate with a frequency $(\widetilde{\epsilon}_k - \epsilon_k)$. The only contribution from the integral will then be from the state with $\widetilde{\epsilon}_k = \epsilon_k$ provided the lifetime of this excited state is much longer than time of averaging of the integrand.

Let us now formally demonstrate that $C^\dagger_{\mathbf{k},H}$ has the properties of a quasi-particle operator by showing that the thermal equilibrium value $\langle C^\dagger_{\mathbf{k},H} C_{\mathbf{k},H}\rangle$ is precisely the equilibrium quasi-particle distribution function $f(\epsilon_k)$. Let

$\psi_n^{(N)}$ be the exact eigenstates in the N-particle space of the Hamiltonian with energies $E_n^{(N)}$. By equation (33.10), the matrix elements of $C^\dagger_{\mathbf{k},H}$ and $C_{\mathbf{k},H}$ in this basis are

$$\langle\psi_n \mid C^\dagger_{\mathbf{k},H} \mid \psi_{n'}\rangle \equiv (C^\dagger_k)_{nn'} = -\frac{i\eta_k}{\sqrt{z_k}}\frac{(c^\dagger_k)_{nn'}}{-\epsilon_k + (E_n^{(N+1)} - E_{n'}^{(N)}) - i\eta_k} \tag{33.11}$$

$$\langle\psi_n|C_{\mathbf{k},H}|\psi_{n'}\rangle \equiv (C_k)_{nn'} = \frac{i\eta_k}{\sqrt{z_k}}\frac{(c_k)_{nn'}}{-\epsilon_k + i\eta_k - (E_n^{(N-1)} - E_{n'}^{(N)})} \tag{33.12}$$

with the obvious definitions of the matrix elements $(c^\dagger_k)_{nn'}$ and $(c_k)_{nn'}$. Using equations (33.11) and (33.12) we can study the thermal equilibrium distribution function $\langle C^\dagger_{\mathbf{k},H} C_{\mathbf{k},H}\rangle$:

$$\begin{aligned}
\langle C^\dagger_{\mathbf{k},H} C_{\mathbf{k},H}\rangle &= \frac{1}{Z_G}\sum_n \langle\psi_n^{(N)} \mid \mathrm{e}^{-\beta(H-\mu N)} C^\dagger_{\mathbf{k},H} C_{\mathbf{k},H} \mid \psi_n^{(N)}\rangle \\
&= \sum_{nn'} \frac{1}{Z_G}\langle\psi_n^{(N)} \mid \mathrm{e}^{-\beta(H-\mu N)} C^\dagger_{\mathbf{k},H} \mid \psi_{n'}^{(N-1)}\rangle\langle\psi_{n'}^{(N-1)} \mid C_{\mathbf{k},H} \mid \psi_n^{(N)}\rangle \\
&= \frac{\eta_k^2}{z_k}\sum_{nn'} \frac{\rho_n (c^\dagger_k)_{nn'}(c_k)_{n'n}}{(\epsilon_k + i\eta_k + E_{n'}^{(N-1)} - E_n^{(N)})(\epsilon_k - i\eta_k + E_{n'}^{(N-1)} - E_n^{(N)})} \\
&= \frac{\eta_k^2}{z_k}\int_{-\infty}^{\infty} \mathrm{d}\xi \frac{1}{(\epsilon_k - \xi - i\eta_k)(\epsilon_k - \xi + i\eta_k)} \\
&\quad \times \sum_{nn'} \rho_n \delta(\xi + E_{n'}^{(N-1)} - E_n^{(N)})(c^\dagger_k)_{nn'}(c_k)_{n'n},
\end{aligned} \tag{33.13}$$

where $\psi_n^{(N)}$ and $\psi_{n'}^{(N-1)}$ are eigenstates with N and $(N-1)$ particles, respectively, and

$$\rho_n = \frac{\mathrm{e}^{-\beta(E_n^{(N)} - \mu N)}}{Z_G} = \frac{1}{Z_G}\langle\psi_n^{(N)} \mid \rho_G \mid \psi_n^{(N)}\rangle$$

with Z_G the partition function. We can cast equation (33.13) in a more transparent form. To do so, we consider the finite-temperature spectral representation of the exact real-time single-particle Green's function in the same basis ψ_n:

$$\begin{aligned}
&G(\mathbf{k},\omega)\\
&= \frac{1}{Z_G}\sum_{nn'}\frac{\mathrm{e}^{-\beta(E_{n'}^{(N-1)}-\mu(N-1))}+\mathrm{e}^{-\beta(E_n^{(N)}-\mu N)}}{\omega-(E_n^{(N)}-\mu N-E_{n'}^{(N-1)}+\mu(N-1))}(c_k^\dagger)_{nn'}(c_k)_{n'n}\\
&= \frac{1}{Z_G}\sum_{nn'}\frac{\mathrm{e}^{-\beta(E_n^{(N)}-\mu N)}+\mathrm{e}^{-\beta(E_{n'}^{(N-1)}-\mu(N-1))}}{\omega-(E_n^{(N)}-E_{n'}^{(N-1)}-\mu)}(c_k^\dagger)_{nn'}(c_k)_{n'n}\\
&= \frac{1}{Z_G}\sum_{nn'}\mathrm{e}^{-\beta(E_n^{(N)}-\mu N)}\frac{1+\mathrm{e}^{\beta(E_n^{(N)}-E_{n'}^{(N-1)}-\mu)}}{\omega-(E_n^{(N)}-E_{n'}^{(N-1)}-\mu)}(c_k^\dagger)_{nn'}(c_k)_{n'n}\\
&= \frac{1}{Z_G}\sum_{nn'}\int_{-\infty}^{\infty}\mathrm{d}\xi\,\mathrm{e}^{-\beta(E_n^{(N)}-\mu N)}\frac{(1+\mathrm{e}^{\beta(\xi-\mu)})}{\omega-(\xi-\mu)}\\
&\quad\times\delta(\xi+E_{n'}^{(N-1)}-E_n^{(N)})(c_k^\dagger)_{nn'}(c_k)_{n'n}\\
&= \int_{-\infty}^{\infty}\mathrm{d}\xi\,\frac{\widetilde{A}_k(\xi)}{\omega-(\xi-\mu)}, \qquad (33.14)
\end{aligned}$$

where the finite-temperature spectral function $\widetilde{A}_k(\xi)$ is defined by

$$\widetilde{A}_k(\xi) = \sum_{nn'}\rho_n\left[1+\mathrm{e}^{\beta(\xi-\mu)}\right](c_k^\dagger)_{nn'}(c_k)_{n'n}\delta(\xi-E_n^{(N)}+E_{n'}^{(N-1)}). \qquad (33.15)$$

From equation (33.15), we see that

$$\sum_{nn'}\rho_n\delta(\xi+E_{n'}^{(N-1)}-E_n^{(N)})(c_k^\dagger)_{nn'}(c_k)_{n'n}=\widetilde{A}_k(\xi)f(\xi) \qquad (33.16)$$

where $f(\xi)$ is the Fermi distribution function

$$f(\xi)=\frac{1}{\mathrm{e}^{\beta(\xi-\mu)+1}}.$$

Equation (33.16) in equation (33.13) then yields

$$\langle C_{\mathbf{k},H}^\dagger C_{\mathbf{k},H}\rangle=\frac{1}{z_k}\int_{-\infty}^{\infty}\mathrm{d}\xi\,\widetilde{A}_k(\xi)f(\xi)\frac{\eta_k^2}{(\epsilon_k-\xi)^2+\eta_k^2}. \qquad (33.17)$$

Near the Fermi surface, we have

$$G(\mathbf{k},\omega)=G_{\mathrm{inc}}+\frac{z_k}{\omega-(\epsilon_k-\mu)}=\int_{-\infty}^{\infty}\mathrm{d}\xi\,\frac{\widetilde{A}_k(\xi)}{\omega-(\xi-\mu)}$$

so here the spectral function $\widetilde{A}_k(\xi)$ can be written as a sum of a singular term due to the quasi-particle and a smooth incoherent term:

$$\widetilde{A}_k(\xi)=\widetilde{A}_{k,\mathrm{inc}}(\xi)+z_k\delta(\xi-\epsilon_k). \qquad (33.18)$$

With equation (33.18) inserted in (33.17), we obtain

$$\langle C^\dagger_{\mathbf{k},H} C_{\mathbf{k},H}\rangle = f(\epsilon_k) + \frac{1}{z_k}\int_{-\infty}^{\infty} \mathrm{d}\xi\, \widetilde{A}_{k,\mathrm{inc}}(\xi) f(\xi) \frac{\eta_k^2}{(\epsilon_k - \xi)^2 + \eta_k^2}. \tag{33.19}$$

The last term in equation (33.19) vanishes as we move onto the Fermi surface because $A_{k,\mathrm{inc}}(\xi)$ is smooth, $f(\xi)$ is bounded and $\eta_k^2/[(\epsilon_k - \xi)^2 + \eta_k^2]$ vanishes as η_k when $\eta_k \to 0$. Hence, we conclude that

$$\langle C^\dagger_{\mathbf{k},H} C_{\mathbf{k},H}\rangle = \frac{1}{\mathrm{e}^{\beta(\epsilon_k - \mu)+1}} \tag{33.20}$$

which is precisely the quasi-particle equilibrium distribution function.

We will now turn to the verification of the properties (2) to (4) of the Landau Fermi liquid theory. These properties are all related to how the system responds to an external perturbation. It is then natural that our starting point is to discuss this response. Once we have done so, we will examine this expression in the limit of long wavelengths and low energies of the perturbation, from which we can verify the properties of the Landau Fermi liquid theory.

In Chapter 27, we derived an expression for the linear response of an observable $A(t)$ due to an external perturbation $H_{\mathrm{ext}}(t')_H$ turned on at time $t = t_0$. The response is

$$\delta\langle A\rangle(t) = i\int_{t_0}^{t} \mathrm{d}t' \langle\Psi_0 \mid [H_{\mathrm{ext}}(t')_H, A(t)_H] \mid \Psi_0\rangle \tag{33.21}$$

where Ψ_0 is the interacting ground state. (We assume in this chapter that all states are normalized.) In terms of the retarded correlation function

$$iD^R(t,t') \equiv \theta(t-t')\langle\Psi_0 \mid [A(t)_H, H_{\mathrm{ext}}(t')_H] \mid \Psi_0\rangle \tag{33.22}$$

we can write $\delta\langle A\rangle(t)$ as

$$\delta\langle A\rangle(t) = \int_{t_0}^{t} \mathrm{d}t'\, D^R(t,t'). \tag{33.23}$$

In most cases, $D^R(t,t')$ depends only on the difference $t - t'$, in which case we can set $t' = 0$ in equation (33.22) and write

$$iD^R(t) = \theta(t)\langle\Psi_0 \mid [A(t)_H, H_{\mathrm{ext}}(0)_H] \mid \Psi_0\rangle. \tag{33.24}$$

The function $D^R(t)$ defined by equation (33.24) is called a retarded correlation function, since it describes an after-effect. In analogy to this function, we may define an *advanced* correlation function $D^A(t)$ by

$$iD^A(t) = \theta(-t)\langle\Psi_0 \mid [A(t)_H, H_{\mathrm{ext}}(0)_H] \mid \Psi_0\rangle. \tag{33.25}$$

We will see later in this section that the retarded and the advanced correlation functions are intimately related to the *real-time* correlation function, which is defined by

$$iD(t) = \langle \Psi_0 \mid T\left\{A(t)_H H_{\mathrm{ext}}(0)_H\right\} \mid \Psi_0 \rangle. \tag{33.26}$$

In fact, one may show that the real-time correlation function completely determines the retarded and advanced correlation functions (see, for example, Fetter and Walecka [22]). The real-time correlation function is usually more convenient to use in zero-temperature calculations than the retarded correlation function. The reason for this is clear if we remind ourselves of the definition of the Green's function $G(\mathbf{r}, t)$:

$$iG(\mathbf{r},t) = \langle \Psi_0 \mid T\left\{\psi(\mathbf{r},t)_H \psi^\dagger(0,0)_H\right\} \mid \Psi_0 \rangle.$$

The structure of the real-time correlation function is then similar to that of the Green's function. In the cases of interest to us, the real-time correlation functions will be proportional to the two-particle Green's function. This means that all the techniques for calculating the Green's functions, such as Feynman diagrams, can be applied to the calculation of the real-time correlation functions. Once the real-time correlation has been calculated, it is easy to obtain the retarded correlation function.

If we consider the response of the density to a perturbation which couples to the density we are thus led to study the real-time density–density correlation function

$$iD_4(\mathbf{q},t) = \langle \Psi_0 \mid T\left\{\rho_{\mathbf{q}}(t)_H \rho_{-\mathbf{q}}(0)_H\right\} \mid \Psi_0 \rangle. \tag{33.27}$$

The density operator $\rho_{\mathbf{q}}(t)_H$ is in the plane-wave representation

$$\rho_{\mathbf{q}}(t)_H = \sum_{\mathbf{k}} c^\dagger_{\mathbf{k}+\frac{1}{2}\mathbf{q}}(t)_H c_{\mathbf{k}-\frac{1}{2}\mathbf{q}}(t)_H.$$

If, on the other hand, we want to calculate the response of the density to a perturbation which couples to the current density, we are led to study the correlation function

$$iD_\alpha(\mathbf{q},t) = \langle \Psi_0 \mid T\left\{\rho_{\mathbf{q}}(t)_H J_{-\mathbf{q},\alpha}(0)_H\right\} \mid \Psi_0 \rangle \tag{33.28}$$

where $\alpha = 1, 2, 3$ denotes the three Cartesian components. The current operator is in the plane-wave representation

$$J_{\mathbf{q},\alpha}(t)_H = \sum_{\mathbf{k}} \frac{k_\alpha}{m} c^\dagger_{\mathbf{k}+\frac{1}{2}\mathbf{q}}(t)_H c_{\mathbf{k}-\frac{1}{2}\mathbf{q}}(t)_H.$$

With these density and current operators in equations (33.27) and (33.28) we see that these correlation functions are proportional to sums over two-particle Green's functions.

We will use the Fourier-transforms of the correlation functions (33.27) and (33.28) with respect to time:

$$D_\mu(\mathbf{q},\omega) = \int_{-\infty}^{\infty} D_\mu(\mathbf{q},t)\mathrm{e}^{i\omega t}\,\mathrm{d}t. \tag{33.29}$$

For convenience, we have here introduced the notation $\mu = 1,2,3,4$. At this point, it is also convenient to introduce a four-vector notation. We will denote $(\mathbf{k},\tilde{\omega})$ by k, where $\mathbf{k}$ and $\tilde{\omega}$ are particle wavevectors and energies, respectively, and we will denote the wavevector $\mathbf{q}$ and frequency ω of the external perturbation by q. We also introduce a four-vector v_k^μ defined by

$$v_k^\mu = \begin{cases} 1 & \text{if } \mu = 4 \\ \dfrac{\partial \epsilon_k}{\partial k_\mu} & \text{if } \mu = 1,2,3. \end{cases}$$

The diagrammatic representation of $D_\mu(\mathbf{q},\omega)$ is given in figure 33.1.

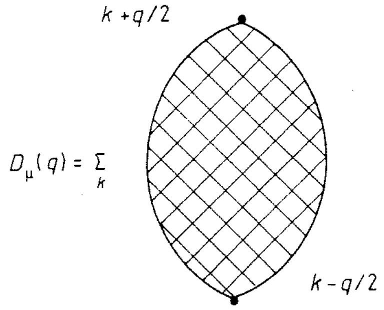


Figure 33.1 *The correlation function $D_\mu(\mathbf{q},\omega)$ is obtained by summing all these polarization diagrams over k.*

With the four-vector notation introduced above, $D_\mu(\mathbf{q},\omega)$ is given by the equation

$$iD_\mu(\mathbf{q},\omega) = \sum_k G(k+q/2)G(k-q/2)\Lambda_\mu(k;q) \tag{33.30}$$

where

$$\sum_k = \sum_{\mathbf{k}} \int \mathrm{d}\tilde{\omega}.$$

In equation (33.30), $\Lambda_\mu(k;q)$ is the so-called vertex function. This function has the diagrammatic representation given in figure 33.2, which yields the equation

$$\Lambda_\mu(k;q) = v_k^\mu + \sum_{k'} v_{k'}^\mu \Gamma(k,k';q)G(k'+q/2)G(k'-q/2). \tag{33.31}$$

Here, $\Gamma(k,k';q)$ is the scattering function, which is the collection of all the

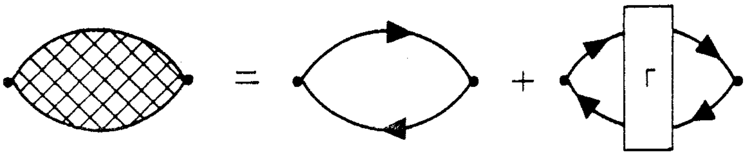


Figure 33.2 *Diagrammatic representation of the vertex function* $\Lambda(k;q)$ *in equation (33.29).*

connected diagrams shown in figure 33.3. This function is the sum of all possible scattering events between a particle and a hole. The scattering function may be decomposed into irreducible parts $I(k,k';q)$ and products of particle and hole propagators. The irreducible parts are represented by diagrams which cannot be separated by cutting one particle and one hole line only. From figure 33.4, we see that $\Gamma(k,k';q)$ satisfies

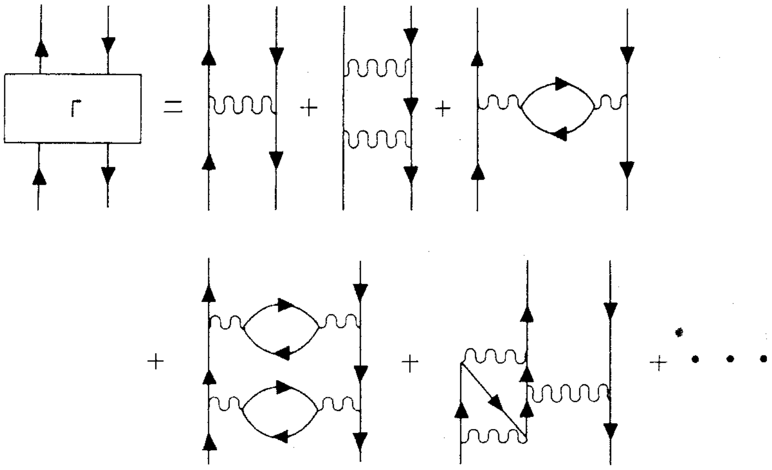


Figure 33.3 *The scattering function* $\Gamma(k,k';q)$ *consists of all possible ways a particle–hole pair of momentum* q *can scatter.*

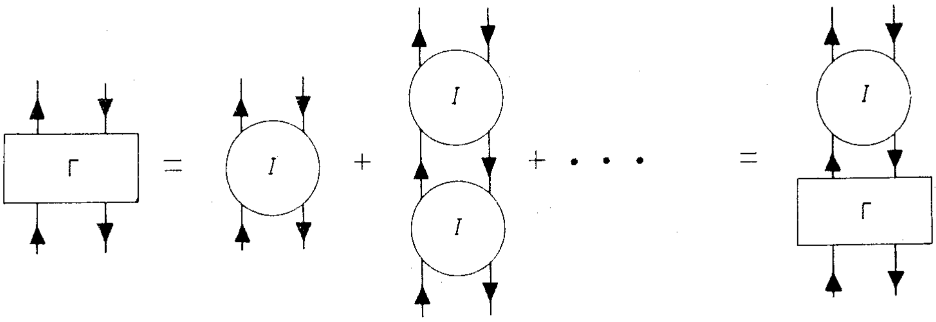


Figure 33.4 *The scattering function can be separated into irreducible parts and products of particle and hole propagators.*

$$\begin{aligned}\Gamma(k,k';q)&\\ = \ & I(k,k';q)+\sum_{k''} I(k,k'';q)G(k''+q/2)G(k''-q/2)I(k'',k';q)+\cdots\end{aligned}$$

or

$$\begin{aligned}\Gamma(k,k';q)&\\ = \ & I(k,k';q)+\sum_{k''} I(k,k'';q)G(k''+q/2)G(k''-q/2)\Gamma(k'',k';q).\end{aligned} \tag{33.32}$$

Using equation (33.32), we can then write the following integral equation for the vertex function:

$$\Lambda_\mu(k,q)=v_k^\mu+\sum_{k'} I(k,k';q)G(k'+q/2)G(k'-q/2)\Lambda_\mu(k',q). \tag{33.33}$$

In the equation for the correlation function, equation (33.30), and in equations (33.33) and (33.32) we see that the quantity

$$G(k+q/2)G(k-q/2) \tag{33.34}$$

enters. This quantity describes the propagation of a dressed particle–hole pair. As we are interested in perturbations with long wavelengths and low energies, which has as a consequence that the excitations of the system will be on the Fermi surface, we will ultimately take the limit $|\mathbf{q}| \to 0$ and $\omega \to 0$ of the correlation function. To do so, we must know how the product equation (33.34) behaves in this limit. Near the Fermi surface, we can write

$$\begin{aligned}G(k+q/2) &= G_{\text{inc}}(k+q/2)+\frac{z_{k+q/2}}{\tilde\omega-(\epsilon_{k+q/2}-\omega/2-\mu)+i\eta}\\ &\approx G_{\text{inc}}(k)+\frac{z_k}{\tilde\omega-(\epsilon_k+\mathbf{q}\cdot\mathbf{v}_k/2-\omega/2-\mu)+i\eta}\end{aligned} \tag{33.35}$$

where ϵ_k can be taken to be real, since the damping of the propagator vanishes as we approach the Fermi surface. Here, $\eta > 0$ if $\epsilon_{k+q/2} > \mu$, which corresponds to a particle, and $\eta < 0$ if $\epsilon_{k-q/2} < \mu$, which corresponds to the propagation of a hole. In the equations involving the product equation (33.34), we have to integrate the particle–hole propagator multiplied by some other function, such as $I(k,k';q)$ or $\Lambda_\mu(k',q)$, over particle frequencies $\tilde\omega$. In general the integral over $\tilde\omega$ can then be written

$$\int_{-\infty}^{\infty} d\tilde\omega\, G(k+q/2)G(k-q/2)F(k,q),$$

where the function $F(k,q)$ is regular as $|\mathbf{q}|,\omega \to 0$. If we insert equation (33.35) and the corresponding expression for $G(k-q/2)$ in this integral, we obtain four terms. Three of these terms contain at least one factor of the incoherent part of the Green's function. These terms have well-defined limits as $q \longrightarrow 0$. The fourth term is

$$\int_{-\infty}^{\infty} \mathrm{d}\tilde{\omega} \left\{ \frac{z_{k+q/2}}{\tilde{\omega} - (\epsilon_{k+q/2} - \omega/2 - \mu) + i\eta'} \right. \times \left. \frac{z_{k-q/2}}{\tilde{\omega} - (\epsilon_{k-q/2} + \omega/2 - \mu) + i\eta''} \right\} F(k,q). \tag{33.36}$$

The structure of this term is complicated due to the fact that the two separate poles of each factor merge on the real axis as $|\mathbf{q}|, \omega \longrightarrow 0$. In the limit of $q \longrightarrow 0$, we can write this integral as

$$\int_{-\infty}^{\infty} \mathrm{d}\tilde{\omega} \left\{ \frac{z_k}{\tilde{\omega} - (\epsilon_k + \mathbf{q}\cdot\mathbf{v}_k/2 - \omega/2 - \mu) + i\eta'} \right. \times \left. \frac{z_k}{\tilde{\omega} - (\epsilon_k - \mathbf{q}\cdot\mathbf{v}_k/2 + \omega/2 - \mu) + i\eta''} \right\} F(k,q). \tag{33.37}$$

Consider the case where $G(k+q/2)$ corresponds to the propagation of a particle. Then $\eta' > 0$, and $G(k-q/2)$ corresponds to the propagation of a hole, so $\eta'' < 0$. By using the identity

$$\frac{1}{x+i\eta} = P\frac{1}{x} - \pi i \delta(x)$$

where P denotes principal value, we can write

$$\begin{aligned} &\frac{z_k}{\tilde{\omega} - (\epsilon_k + \mathbf{q}\cdot\mathbf{v}_k/2 - \omega/2 - \mu) + i|\eta'|} \\ &\quad = \left\{ \frac{z_k}{\tilde{\omega} - (\epsilon_k + \mathbf{q}\cdot\mathbf{v}_k/2 - \omega/2 - \mu) - i|\eta'|} \right. \\ &\qquad \left. -2\pi i z_k \delta[\tilde{\omega} - (\epsilon_k + \mathbf{q}\cdot\mathbf{v}_k/2 - \omega/2 - \mu)] \right\} \theta(\epsilon_{k+q/2} - \mu). \end{aligned} \tag{33.38}$$

where the step-function ensures that $\mathbf{k} + \mathbf{q}/2$ is outside the Fermi surface. The integral equation (33.37) then becomes

$$\left\{ \frac{2\pi i z_k^2}{\omega - \mathbf{q}\cdot\mathbf{v}_k - i\eta} + \int_{-\infty}^{\infty} \mathrm{d}\tilde{\omega} \left[\frac{z_k}{\tilde{\omega} - (\epsilon_k - \mu) - i\eta} \right]^2 \right\} \times \theta(\epsilon_{k+q/2} - \mu) F(k_F, q=0). \tag{33.39}$$

Consider now the case where $G(k-q/2)$ corresponds to the propagation of a particle. Going through the same algebra that led to equation (33.39), we arrive at

$$\left\{-\frac{2\pi i z_k^2}{\omega - \mathbf{q}\cdot\mathbf{v}_k - i\eta} + \int_{-\infty}^{\infty} \mathrm{d}\tilde{\omega} \left[\frac{z_k}{\tilde{\omega} - (\epsilon_k - \mu) - i\eta}\right]^2\right\}$$
$$\times\theta(\epsilon_{k-q/2} - \mu)F(k_F, q = 0). \tag{33.40}$$

In these two equations, the function $F(k,q)$ can be evaluated at the Fermi surface, since this function is regular. Combining equations (33.39) and (33.40) and using

$$\left[\theta(\epsilon_{k+q/2} - \mu) - \theta(\epsilon_{k-q/2} - \mu)\right] = \mathbf{q}\cdot\mathbf{v}_k\delta(\epsilon_k - \mu)$$

as $|\mathbf{q}| \to 0$, we can finally write

$$\int_{-\infty}^{\infty} \mathrm{d}\tilde{\omega} G(k+q/2)G(k-q/2)F(k,q)$$
$$= \int_{-\infty}^{\infty} \mathrm{d}\tilde{\omega}\left[G^2(k) + \frac{2\pi i z_k^2 \mathbf{q}\cdot\mathbf{v}_k\delta(\epsilon_k - \mu)\delta(\tilde{\omega})}{\omega - \mathbf{q}\cdot\mathbf{v}_k - i\eta}\right]F(k_F, 0). \tag{33.41}$$

Here $G^2(k)$ is the term obtained by first taking the limit $q \to 0$ separately in the Green's functions, and then squaring:

$$G^2(k) = \left[\lim_{q\to 0} G(k+q/2)\right]\left[\lim_{q\to 0} G(k-q/2)\right].$$

This term contains the second-order poles in equations (33.39) and (33.40), which are well-defined as $q \to 0$. Thus

$$\lim_{q\to 0} G(k+q/2)G(k-q/2) = G^2(k) + R(k;\omega) \tag{33.42}$$

where the singular part $R(k;\omega)$ is

$$R(k;\omega) = 2\pi i z_k^2 \frac{\mathbf{q}\cdot\mathbf{v}_k}{\omega - \mathbf{q}\cdot\mathbf{v}_k - i\eta}\delta(\tilde{\omega})\delta(\epsilon_k - \mu). \tag{33.43}$$

The singular part $R(k;\omega)$ enters only on the Fermi surface because of the two δ-functions. It is clear that this singular part has a limit $q \to 0$ which is not unique but depends on $\mathbf{r} = \mathbf{q}/\omega$. We will distinguish three limiting cases: $|\mathbf{r}|$ constant, so that $|\mathbf{q}|$ and ω go to zero simultaneously; $|\mathbf{r}| = 0$, and $|\mathbf{r}| = \infty$. These limits will be denoted by superscripts. Thus

$$R^r(k) = 2\pi i z_k^2 \frac{\mathbf{r}\cdot\mathbf{v}_k}{1 - \mathbf{r}\cdot\mathbf{v}_k - i\eta}\delta(\tilde{\omega})\delta(\epsilon_k - \mu) \tag{33.44}$$
$$R^0(k) = 0 \tag{33.45}$$
$$R^\infty(k) = -2\pi i z_k^2 \delta(\tilde{\omega})\delta(\epsilon_k - \mu). \tag{33.46}$$

We now examine the limit $|\mathbf{q}| \to 0$, $\omega \to 0$ of the scattering function Γ. From equation (33.32) we see that the singularities that arise in Γ are due to the product $G(k+q/2)G(k-q/2)$. Combining equations (33.32) and (33.43), we can write

$$\Gamma^r(k,k') = I(k,k') + \sum_{k''} I(k,k'')\left\{G^2(k'') + R^r(k'')\right\}\Gamma^r(k'',k'). \quad (33.47)$$

In the case $r = 0$, we have

$$\Gamma^0(k,k') = I(k,k') + \sum_{k''} I(k,k'')G^2(k'')\Gamma^0(k'',k'). \quad (33.48)$$

We manipulate these two equations. Equation (33.47) leads to

$$\begin{aligned}&\sum_{k''}\left[\delta_{k,k''} - I(k,k'')G^2(k'')\right]\Gamma^r(k'',k')\\ &= \quad I(k,k') + \sum_{k''} I(k,k'')R^r(k'')\Gamma^r(k'',k').\end{aligned}$$

We multiply this expression from the left with the inverse of $\left[\delta_{\tilde{k},k} - I(\tilde{k},k)G^2(k)\right]$, and sum over k. The result is

$$\begin{aligned}\Gamma^r(\tilde{k},k') \quad &= \quad \sum_{k}\left[\delta_{\tilde{k},k} - I(\tilde{k},k)G^2(\tilde{k})\right]^{-1}\\ &\quad\times\left[I(k,k') + \sum_{k''} I(k,k'')R^r(k'')\Gamma^r(k'',k')\right].\end{aligned} \quad (33.49)$$

From equation (33.48) we obtain

$$\sum_{k''}\left[\delta_{k,k''} - I(k,k'')G^2(k'')\right]\Gamma^0(k'',k') = I(k,k').$$

We multiply this equation on the left with $\left[\delta_{\tilde{k},k} - I(\tilde{k},k)G^2(k)\right]^{-1}$ and sum over k, which yields

$$\Gamma^0(\tilde{k},k') = \sum_{k}\left[\delta_{\tilde{k},k} - I(\tilde{k},k)G^2(k)\right]^{-1} I(k,k'). \quad (33.50)$$

We insert equation (33.50) in equation (33.49) and relabel dummy indices $\tilde{k} \to k$, $k \to k''$ to obtain

$$\Gamma^r(k,k') = \Gamma^0(k,k') + \sum_{k''}\Gamma^0(k,k'')R^r(k'')\Gamma^r(k'',k'). \quad (33.51)$$

Similarly, it is easy to verify that

$$\Gamma^r(k,k') = \Gamma^\infty(k,k') + \sum_{k''} \Gamma^\infty(k,k'')\left[R^r(k'') - R^\infty(k'')\right]\Gamma^r(k'',k'). \tag{33.52}$$

On the Fermi surface, it is convenient to introduce

$$\begin{aligned} f(k,k') &= 2\pi i z_k z_{k'} \Gamma^0(k,k') && (33.53)\\ f^r(k,k') &= 2\pi i z_k z_{k'} \Gamma^r(k,k') && (33.54)\end{aligned}$$

with k, k' on the Fermi surface. In terms of these functions, we can then write (33.51) as

$$\begin{aligned} &f^r(k,k')\\ &= f(k,k') + \sum_{k''} f(k,k'')\frac{\mathbf{r}\cdot\mathbf{v}_{k''}}{1-\mathbf{r}\cdot\mathbf{v}_{k''}-i\eta}\delta(\tilde{\omega})\delta(\epsilon_{k''}-\mu)f^r(k'',k')\end{aligned} \tag{33.55}$$

Manipulating equation (33.31) in the same way as equation (33.47), and using equations (33.53) and (33.54), we can write the following equations for the vertex function on the Fermi surface

$$z_k\Lambda^r_\mu(k) = \begin{cases} z_k\Lambda^0_\mu(k) + \sum_{k'} f(k,k')\dfrac{\mathbf{r}\cdot\mathbf{v}_{k'}\,\delta(\tilde{\omega})}{1-\mathbf{r}\cdot\mathbf{v}_{k'}-i\eta}\delta(\mu-\epsilon_{k'})z_{k'}\Lambda^r_\mu(k') \\[2ex] z_k\Lambda^0_\mu(k) + \sum_{k'} f^r(k,k')\dfrac{\mathbf{r}\cdot\mathbf{v}_{k'}\,\delta(\tilde{\omega})}{1-\mathbf{r}\cdot\mathbf{v}_{k'}-i\eta}\delta(\mu-\epsilon_{k'})z_{k'}\Lambda^0_\mu(k') \\[2ex] z_k\Lambda^\infty_\mu(k) + \sum_{k'} f^r(k,k')\dfrac{\delta(\tilde{\omega})}{1-\mathbf{r}\cdot\mathbf{v}_{k'}-i\eta}\delta(\mu-\epsilon_{k'})z_{k'}\Lambda^\infty_\mu(k'). \end{cases} \tag{33.56}$$

We will need these results later at the final stage of the derivation of the Landau Fermi liquid theory.

To complete this section and verify the Landau Fermi liquid theory, we will relate the values of the vertex functions $\Lambda^0_\mu(k)$ and $\Lambda^\infty_\mu(k)$ on the Fermi surface to the self-energy. These relationships are established by the Ward identities.

We consider first the self-energy $M(\mathbf{k},\tilde{\omega})$. A diagram for $M(\mathbf{k},\tilde{\omega})$ with an internal line k' explicitly indicated is shown in figure 33.5. If we remove an internal line k' in all possible ways from $M(\mathbf{k},\tilde{\omega})$ we obtain the irreducible scattering function $I(k,k')$ (see figure 33.5). From this figure it is clear that we can write

$$M(\mathbf{k},\tilde{\omega}) = \sum_{k'} I(k,k')G(k'). \tag{33.57}$$

We want to take the partial derivative of $M(\mathbf{k},\tilde{\omega})$ with respect to $\tilde{\omega}$. This

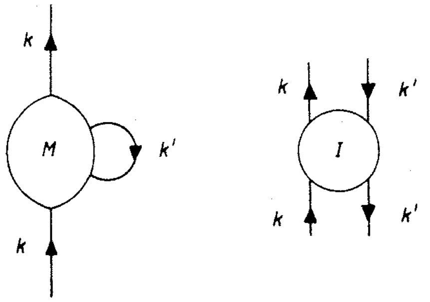


Figure 33.5 *Diagrammatic representation of the relation between the self-energy and the irreducible scattering function.*

is by definition

$$\lim_{\epsilon \to 0} \frac{M(\mathbf{k}, \widetilde{\omega} + \epsilon) - M(\mathbf{k}, \widetilde{\omega})}{\epsilon}.$$

By conservation of energy $\widetilde{\omega}$ at each vertex, increasing $\widetilde{\omega}$ to $\widetilde{\omega} + \epsilon$ is the same as on the right-hand side of equation (33.57) increasing all frequencies $\widetilde{\omega}'$ to $\widetilde{\omega}' + \epsilon$. We then immediately obtain

$$\frac{\partial M}{\partial \widetilde{\omega}} = \sum_{k'} I(k, k') \frac{\partial}{\partial \widetilde{\omega}'} G(k'). \qquad (33.58)$$

This is illustrated in the low-order example in figure 33.6. But

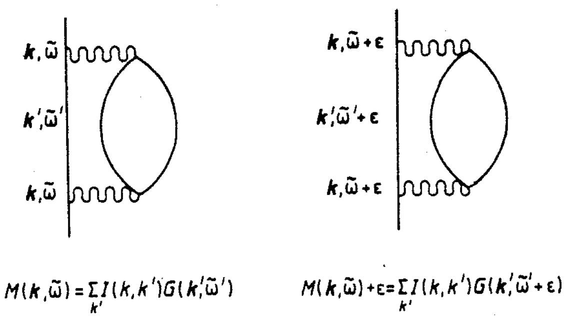


Figure 33.6 *This second-order example illustrates equation 33.57.*

$$\frac{\partial G}{\partial \widetilde{\omega}} = -G^2(k) \left[1 - \frac{\partial M(k')}{\partial \widetilde{\omega}}\right]$$

so

$$-\frac{\partial M(k)}{\partial \widetilde{\omega}} = \sum_{k'} I(k, k') G^2(k') \left[1 - \frac{\partial M(k')}{\partial \widetilde{\omega}}\right]. \qquad (33.59)$$

From equations (33.33) and (33.42) we have in the $r = 0$ limit

$$\Lambda_4^0(k) = 1 + \sum_{k'} I(k, k') G^2(k') \Lambda_4^0(k'). \qquad (33.60)$$

By comparing equation (33.59) and equation (33.60) we arrive at the first Ward identity:

$$\Lambda_4^0(k) = 1 - \frac{\partial M(k)}{\partial \tilde{\omega}}. \tag{33.61}$$

For the second Ward identity, we consider $\partial M(\mathbf{k},\tilde{\omega})/\partial k_\alpha$. Now $M(\mathbf{k},\tilde{\omega})$ depends on k_α only through the matrix elements of the interaction potential. These matrix elements are all invariant if all momenta are increased by the same amount. Therefore, instead of differentiating the right-hand side of equation (33.57) with respect to k_α, we may differentiate every internal line, given by $G(\mathbf{k},\tilde{\omega})$, with respect to k'_α. Thus

$$\frac{\partial M(\mathbf{k},\tilde{\omega})}{\partial k_\alpha} = \sum_{k'} I(k,k') \frac{\partial}{\partial k'_\alpha} G(\mathbf{k}',\tilde{\omega}').$$

But

$$\begin{aligned} \frac{\partial}{\partial k'_\alpha} G(\mathbf{k}',\tilde{\omega}') &= \lim_{q_\alpha \to 0} \frac{G(\mathbf{k}'+q_\alpha,\tilde{\omega}') - G(\mathbf{k}',\tilde{\omega}')}{q_\alpha} \\ &= \lim_{q_\alpha \to 0} \frac{q_\alpha k'_\alpha/m + M(\mathbf{k}'+q_\alpha,\tilde{\omega}') - M(\mathbf{k}',\tilde{\omega}')}{q_\alpha} G(\mathbf{k}',\tilde{\omega}')G(\mathbf{k}'+q_\alpha,\tilde{\omega}'). \end{aligned}$$

The last factor is just the $r = \infty$ limit of $G(\mathbf{k}',\tilde{\omega}')G(\mathbf{k}',\tilde{\omega}')$, so we obtain

$$\frac{\partial}{\partial k'_\alpha} G(\mathbf{k}',\tilde{\omega}') = \left[G^2(\mathbf{k}',\tilde{\omega}') + R^\infty(\mathbf{k}',\tilde{\omega}')\right] \left[\frac{k'_\alpha}{m} + \frac{\partial M(\mathbf{k}',\tilde{\omega}')}{\partial k'_\alpha}\right].$$

Thus

$$\frac{\partial M(\mathbf{k},\tilde{\omega})}{\partial k_\alpha} = \sum_{k'} I(k,k') \left[G^2(\mathbf{k}',\tilde{\omega}') + R^\infty(\mathbf{k}',\tilde{\omega}')\right] \left[\frac{k'_\alpha}{m} + \frac{\partial M(\mathbf{k}',\tilde{\omega}')}{\partial k'_\alpha}\right]. \tag{33.62}$$

But according to the $r = \infty$ limit of equation (33.33) we have

$$\Lambda_\alpha^\infty(\mathbf{k},\tilde{\omega}) = \frac{k_\alpha}{m} + \sum_{k'} I(k,k') \left[G^2(k') + R^\infty(k')\right] \Lambda_\alpha^\infty(k'). \tag{33.63}$$

By comparing (33.62) and (33.63), we obtain

$$\Lambda_\alpha^\infty(\mathbf{k},\tilde{\omega}) = \frac{k_\alpha}{m} + \frac{\partial M(\mathbf{k},\tilde{\omega})}{\partial k_\alpha}. \tag{33.64}$$

For the remaining two Ward identities, which involve Λ_α^0 and Λ_4^∞, we consider a simultaneous translation of the wavevector $\mathbf{k}$ and the Fermi surface by an amount q_α. We denote by $M(\mathbf{k}+q_\alpha,\tilde{\omega};q_\alpha)$ the value of the self-energy under such a translation. This is nothing but the self-energy in a reference frame moving with a velocity $-q_\alpha/m$. With this translation, we may define a 'total', or 'convective', derivative:

$$\frac{\mathrm{d}M(\mathbf{k},\tilde{\omega})}{\mathrm{d}k_\alpha} \equiv \lim_{q_\alpha \to 0} \frac{1}{q_\alpha}\left[M(\mathbf{k}+q_\alpha,\tilde{\omega};q_\alpha) - M(\mathbf{k},\tilde{\omega})\right]. \tag{33.65}$$

Note that in this derivative, the Fermi surface follows the motion of $\mathbf{k}$. It is now straightforward to evaluate $\mathrm{d}M/\mathrm{d}k_\alpha$. We have

$$\frac{\mathrm{d}M(\mathbf{k},\tilde{\omega})}{\mathrm{d}k_\alpha} = \sum_{k'} I(k,k')\frac{\mathrm{d}}{\mathrm{d}k'_\alpha}G(\mathbf{k}',\tilde{\omega}').$$

Now

$$\frac{\mathrm{d}}{\mathrm{d}k'_\alpha}G(\mathbf{k}',\tilde{\omega}') = \left[\frac{\mathrm{d}M(\mathbf{k}',\tilde{\omega}')}{\mathrm{d}k'_\alpha} + \frac{k'_\alpha}{m}\right]\lim_{q_\alpha \to 0} G(\mathbf{k}',\tilde{\omega}')G(\mathbf{k}'+q_\alpha,\tilde{\omega}';q_\alpha).$$

In the second factor, both $\mathbf{k}'$ and the Fermi surface are translated simultaneously so that their relative positions do not change. But then the poles of $G(\mathbf{k}',\tilde{\omega}')$ and $G(\mathbf{k}'+q_\alpha,\tilde{\omega}';q_\alpha)$ are on the same side of the Fermi surface, so according to (33.42) we have

$$\lim_{q_\alpha \to 0} G(\mathbf{k}',\tilde{\omega}')G(\mathbf{k}'+q_\alpha,\tilde{\omega}';q_\alpha) = G^2(\mathbf{k}',\tilde{\omega}').$$

Thus,

$$\frac{\mathrm{d}M(\mathbf{k},\tilde{\omega})}{\mathrm{d}k_\alpha} = \sum_{k'} I(k,k')G^2(\mathbf{k}',\tilde{\omega}')\left[\frac{\mathrm{d}M(\mathbf{k}',\tilde{\omega}')}{\mathrm{d}k'_\alpha} + \frac{k'_\alpha}{m}\right].$$

If we compare this with the $r = 0$ limit of equation (33.33)

$$\Lambda^0_\alpha(\mathbf{k},\tilde{\omega}) = \frac{k_\alpha}{m} + \sum_{k'} I(k,k')G^2(\mathbf{k}',\tilde{\omega}')\Lambda^0_\alpha(\mathbf{k}',\tilde{\omega}')$$

we see that

$$\Lambda^0_\alpha(\mathbf{k},\tilde{\omega}) = \frac{k_\alpha}{m} + \frac{\mathrm{d}M(\mathbf{k},\tilde{\omega})}{dk_\alpha}. \tag{33.66}$$

For the last Ward identity, we consider an increase $\mathrm{d}\mu$ in the chemical potential ($\mathrm{d}\mu > 0$). Due to this increase, the volume enclosed by the Fermi surface must expand to accommodate the increase in particles, hence k_F must increase an amount $\mathrm{d}k_F$ (which depends on direction in anisotropic systems), with

$$\mathrm{d}k_F = \frac{\partial k_F}{\partial \mu}\mathrm{d}\mu.$$

A quasi-particle is by definition an excitation on the Fermi surface, so its energy is equal to the chemical potential. Thus, the energies of the quasi-particles increase when μ increases. Consider a point A on the Fermi surface. As μ increases, this point is translated to a point B. The energies of a quasi-particle at A and one at B must then satisfy

$$\epsilon(k_B, \mu + \mathrm{d}\mu) - \epsilon(k_A, \mu) = \frac{\partial \epsilon_F}{\partial \mu}\mathrm{d}\mu + v_k \mathrm{d}k_F = \mathrm{d}\mu,$$

so

$$\frac{\partial \epsilon_F}{\partial \mu} = 1 - v_k \frac{\partial k_F}{\partial \mu}. \tag{33.67}$$

This equation shows how the energy of a quasi-particle changes with μ. We will use this relation shortly.

Now consider the self-energy $M(\mathbf{k}, \omega)$. As μ increases to $\mu + \mathrm{d}\mu$, the self-energy changes. We then have

$$\frac{\partial M(\mathbf{k}, \omega)}{\partial \mu} = \lim_{\mathrm{d}\mu \to 0} \frac{M(\mathbf{k}, \omega; \mu + \mathrm{d}\mu) - M(\mathbf{k}, \omega; \mu)}{\mathrm{d}\mu}. \tag{33.68}$$

Using the same construction as for the other Ward identities, we arrive at

$$\begin{aligned}\frac{\partial M(\mathbf{k}, \omega)}{\partial \mu} &= \lim_{\mathrm{d}\mu \to 0} \sum_{k'} I(k, k') \left[\frac{G(\mathbf{k}', \omega'; \mu + \mathrm{d}\mu) - G(\mathbf{k}', \omega'; \mu)}{\mathrm{d}\mu}\right] \\ &= \sum_{k'} I(k, k') \left[\frac{\partial M(\mathbf{k}, \omega')}{\partial \mu} - 1\right] \lim_{\mathrm{d}\mu \to 0} G(\mathbf{k}', \omega'; \mu + \mathrm{d}\mu) G(\mathbf{k}', \omega'; \mu).\end{aligned} \tag{33.69}$$

We examine the last factor of this expression. With $\mathbf{k}'$ between the Fermi surfaces at μ and $\mu + \mathrm{d}\mu$, this wavevector passes from the exterior of the Fermi surface to the interior of the Fermi surface as $\mu \to \mu + \mathrm{d}\mu$, hence its pole crosses the real axis in the complex $\tilde{\omega}'$–plane. From equation (33.38), the last factor is in this case

$$\left[\frac{z_k}{\tilde{\omega}' - (\epsilon_k - \mu) + i\eta}\right]^2 + \frac{z_{k'}^2}{\left[\tilde{\omega}' - (\epsilon_{k'} + \frac{\partial \epsilon_{k'}}{\partial \mu} - \mu - d\mu) + i\eta\right] \left[\tilde{\omega}' - (\epsilon_{k'} - \mu) - i\eta\right]}, \quad \eta > 0.$$

If $\mathbf{k}'$ is not in the region between the Fermi surfaces at μ and $\mu + \mathrm{d}\mu$, the limit is simply $G^2(\mathbf{k}', \tilde{\omega}')$. Since the extra term appears only if $\mathbf{k}'$ is on the Fermi surface at μ, we can write

$$\lim_{\mathrm{d}\mu \to 0} G(\mathbf{k}', \tilde{\omega}'; \mu + \mathrm{d}\mu) G(\mathbf{k}', \tilde{\omega}'; \mu) = G^2(\mathbf{k}', \tilde{\omega}'; \mu) + 2\pi i z_{k'}^2 \delta(\epsilon_{k'} - \mu) \delta(\tilde{\omega}')$$

which is just the $r \to \infty$ limit of the product of the Green's functions. With this in (33.69), we have

$$\frac{\partial M(\mathbf{k},\tilde{\omega})}{\partial \mu} = \sum_{k'} I(k,k') \left[G^2(\mathbf{k}',\tilde{\omega}') + R^{\infty}(\mathbf{k}',\tilde{\omega}')\right] \left[\frac{\partial M(\mathbf{k}',\tilde{\omega}')}{\partial \mu} - 1\right].$$

If we compare this with the $r = \infty$ limit of (33.33), we deduce that

$$\Lambda_4^{\infty}(\mathbf{k},\tilde{\omega}) = 1 - \frac{\partial M(\mathbf{k},\tilde{\omega})}{\partial \mu}. \tag{33.70}$$

All that remains is to write down the Ward identities on the Fermi surface ($k = k_F$, $\epsilon_k = \mu$, $\tilde{\omega} = 0$). We first note that the residue z_k is

$$z_k = \frac{1}{1 - \left.\frac{\partial M(\mathbf{k},\tilde{\omega})}{\partial \tilde{\omega}}\right|_{\tilde{\omega}=0}}.$$

If we compare this with the first Ward identity, equation (33.61), we see that

$$\Lambda_4^{0}(\mathbf{k},\tilde{\omega}) = \frac{1}{z_k}.$$

Furthermore, the quasi-particle energy is at the pole of the Green's function. The location of this pole is given by

$$\epsilon_k - \frac{k^2}{2m} - M(\mathbf{k},\tilde{\omega}) = 0. \tag{33.71}$$

If we differentiate this expression with respect to k_α, we obtain

$$\frac{\partial \epsilon_k}{\partial k_\alpha}\left[1 - \left.\frac{\partial M(\mathbf{k},\tilde{\omega})}{\partial \tilde{\omega}}\right|_{\tilde{\omega}=0}\right] - \left[\frac{k_\alpha}{m} + \frac{\partial M(\mathbf{k},0)}{\partial k_\alpha}\right] = 0. \tag{33.72}$$

From the second Ward identity, equation (33.64), and equation (33.72), we then have

$$\Lambda_\alpha^{\infty}(\mathbf{k},\tilde{\omega}) = \frac{1}{z_k}\frac{\partial \epsilon_k}{\partial k_\alpha} = \frac{1}{z_k} v_{k,\alpha}.$$

If, on the other hand, we take the total derivative as defined in equation (33.65) of (33.71) with respect to k_α, and use the third Ward identity (33.66), we obtain

$$\Lambda_\alpha^{0}(\mathbf{k},\tilde{\omega}) = \frac{1}{z_k}\frac{\mathrm{d}\epsilon_k}{\mathrm{d}k_\alpha}. \tag{33.73}$$

To evaluate the final Ward identity on the Fermi surface, we differentiate (33.71) with respect to the chemical potential. The result is

$$\frac{\partial \epsilon_k}{\partial \mu}\left[1 - \left.\frac{\partial M(\mathbf{k},\tilde{\omega})}{\partial \tilde{\omega}}\right|_{\tilde{\omega}=0}\right] - \frac{\partial M(\mathbf{k},0)}{\partial \mu} = 0.$$

Using equation (33.68), the equation for the residue z_k and the fourth Ward identity, equation (33.70), we obtain

$$\frac{1}{z_k}\frac{\partial \epsilon_k}{\partial \mu} = \frac{1}{z_k} - \Lambda_4^{\infty}. \tag{33.74}$$

But according to (33.67), we have

$$\frac{\partial \epsilon_k}{\partial \mu} = 1 - v_k \frac{\partial k_F}{\partial \mu}$$

which in (33.74) yields

$$\Lambda_4^{\infty}(\mathbf{k}, \tilde{\omega}) = \frac{1}{z_k} v_k \frac{\partial k_F}{\partial \mu}.$$

We can evaluate $\mathrm{d}\epsilon_k/\mathrm{d}k_\alpha$ by transforming to a coordinate system moving with a uniform velocity $-q_\alpha/m$. In this coordinate system, the Hamiltonian is

$$H_q = \sum_{\mathbf{k}} \frac{(\mathbf{k}+q_\alpha)^2}{2m} + V = H + q_\alpha \sum_{\mathbf{k}} \frac{k_\alpha}{m} + N\frac{q_\alpha^2}{2m}.$$

If we let E_q denote the expectation value of the energy in a state $\mid \psi_n\rangle$ seen in this reference frame, then

$$E_q = \sum_{\mathbf{k}} \langle \psi_n \mid \frac{k^2}{2m} \mid \psi_n\rangle + q_\alpha \sum_{\mathbf{k}} \langle \psi_n \mid \frac{k_\alpha}{m} \mid \psi_n\rangle + N\frac{q_\alpha^2}{2m} + \langle \psi_n \mid V \mid \psi_n\rangle.$$

From the definition (33.65) we have

$$\frac{\mathrm{d}E}{\mathrm{d}k_\alpha} = \frac{\partial E_q}{\partial q_\alpha} = \sum_{\mathbf{k}} \langle \frac{k_\alpha}{m} \rangle = J_\alpha$$

where J_α is the α-component of the total current density. Hence, it follows that $\mathrm{d}\epsilon_k/\mathrm{d}k_\alpha$ is the component $j_{\mathbf{k},\alpha}$ of the current carried by the quasi-particle $\mathbf{k}$. If the interactions are translationally invariant and thus conserve momentum, the current carried in the presence of a quasi-particle in the interacting system is the same as the current carried in the absence of interactions. This current is simply $\mathbf{k}/m$, so we have

$$\mathbf{j_k} = \nabla_{\mathbf{k}} \epsilon_k = \frac{\mathbf{k}}{m}$$

so

$$\Lambda_\alpha^0(\mathbf{k}, \tilde{\omega}) = \frac{1}{z_k} j_{\mathbf{k},\alpha}.$$

We can then summarize the Ward identities as follows:

$$z_k \Lambda_4^0(\mathbf{k},\tilde{\omega}) = 1 \tag{33.75}$$

$$z_k \Lambda_4^\infty(\mathbf{k},\tilde{\omega}) = v_k \frac{\partial k_F}{\partial \mu} \tag{33.76}$$

$$z_k \Lambda_\alpha^\infty(\mathbf{k},\tilde{\omega}) = v_{k,\alpha} \tag{33.77}$$

$$z_k \Lambda_\alpha^0(\mathbf{k},\tilde{\omega}) = j_{\mathbf{k},\alpha}. \tag{33.78}$$

If we now use these forms of the Ward identities in equations (33.56), we obtain

$$j_{\mathbf{k},\alpha} = v_{k,\alpha} + \sum_{\mathbf{k}'} f_{\mathbf{k}\mathbf{k}'} v_{k',\alpha} \delta(\epsilon_{k'} - \mu) \tag{33.79}$$

$$v_k \frac{\partial k_F}{\partial \mu} = 1 - \sum_{\mathbf{k}'} f_{\mathbf{k},\mathbf{k}'} v_{k'} \frac{\mathrm{d}k'_F}{\mathrm{d}\mu} \delta(\epsilon_{k'} - \mu) \tag{33.80}$$

These two equations are precisely the properties (2)–(3) of the Landau Fermi liquid theory. We have then finished verifying these two properties, when we add the fact that it is obvious from perturbation theory that one quasi-particle contains precisely one bare particle. In addition, in the verification of these properties we have made the identification

$$f_{\mathbf{k},\mathbf{k}'} = 2\pi i z_k z_{k'} \Gamma^0(k,k'). \tag{33.81}$$

Thus, we have obtained the microscopic expression for $f_{\mathbf{k},\mathbf{k}'}$. Equation (33.81) states that the Landau f-function is given by the scattering function in the limit of long wavelengths and low energies.

All that we have left to do is to verify the transport equation of the Landau Fermi liquid theory. To this end, we consider the response of the quasi-particles to a perturbation which couples to the density of the system. To be specific, we take the perturbation to be of the form

$$H_1(\mathbf{q},t) = V_{\mathbf{q}} \rho_{-\mathbf{q}} \mathrm{e}^{-i\omega t}$$

where $V_{\mathbf{q}}$ is an amplitude. The perturbation is macroscopic in the sense that $q/k_F \ll 1$ and $\omega/\epsilon_F \ll 1$. We seek the response of the quasi-particle density, so we must find an expression for this quantity. Previously, we introduced the operator $C^\dagger_{\mathbf{k}}(t)_H$, which we argued is a quasi-particle creation operator. In analogy with the *particle*-density operator

$$\sum_{\mathbf{k},\mathbf{q}} c^\dagger_{\mathbf{k}-\mathbf{q}/2}(t)_H c_{\mathbf{k}+\mathbf{q}/2}(t)_H \mathrm{e}^{i\mathbf{q}\cdot\mathbf{r}}$$

we introduce the *quasi*-particle density operator

$$\sum_{\mathbf{k},\mathbf{q}} C^\dagger_{\mathbf{k}-\mathbf{q}/2}(t)_H C_{\mathbf{k}+\mathbf{q}/2}(t)_H \mathrm{e}^{i\mathbf{q}\cdot\mathbf{r}}$$

so that

$$\sum_{\mathbf{q}} C^{\dagger}_{\mathbf{k}-\mathbf{q}/2}(t)_H C_{\mathbf{k}+\mathbf{q}/2}(t)_H \mathrm{e}^{i\mathbf{q}\cdot\mathbf{r}}$$

is the density of quasi-particles $\mathbf{k}$ at $\mathbf{r}$. The response of this density to the perturbation $H_1(\mathbf{q},t)$ is then (see Chapter 27)

$$\begin{aligned}\delta n_{\mathbf{k}}(\mathbf{q},t) &= \delta n_{\mathbf{k}}(\mathbf{q},\omega)\mathrm{e}^{-i\omega t}\\ &= -iV_{\mathbf{q}}\int_{-\infty}^{t}\mathrm{d}t'\,\mathrm{e}^{\eta t'}\mathrm{e}^{-i\omega t'}\\ &\quad\times\langle\Psi_0\mid\left[C^{\dagger}_{\mathbf{k}-\mathbf{q}/2}(t)_H C_{\mathbf{k}+\mathbf{q}/2}(t)_H,\rho_{-\mathbf{q}}(t')_H\right]\mid\Psi_0\rangle\end{aligned} \tag{33.82}$$

where η is a positive infinitesimal which assures that we turn on the perturbation adiabatically. In particular, at $t = 0$ we have

$$\delta n_{\mathbf{k}}(\mathbf{q},\omega) = -iV_{\mathbf{q}}\int_{-\infty}^{0}\mathrm{d}t\,\mathrm{e}^{-i\omega t}\mathrm{e}^{\eta t}\langle\Psi_0\mid\left[C^{\dagger}_{\mathbf{k}-\mathbf{q}/2}C_{\mathbf{k}+\mathbf{q}/2},\rho_{-\mathbf{q}}(t)_H\right]\mid\Psi_0\rangle. \tag{33.83}$$

If we define a renormalized real-time correlation function $\widetilde{D}_4(\mathbf{k},t-t';\mathbf{q},\omega)$ by

$$\begin{aligned}&i\widetilde{D}_4(\mathbf{k},t-t';\mathbf{q},\omega)\\ &= \int_{-\infty}^{\infty}\mathrm{d}t''\,\mathrm{e}^{-i\omega t''}\mathrm{e}^{-\eta|t''|}\\ &\quad\times\langle\Psi_0\mid T\left\{C^{\dagger}_{\mathbf{k}-\mathbf{q}/2}(t')_H C_{\mathbf{k}+\mathbf{q}/2}(t)_H\rho_{-\mathbf{q}}(t'')_H\right\}\mid\Psi_0\rangle,\end{aligned} \tag{33.84}$$

we can write the quasi-particle response as

$$\delta n_{\mathbf{k}\sigma}(\mathbf{q},\omega) = V_{\mathbf{q}}\widetilde{D}_4(\mathbf{k},0^+;\mathbf{q},\omega). \tag{33.85}$$

To show the equality between equations (33.83) and (33.85) we must show under what conditions

$$\begin{aligned}&\int_{-\infty}^{\infty}\mathrm{d}t\,\mathrm{e}^{-i\omega t}\mathrm{e}^{-\eta|t|}\langle\Psi_0\mid T\left\{A(0)_H B(t)_H\right\}\mid\Psi_0\rangle\\ &= \int_{-\infty}^{0}\mathrm{d}t\,\mathrm{e}^{-i\omega t}\mathrm{e}^{\eta t}\langle\Psi_0\mid[A(0)_H,B(t)_H]\mid\Psi_0\rangle\end{aligned} \tag{33.86}$$

for any two bosonic Heisenberg operators $A(t)_H$ and $B(t)_H$ (*e.g.*, $A = C^{\dagger}_{\mathbf{k}-\mathbf{q}/2}C_{\mathbf{k}+\mathbf{q}/2}$ and $B = \rho_{\mathbf{q}}$). By inserting a complete set of eigenstates

ψ_n, the left side of equation (33.86) becomes

$$\begin{aligned}
&\sum_n \int_{-\infty}^{\infty} \mathrm{d}t\, \mathrm{e}^{-i\omega t-\eta|t|} \\
&\qquad \times \left[\mathrm{e}^{-i(E_0-E_n)t} A_{0n} B_{n0}\theta(-t) + \mathrm{e}^{i(E_0-E_n)t} B_{0n} A_{n0}\theta(t)\right] \\
&= i\sum_n \frac{A_{0n}B_{n0}}{\omega+(E_0-E_n)+i\eta} + i\sum_n \frac{B_{0n}A_{n0}}{(E_0-E_n)-\omega+i\eta}.
\end{aligned} \tag{33.87}$$

The right-hand side of equation (33.86), on the other hand, is

$$\begin{aligned}
&\sum_n \int_{-\infty}^{0} \mathrm{d}t\, \mathrm{e}^{-i\omega t+\eta t} \left[\mathrm{e}^{-i(E_0-E_n)t} A_{0n} B_{n0} - \mathrm{e}^{i(E_0-E_n)t} B_{0n} A_{n0}\right] \\
&= i\sum_n \frac{A_{0n}B_{n0}}{\omega+(E_0-E_n)+i\eta} - i\sum_n \frac{B_{0n}A_{n0}}{\omega-(E_0-E_n)+i\eta}
\end{aligned} \tag{33.88}$$

We define a function $S_1(\omega')$ by

$$S_1(\omega') = \sum_n A_{0n}B_{n0}\delta\left(\omega' - (E_n - E_0)\right)$$

and a function $S_2(\omega')$ by

$$S_2(\omega') = \sum_n B_{0n}A_{n0}\delta\left(\omega' - (E_n - E_0)\right).$$

These functions are essentially generalizations of the spectral functions $A(\mathbf{k},\omega')$ and $B(\mathbf{k},\omega')$ introduced in Chapter 15 (see equation (15.30)). Since $E_n \geq E_0$, it follows that $S_1(\omega')$ and $S_2(\omega')$ vanish if $\omega' \leq 0$. Equation (33.87) can then be written as

$$i\int_{-\infty}^{\infty} \mathrm{d}\omega' \frac{S_1(\omega')}{\omega-\omega'+i\eta} - i\int_{-\infty}^{\infty} \mathrm{d}\omega' \frac{S_2(\omega')}{\omega+\omega'-i\eta} \tag{33.89}$$

and equation (33.88) can be written as

$$i\int_{-\infty}^{\infty} \mathrm{d}\omega' \frac{S_1(\omega')}{\omega-\omega'+i\eta} - i\int_{-\infty}^{\infty} \mathrm{d}\omega' \frac{S_2(\omega')}{\omega+\omega'+i\eta}. \tag{33.90}$$

Using the by now familiar identity

$$\frac{1}{x \pm i\eta} = P\frac{1}{x} \mp i\pi\delta(x)$$

these two equations become

$$iP\int d\omega'\frac{S_1(\omega')}{\omega-\omega'}+\pi S_1(\omega)-iP\int d\omega'\frac{S_2(\omega')}{\omega-\omega'}-\pi S_2(-\omega)$$

and

$$iP\int d\omega'\frac{S_1(\omega')}{\omega-\omega'}+\pi S_1(\omega)-iP\int d\omega'\frac{S_2(\omega')}{\omega-\omega'}+\pi S_2(-\omega)$$

respectively. These two expressions are identical if $\omega > 0$, and differ by the sign of the term $\pi S_2(-\omega)$ if $\omega < 0$. To avoid any complications, we will assume that $\omega > 0$. This is in any case not unreasonable, since ω is the frequency with which the perturbation is driving the system.

The correlation function $\widetilde{D}_4(\mathbf{k}, t-t'; \mathbf{q}, \omega)$ is a real-time correlation function which is closely related to the real-time correlation function $D_4(q)$ which we studied earlier. $D_4(q)$ could be decomposed into a vertex part and a particle–hole propagator:

$$iD_4(q)=\sum_k \Lambda_4(k;q)G(k+q/2)G(k-q/2)\equiv i\sum_k D_4(k,q). \tag{33.91}$$

The Fourier transform $\widetilde{D}_4(k,q)$ of $\widetilde{D}(\mathbf{k},t-t';\mathbf{q},\omega)$ is a renormalized version of $D_4(k,q)$ which satisfies the same equation, but with the two Green's functions replaced by mixed Green's functions $g(k)$ and $\widetilde{g}(k)$ defined by

$$\begin{aligned} ig(\mathbf{k},t-t') &= \langle\Psi_0 \mid T\left\{C_{\mathbf{k}}(t)_H c_{\mathbf{k}}^\dagger(t')_H\right\} \mid \Psi_0\rangle \\ i\widetilde{g}(\mathbf{k},t-t') &= \langle\Psi_0 \mid T\left\{c_{\mathbf{k}}(t)_H C_{\mathbf{k}}^\dagger(t')_H\right\} \mid \Psi_0\rangle \end{aligned}$$

so that

$$i\widetilde{D}_4(k,q)=\Lambda_4(k,q)g(k+q/2)\widetilde{g}(k-q/2). \tag{33.92}$$

To cast this equation in a more transparent form, we start by writing out the zero-temperature form of the mixed Green's function $g(\mathbf{k},t-t')$:

$$\begin{aligned} & ig(\mathbf{k},t-t') \\ &= \sum_n e^{i(E_0^{(N)}-E_n^{(N+1)})(t-t')}\frac{(c_k)_{0n}\left(c_k^\dagger\right)_{n0}}{-\epsilon_k-(E_0^{(N)}-E_n^{(N+1)})+i\eta_k}\frac{i\eta_k}{\sqrt{z_k}}\theta(t-t') \\ &- \sum_n e^{-i(E_0^{(N)}-E_n^{(N-1)})(t-t')}\frac{\left(c_k^\dagger\right)_{0n}(c_k)_{n0}}{-\epsilon_k-(E_n^{(N-1)}-E_0^{(N)})+i\eta_k}\frac{i\eta_k}{\sqrt{z_k}}\theta(t'-t) \end{aligned} \tag{33.93}$$

where we have used equations (33.11) and (33.12). On the other hand, the Lehmann representation for the Green's function $G(\mathbf{k},\widetilde{\omega})$ is

$$
\begin{aligned}
G(\mathbf{k},\omega)& \\
&= \sum_n \frac{(c_k)_{0n}\left(c_k^\dagger\right)_{n0}}{\omega-(E_n^{(N+1)}-E_0^{(N)})+i\eta}+\sum_n \frac{\left(c_k^\dagger\right)_{0n}(c_k)_{n0}}{\omega+(E_n^{(N-1)}-E_0^{(N)})-i\eta} \\
&= \int_0^\infty \mathrm{d}\omega' \left[\frac{A(\mathbf{k},\omega')}{\omega-\omega'+i\eta}+\frac{B(\mathbf{k},\omega')}{\omega+\omega'-i\eta}\right]. \qquad (33.94)
\end{aligned}
$$

Here, $A(\mathbf{k},\omega')$ and $B(\mathbf{k},\omega')$ are the spectral functions

$$
\begin{aligned}
A(\mathbf{k},\omega') &= \sum_n (c_k)_{0n}\left(c_k^\dagger\right)_{n0}\delta(\omega'-(E_n^{(N+1)}-E_0^{(N)})) \\
B(\mathbf{k},\omega') &= \sum_n \left(c_k^\dagger\right)_{0n}(c_k)_{n0}\,\delta(\omega'-(E_n^{(N-1)}-E_0^{(N)})).
\end{aligned}
$$

By comparing (33.93) and (33.94), we see that we have

$$
\begin{aligned}
ig(\mathbf{k},t-t')& \\
&= \int_{-\infty}^\infty \mathrm{d}\omega \left(\frac{i\eta_k}{\sqrt{z_k}}\right)\frac{\mathrm{e}^{-i(t-t')\omega}\left[A(\mathbf{k},\omega)\theta(t-t')-B(\mathbf{k},-\omega)\theta(t'-t)\right]}{\omega-\epsilon_k+i\eta_k}.
\end{aligned}
\qquad (33.95)
$$

If $\mathbf{k}$ is near the Fermi surface, we use

$$
\begin{aligned}
A(\mathbf{k},\omega) &= A_{\mathrm{inc}}(\mathbf{k},\omega)+z_k\delta(\omega-\epsilon_k)\theta(\epsilon_k-\mu) \\
B(\mathbf{k},\omega) &= B_{\mathrm{inc}}(\mathbf{k},\omega)+z_k\delta(\omega+\epsilon_k)\theta(\mu-\epsilon_k)
\end{aligned}
$$

where $A_{\mathrm{inc}}(\mathbf{k},\omega)$ and $B_{\mathrm{inc}}(\mathbf{k},\omega)$ are the incoherent parts of the spectral functions. We have explicitly written out the θ-functions to demonstrate that the two terms correspond to quasi-particle and quasi-hole excitations, respectively. These parts are analytic at the Fermi surface. The incoherent part of the spectral densities do not contribute anything as $\eta_k \to 0$. In this limit, we then have

$$
\begin{aligned}
ig(\mathbf{k},t-t')& \\
&= \mathrm{e}^{-i\epsilon_k(t-t')}\sqrt{z_k}\theta(\epsilon_k-\mu)\theta(t-t')-\mathrm{e}^{-i\epsilon_k(t-t')}\sqrt{z_k}\theta(\mu-\epsilon_k)\theta(t'-t).
\end{aligned}
$$

In other words, the function $g(\mathbf{k},t-t')$ is a renormalized conventional unperturbed propagator with the unperturbed energies replaced by the exact quasi-particle energies. Going through the same analysis for $\widetilde{g}(\mathbf{k},t-t')$, we find precisely the same result. By Fourier transforming $g(\mathbf{k},t-t')$ and $\widetilde{g}(\mathbf{k},t-t')$ and inserting the results in equation (33.92) we arrive at

$$
\begin{aligned}
i\widetilde{D}_4(\mathbf{k},0,0;\mathbf{q},\omega) \\
&= \int_{-\infty}^{\infty} \frac{d\widetilde{\omega}}{2\pi}\Lambda_4(k,q) \\
&\times \frac{z_k}{\left(\epsilon_{k+q/2}-\widetilde{\omega}+\mu-\omega/2+i\eta'\right)\left(\epsilon_{k-q/2}+\mu-\widetilde{\omega}+\omega/2+i\eta''\right)}.
\end{aligned}
\tag{33.96}
$$

In this expression, the poles of the integrand are on different sides of the real $\widetilde{\omega}$–axis, and the contributions from the poles dominate the integral. In the limit $|\mathbf{q}| \to 0$, $\omega \to 0$ (the r-limit), the factor

$$g(k+q/2)\widetilde{g}(k-q/2)$$

behaves precisely as the r-limit of $G(k+q/2)G(k-q/2)$, except for the fact that $g(k+q/2)$ and $\widetilde{g}(k-q/2)$ are renormalized by a factor of $z_k^{-1/2}$ each compared to the interacting Green's functions $G(k \pm q/2)$. Hence, this r-limit is the r-limit of $G(k+q/2)G(k-q/2)$ divided by z_k, so the result is

$$i\widetilde{D}_4(\mathbf{k},0,0;\mathbf{q},\omega) = -\frac{z_k}{2\pi}\Lambda_4^r(\mathbf{k},0;q)\frac{2\pi i}{\mathbf{q}\cdot\mathbf{v}_k-\omega-i\eta}\mathbf{q}\cdot\mathbf{v}_k\delta(\epsilon_k-\mu). \tag{33.97}$$

This result inserted in equation (33.85) yields

$$\delta n_{\mathbf{k}}(\mathbf{q},\omega) = -V_{\mathbf{q}}\frac{\mathbf{q}\cdot\mathbf{v}_k}{\mathbf{q}\cdot\mathbf{v}_k-\omega-i\eta}\delta(\epsilon_k-\mu)z_k\Lambda_4^r(\mathbf{k},0;q). \tag{33.98}$$

By using equation (33.52) and the Ward identity equation (33.75), we can write

$$z_k\Lambda_4^r(\mathbf{k},0;q) = 1+\sum_{\mathbf{k}'} f_{\mathbf{k},\mathbf{k}'}\frac{\mathbf{q}\cdot\mathbf{v}_{k'}}{\omega-\mathbf{q}\cdot\mathbf{v}_k-i\eta}\delta(\epsilon_{k'}-\mu)z_{k'}\Lambda_4^r(\mathbf{k}',0;q). \tag{33.99}$$

We can eliminate Λ_4^r between these two equations. By inserting equation (33.99) in (33.98), we obtain

$$
\begin{aligned}
(\omega-\mathbf{q}\cdot\mathbf{v}_{\mathbf{k}})\delta n_{\mathbf{k}}(\mathbf{q},\omega) \\
&= V_{\mathbf{q}}\mathbf{q}\cdot\mathbf{v}_{\mathbf{k}}\delta(\epsilon_k-\mu) && (33.100) \\
&\times \left[1+\sum_{\mathbf{k}'} f_{\mathbf{k},\mathbf{k}'}\frac{\mathbf{q}\cdot\mathbf{v}_{\mathbf{k}'}}{\omega-\mathbf{q}\cdot\mathbf{v}_{\mathbf{k}'}-i\eta}\delta(\epsilon_{k'}-\mu)z_{k'}\Lambda(\mathbf{k}',0;q)\right].
\end{aligned}
\tag{33.101}
$$

On the other hand, if we relabel $\mathbf{k} \to \mathbf{k}'$ in equation (33.98), multiply by $f_{\mathbf{k},\mathbf{k}'}$ and sum over $\mathbf{k}'$, we have

$$\sum_{\mathbf{k},\mathbf{k}'} f_{\mathbf{k},\mathbf{k}'}\delta_{\mathbf{k}'}(\mathbf{q},\omega) = V_{\mathbf{q}}\sum_{\mathbf{k},\mathbf{k}'} f_{\mathbf{k},\mathbf{k}'}\frac{\mathbf{q}\cdot\mathbf{v}_{\mathbf{k}'}}{\omega-\mathbf{q}\cdot\mathbf{v}_{\mathbf{k}'}-i\eta}\delta(\epsilon_{k'}-\mu)z_{k'}\Lambda(\mathbf{k}',0;q). \tag{33.102}$$

Inserting equation (33.102) in (33.101) yields

$$\begin{aligned}(\omega - \mathbf{q}\cdot\mathbf{v}_k)\,\delta n_{\mathbf{k}}(\mathbf{q},\omega) &= V_{\mathbf{q}}\mathbf{q}\cdot\mathbf{v}_k\delta(\epsilon_k-\mu) \\ &\quad +\mathbf{q}\cdot\mathbf{v}_k\delta(\epsilon_k-\mu)\sum_{\mathbf{k}'} f_{\mathbf{k},\mathbf{k}'}\delta n_{\mathbf{k}'}(\mathbf{q},\omega).\end{aligned} \tag{33.103}$$

If we introduce the amplitude $\mathcal{F}$ of the force created by the perturbation,

$$\mathcal{F} = -i\mathbf{q}V_{\mathbf{q}}$$

Equation (33.103) takes the form

$$\begin{aligned}0 &= (\mathbf{q}\cdot\mathbf{v}_k-\omega)\,\delta n_{\mathbf{k}}(\mathbf{q},\omega)+i\mathcal{F}\cdot\mathbf{v}_k\delta(\epsilon_k-\mu) \\ &\quad +\mathbf{q}\cdot\mathbf{v}_k\delta(\epsilon_k-\mu)\sum_{\mathbf{k}'} f_{\mathbf{k},\mathbf{k}'}\delta n_{\mathbf{k}'}(\mathbf{q},\omega).\end{aligned} \tag{33.104}$$

This is precisely the transport equation in the absence of collisions of the Landau Fermi liquid theory and the verification of the Landau Fermi liquid theory is complete.

We conclude with a comment on the expression (33.83) for $\delta n_{\mathbf{k}}(\mathbf{q},\omega)$:

$$\begin{aligned}&\delta n_{\mathbf{k}}(\mathbf{q},\omega) \\ &\quad = -iV_{\mathbf{q}}\int_{-\infty}^{0} dt\, e^{-i\omega t}e^{\eta t}\langle\Psi_0\mid\left[C^{\dagger}_{\mathbf{k}-\mathbf{q}/2}C_{\mathbf{k}+\mathbf{q}/2},\rho_{-\mathbf{q}}(t)_H\right]\mid\Psi_0\rangle.\end{aligned}$$

This expression shows that $\delta n_{\mathbf{k}}(\mathbf{q},\omega)$ can be interpreted as a probability amplitude for finding a quasi-particle–quasi-hole pair of momentum $\mathbf{q}$ and energy ω. Note that the expression is *not* positive definite, so that an interpretation as a *probability* is not permissible.

Chapter 34

Application to the Kondo problem

A standard result due to Bloch in transport theory predicts that the resistivity $\rho(T)$ of metals should vary as T^5 at low temperatures, due to normal electron–phonon scattering. In real metals, even the simplest ones, such as potassium and sodium, the resistivity exhibits a more complex temperature dependence than this. Although the normal electron–phonon scattering term can in some cases be identified, there are also contributions to the resistivity from many other scattering processes, such as electron–electron scattering and electron–impurity scattering. The contribution to the resistivity from these two processes is proportional to T^2 at low temperatures and low impurity concentrations (for an extensive review, see Bass *et al.* [40]). If a small amount of magnetic impurities, such as iron, chromium or manganese, is added to the metal, the resistivity exhibits a *minimum*. The temperature at which this minimum occurs seems to vary with the density n_i of the impurity, and the depth of the minimum, $\rho(0) - \rho(T_{\text{min}})$, is proportional to n_i. Since $\rho(0)$ itself is proportional to n_i, the relative minimum in the resistivity is roughly independent of n_i, and is usually equal to about ten percent of $\rho(0)$.

The explanation for the effect, but by no means a complete theory of the temperature dependence of the system, was provided by Kondo in 1964. He considered the problem of a single magnetic impurity in the sea of conduction electrons. The conduction electrons may suffer a spin-flip as they scatter off the impurity. This makes the problem a very difficult many-body problem, since the Pauli exclusion principle has to be taken into account when the scattering rates off the internal degrees of freedom of the impurity are calculated. It is found that a low-temperature regime is entered when the temperature is much less than a characteristic temperature, the Kondo temperature T_K, of the system. Exactly what happens near this temperature could not be sorted out until renormalization group techniques were applied to the problem by Wilson [42]. He showed that when T goes below T_K, the system enters into an effective strong-coupling regime, where the system behaves as though the coupling J between the impurity and the conduction electrons goes to infinity. Once in this strong coupling regime, Nozières [31] showed that Fermi liquid theory could adequately describe the system. We will here briefly review this application of Fermi liquid theory by Nozières.

We consider a single magnetic spin-$\frac{1}{2}$ impurity in the sea of N Bloch electrons. The appropriate Hamiltonian for this problem is the Kondo Hamiltonian, which consists of the kinetic energy of the conduction electrons and an anti-ferromagnetic coupling to the spin of the impurity:

$$H = \sum_{\mathbf{k}\sigma} \epsilon_k c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + J/N \sum_{\mathbf{k}\sigma,\mathbf{k}'\sigma'} \mathbf{S} \cdot \mathbf{s}_{\sigma\sigma'} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}'\sigma'}. \qquad (34.1)$$

Here, $\mathbf{S}$ is the spin operator of the impurity, $\mathbf{s}_{\sigma\sigma'}$ is the spin operator of the conduction electrons, and $J > 0$. For our purposes here, it is better to write the Hamiltonian in a real-space representation. We imagine that the system is on a lattice, so that $c^\dagger_{i\sigma}$ creates an electron of spin σ at site i with a spatial wavefunction $\phi(\mathbf{r} - \mathbf{R}_i)$. By a simple transformation, the Hamiltonian (34.1) can then be written

$$H = \sum_{ij} T_{ij} c^\dagger_{i\sigma} c_{j\sigma} + J\mathbf{S} \cdot \mathbf{s}_{\sigma\sigma'} c^\dagger_{0\sigma} c_{0\sigma'} \qquad (34.2)$$

where 0 is the impurity site. The T_{ij} are the hopping integrals given by

$$T_{ij} = \int d^3r \phi^*(\mathbf{r} - \mathbf{R}_i) H_{\text{Bloch}} \phi(\mathbf{r} - \mathbf{R}_j)$$

with H_{Bloch} the Bloch Hamiltonian of the conduction electrons.

We will follow Nozières and apply Fermi liquid theory to the low-temperature regime of this problem. This means that we start by assuming that at low temperatures, the coupling J is very large compared to all other dynamic degrees of freedom. A single electron can then substantially lower its energy by binding to the impurity in a singlet state. As $J \to \infty$, the binding energy goes to infinity, so that it requires an infinite amount of energy to remove the electron from the singlet state. Hence, the impurity will trap a single conduction electron into a singlet state. By the Pauli exclusion principle, no more electrons can occupy the singlet state, so the impurity now acts as an infinitely repulsive site for the $N-1$ remaining electrons. We will identify *this* state of the system as our ideal 'non-interacting' reference system of the Fermi liquid theory.

At large, but finite J, it is still impossible to break the singlet state, but virtual excitations of the singlet state are possible. The impurity site may be excited virtually to the states of 0 and 2 electrons at the impurity, and eventually to the triplet state with one electron at the impurity. As a consequence of these virtual excitations, the impurity is now polarizable. This is in analogy with virtual excitations in atoms, molecules and solids – the virtual excitations do not give rise to any real transitions, such as light absorption, but they change the polarization of the medium. In analogy with these system, the polarization of the impurity acts as an effective interaction between conduction electrons – first one electron passes by the impurity and polarizes it, and this polarization affects a second electron which passes by the impurity, just as optical phonons in solids. We identify the eigenstates of the system in this regime as those of our 'real' interacting system of the Fermi liquid theory.

We then assume that there is a one-to-one correspondence between the eigenstates of the 'ideal' $J \to \infty$ system and those of the 'real' system with J large but finite. For J large but finite, the state of the system is described by the distribution function n_α of quasi-particle scattering states, and all physical properties of the system are functionals of n_α.

The quasi-particles α are scattering states, which are described by phase shifts. We limit ourselves to s-wave scattering, so there is only one phase shift δ_α for each quasi-particle. The phase shift δ_α in general depends on the energy ϵ_α of the quasi-particle. In addition, because of the impurity-mediated effective interaction between the quasi-particles, the phase shift will also depend on the distribution n_β of all quasi-particles. The phase shift is then of the form

$$\delta_\alpha = \delta[\epsilon_\alpha, n_\beta]. \tag{34.3}$$

It is the phase shift of the quasi-particle that plays the role of the free energy in the conventional Fermi liquid theory. Consequently, we expand the phase shift in powers of the quasi-particle energy $\epsilon_\alpha - \mu$ and in the departure of the quasi-particle distribution from the ground state

$$\delta n_\beta \equiv n_\beta - n_\beta^{(0)}.$$

The expansion of the phase shift is then

$$\delta_\sigma(\epsilon) = \delta_0(\epsilon) + \sum_{\epsilon'\sigma'} \phi_{\epsilon\sigma,\epsilon'\sigma'} \delta n_{\sigma'}(\epsilon'). \tag{34.4}$$

We furthermore assume that all quantities are analytic near the Fermi surface, so we can expand

$$\delta_0(\epsilon) = \delta_0 + \alpha(\epsilon - \mu) + \dots \tag{34.5}$$

and

$$\phi_{\epsilon\sigma,\epsilon'\sigma'} = \phi_{\sigma\sigma'} + \dots \tag{34.6}$$

where we have carried out the expansion only to first order. The quantities δ_0, α and $\phi_{\sigma\sigma'}$ are numbers which permit a phenomenological description of the low-temperature behavior of the system. These numbers correspond to the parameters of the conventional Fermi liquid theory. Only the four quantities δ_0, α and $\phi_{\sigma,\pm\sigma} = \phi^s \pm \phi^a$ enter. Here we have defined symmetric and antisymmetric parts of $\phi_{\sigma\sigma'}$, in analogy with f^a and f^s. The total number of electrons is constant and ϕ^s never shows up. If we define

$$n_\uparrow - n_\downarrow = m$$

and sum over quasi-particles in equation (34.4), we obtain

$$\delta_\sigma(\epsilon) = \delta_0 + \alpha(\epsilon - \mu) + \sigma\phi^a m. \tag{34.7}$$

A theorem due to Fumi [41] relates the total energy of the impurity due to its interactions with the conduction electrons to the scattering phase shifts. From our point of view, the impurity causes an effective electron–electron interaction, so the energy of the impurity is expressed as a shift in the energies of the conduction electron, such that the sum of these shifts is equal to the total energy of the impurity. Fumi's theorem then states that the energy shifts are $-\delta_0/[\pi\nu'(0)]$. Here, $\nu'(0)$ is the density-of-states at the Fermi surface for one spin direction for an impurity-free system, *i.e.,* the number of electron states per unit energy at the Fermi surface (as opposed to our definition of $\nu(0)$ from before, which is the number of states per unit energy *and unit volume*). The quasi-particle energies due to the interactions are then

$$\widetilde{\epsilon}_\sigma = \epsilon - \frac{\delta_0}{\pi\nu'(0)}. \tag{34.8}$$

As a result of scattering off the impurity, new states will appear in the electron spectrum, for example, the bound singlet state. Consequently, there will be a change $\delta\nu'(0)$ in the density-of-state at the Fermi surface. By combining equation (34.7) and (34.8), we obtain this change as

$$\delta\nu'(0) = \nu'(0)\left[\frac{\partial\epsilon}{\partial\widetilde{\epsilon}} - 1\right] = \frac{\alpha}{\pi}. \tag{34.9}$$

The change in the density-of-states leads to a change δC_v in the specific heat

$$\frac{\delta C_v}{C_v} = \frac{\alpha}{\pi\nu'(0)}.$$

Measurement of the specific heat will thus yield α. Note that the change in C_v change is of order $1/N$, since we are studying the effects of a *single* impurity.

In the presence of an applied external magnetic field H, the quasi-particle energies will shift, depending on the orientation of the spin relative to the direction of the magnetic field (see equations (34.7) and (34.8)):

$$\begin{aligned}\tilde{\epsilon}_\uparrow &= \epsilon - g\mu_B H - \frac{\alpha(\epsilon-\mu)}{\pi\nu'(0)} - \frac{\phi^a}{\pi\nu'(0)}m\\ \tilde{\epsilon}_\downarrow &= \epsilon + g\mu_B H - \frac{\alpha(\epsilon-\mu)}{\pi\nu'(0)} + \frac{\phi^a}{\pi\nu'(0)}m.\end{aligned}$$

To first order in the magnetic field strength, the chemical potential remains unchanged, so the Fermi levels for the two spin directions must be equal to μ. The density of electrons with spin up induced by the magnetic field is then

$$n_\uparrow = -\tilde{\epsilon}_\uparrow \nu'(0)[1 + \frac{\delta\nu'(0)}{\nu'(0)}]$$

and the induced down-spin density is

$$n_\downarrow = -\tilde{\epsilon}_\downarrow \nu'(0)[1 + \frac{\delta\nu'(0)}{\nu'(0)}].$$

In these two expressions, we have taken into account the change in the density-of-states due to the impurity. We obtain the magnetization m from

$$m = n_\uparrow - n_\downarrow = \left[2g\mu_B H + \frac{2\phi^a}{\pi\nu'(0)}m\right]\nu'(0)\left[1 + \frac{\delta\nu'(0)}{\nu'(0)}\right]$$

with the result

$$\begin{aligned} m &= \frac{2g\mu_B H\nu'(0)\left[1+\frac{\alpha}{\pi\nu'(0)}\right]}{1-\frac{2\phi^a}{\pi\nu'(0)}\nu'(0)\left[1+\frac{\alpha}{\pi\nu'(0)}\right]}\\ &\approx \frac{2g\mu_B H\nu'(0)\left[1+\frac{\alpha}{\pi\nu'(0)}\right]}{1-\frac{2\phi^a}{\pi}}\\ &\approx 2g\mu_B H\nu'(0)\left[1+\frac{\alpha}{\pi\nu'(0)}+\frac{2\phi^a}{\pi}\right]\end{aligned}$$

where we used equation (34.9). The spin susceptibility is then

$$\chi = \frac{g\mu_B m}{H} = 2\nu'(0)\,(g\mu_B)^2\left[1+\frac{\alpha}{\pi\nu'(0)}+\frac{2\phi^a}{\pi}\right].$$

This result is easily understood. The terms in the bracket give the enhancement of the susceptibility. The term $\alpha/[\pi\nu'(0)]$ is an enhancement due to the increased density-of-states at the Fermi surface (equation (34.9)), and the term $2\phi^a/\pi$ comes from the impurity-mediated electron–electron interaction.

We have now obtained two expressions containing the two parameters α and ϕ^a. We would like to obtain an expression for a third property, which can then test the predictive powers of the theory. To this end, we will now calculate the zero-temperature conductivity of the system. In the end, we also want to calculate the low-temperature conductivity of the system, to verify that we obtain a conductivity which increases with temperature, consistent with a minimum in the resistivity at a finite temperature.

Because we are only including s-wave scattering, every collision restores angular momentum $\ell = 0$. The collision integral that enters the Boltzmann equation then takes the simple form

$$I(n) = -n_{1\sigma} W_\sigma(\epsilon),$$

where $n_1 = n - n_0(T)$ is the current carrying departure from thermal equilibrium and $W_\sigma(\epsilon)$ is the total relaxation rate of $n_\sigma(\epsilon)$, which includes relaxation both due to elastic and inelastic scattering. The conductivity is then directly found from the Boltzmann transport theory [37] as

$$\sigma = -\frac{\nu'(0)e^2 v_F^2}{3} \sum_\sigma \int \mathrm{d}\epsilon \, \frac{\partial f(\epsilon)/\partial \epsilon}{W_\sigma(\epsilon)}. \quad , \tag{34.10}$$

Here, $f(\epsilon)$ is the Fermi distribution function.

At zero temperature, only elastic scattering is possible. For elastic s-wave scattering, the relaxation rate can be found fairly easily in the following way. The scattering problem can be formulated in terms of the so-called T-matrix [43], defined as

$$T_{\mathbf{k}'\sigma',\mathbf{k}\sigma} = \int \mathrm{d}^3 r \, \varphi_{\mathbf{k}'\sigma'}(\mathbf{r})^* V_{\sigma,\sigma'}(r) \psi_{\mathbf{k}\sigma}(\mathbf{r}),$$

where $\varphi_{\mathbf{k}'\sigma'}$ is the incoming Bloch state, $\psi_{\mathbf{k}\sigma}$ is the exact wavefunction, and $V_{\sigma,\sigma'}(r)$ is the scattering potential. With outgoing-wave boundary conditions, the diagonal T-matrix is given in terms of the phase-shifts as

$$T_{k,k} = -\frac{1}{2mk} \mathrm{e}^{+i\delta_\ell(k)} \sin \delta_\ell(k).$$

The self-energy is related to the scattering matrix by

$$M(\mathbf{k}, \tilde{\omega}) = n_i T_{k,k} = -\frac{2\pi n_i}{mk} \sum_\ell (2\ell + 1) \mathrm{e}^{+i\delta_\ell(k)} \sin[\delta_\ell(k)] \tag{34.11}$$

where n_i is the impurity concentration. The relaxation rate is the magnitude of the imaginary part of the self-energy, so equation (34.11) gives

$$W_\sigma(\epsilon) = \frac{2n_i}{\pi \nu'(0)} \sin^2 \delta_\sigma(\epsilon).$$

In the absence of magnetic fields, $\delta_\sigma(\mu) = \delta_0$, so we obtain

$$\sigma(0) = \frac{1}{3}\frac{\pi\nu'(0)^2 v_F^2 e^2}{n_i \sin^2 \delta_0}.$$

We now consider the low-temperature conductivity $\sigma(T)$. At low, but finite, temperatures, the Fermi function in the expression (34.10) broadens over a range of width T. We consider only elastic scattering. We can use equation (34.10) directly, and we expand $\sin^2\delta(\epsilon)$ to order $(\epsilon-\mu)^2$. Unless $\delta \approx \pi/2$, such an expansion involves coefficients of higher order than given in equation (34.5). However, in the case of strong coupling and particle–hole symmetry, one can show that $\delta_0 \approx \pi/2$, so that the expansion yields

$$\sin^2\delta(\epsilon) = 1 - \alpha^2(\epsilon-\mu)^2$$

and we obtain for the conductivity

$$\frac{\sigma(T)}{\sigma(0)} = 1 + \frac{1}{3}\pi^2\alpha^2T^2. \tag{34.12}$$

The result (34.12) shows that the conductivity increases as the temperature increases from $T = 0$, consistent with a minimum in the resistivity at a finite temperature.

For a rigorous result, we should also consider inelastic scattering. In this case, processes in which one electron scatters off the impurity and excites one or several electron–hole pairs have to be included. We will not go through the actual calculation here. The result is the same as equation (34.12) for the case $\delta_0 \approx \frac{\pi}{2}$, with an additional term proportional to T^2, which arises from inelastic particle–particle scattering (see Nozières [31] for details).

We have then concluded our discussions of interacting many-particle systems. Our discussions have been on an introductory level, aimed at making the reader familiar with basic ideas and, by now, classical results, such as the Gell-Mann–Brueckner theory of the electron gas. There are, of course, many topics that we have not discussed at all. One important topic is density functional theory, which is a method (for extended systems essentially *the only* method) which can deal with inhomogeneous systems in a systematic way (see, for example, Dreizler and Gross [44]). Another topic is highly correlated electron systems, which are systems in which electron correlations dominate. As a consequence, approximations such as the random-phase approximation are inadequate. Other methods, for example variational methods using trial wavefunctions, provide a viable approach. The importance of such systems is illustrated by pointing out that they include the fractional quantum Hall effect (see Chakraborty and Pietiläinen [45]), heavy fermions and, most likely, high-temperature superconductors. It is our hope that the interested reader has at this point achieved a sufficient understanding of basic many-body theories to be able to turn to these more recent and still developing areas.

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