Exercises FYS-KJM4480

Exercise 1

Consider the Slater determinant

$$\Phi_{\lambda}^{AS}(x_1x_2\dots x_N;\alpha_1\alpha_2\dots\alpha_N)=\frac{1}{\sqrt{N!}}\sum_p(-)^pP\prod_{i=1}^N\psi_{\alpha_i}(x_i).$$

where P is an operator which permutes the coordinates of two particles. We have assumed here that the number of particles is the same as the number of available single-particle states, represented by the greek letters $\alpha_1\alpha_2\dots\alpha_N$.

a) Write out Φ^{AS} for $N=3$.

b) Show that

$$\int dx_1dx_2\dots dx_N\left|\Phi_{\lambda}^{AS}(x_1x_2\dots x_N;\alpha_1\alpha_2\dots\alpha_N)\right|^2=1.$$

c) Define a general onebody operator $\hat{F}=\sum_i^N\hat{f}(x_i)$ and a general twobody operator $\hat{G}=\sum_{i>j}^N\hat{g}(x_i,x_j)$ with g being invariant under the interchange of the coordinates of particles i and j. Calculate the matrix elements for a two-particle Slater determinant

$$\left\langle\Phi_{\alpha_1\alpha_2}^{AS}\right|\hat{F}\left|\Phi_{\alpha_1\alpha_2}^{AS}\right\rangle,$$

and

$$\left\langle\Phi_{\alpha_1\alpha_2}^{AS}\right|\hat{G}\left|\Phi_{\alpha_1\alpha_2}^{AS}\right\rangle.$$

Explain the short-hand notation for the Slater determinant. Which properties do you expect these operators to have in addition to an eventual permutation symmetry?

d) Compute the corresponding matrix elements for N particles which can occupy N single particle states.

Exercise 2

We will now consider a simple three-level problem, depicted in the figure below. The single-particle states are labelled by the quantum number p and can accomodate up to two single particles, viz., every single-particle state is doubly degenerate (you could think of this as one state having spin up and the other spin down). We let the spacing between the doubly degenerate single-particle states be constant, with value d. The first state has energy d. There are only three available single-particle states, $p=1$, $p=2$ and $p=3$, as illustrated in the figure.

a) How many two-particle Slater determinants can we construct in this space?

b) We limit ourselves to a system with only the two lowest single-particle orbits and two particles, $p=1$ and $p=2$. We assume that we can write the Hamiltonian as

$$\hat{H}=\hat{H}_0+\hat{H}_I,$$

and that the onebody part of the Hamiltonian with single-particle operator $\hat{h}_0$ has the property

$$\hat{h}_0\psi_{p\sigma}=p\times d\psi_{p\sigma},$$

where we have added a spin quantum number σ. We assume also that the only two-particle states that can exist are those where two particles are in the same state p, as shown by the two possibilities to the left in the figure. The two-particle matrix elements of $\hat{H}_I$ have all a constant value, $-g$. Show then that the Hamiltonian matrix

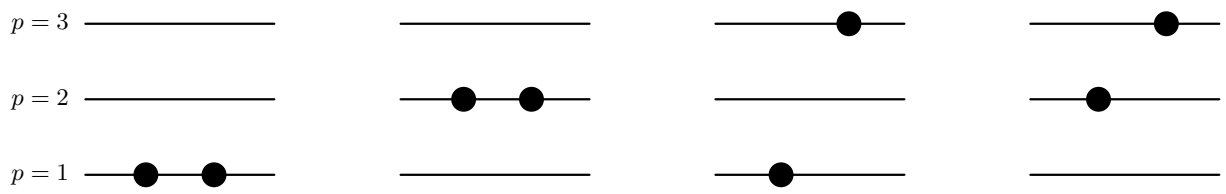


FIG. 1: Schematic plot of the possible single-particle levels with double degeneracy. The filled circles indicate occupied particle states. The spacing between each level p is constant in this picture. We show some possible two-particle states.

can be written as

$$\begin{pmatrix} 2d-g & -g \\ -g & 4d-g \end{pmatrix},$$

and find the eigenvalues and eigenvectors. What is mixing of the state with two particles in $p = 2$ to the wave function with two-particles in $p = 1$? Discuss your results in terms of a linear combination of Slater determinants.

c) Add the possibility that the two particles can be in the state with $p = 3$ as well and find the Hamiltonian matrix, the eigenvalues and the eigenvectors. We still insist that we only have two-particle states composed of two particles being in the same level p. You can diagonalize numerically your 3×3 matrix.

This simple model catches several birds with a stone. It demonstrates how we can build linear combinations of Slater determinants and interpret these as different admixtures to a given state. It represents also the way we are going to interpret these contributions. The two-particle states above $p = 1$ will be interpreted as excitations from the ground state configuration, $p = 1$ here. The reliability of this ansatz for the ground state, with two particles in $p = 1$, depends on the strength of the interaction g and the single-particle spacing d. Finally, this model is a simple schematic ansatz for studies of pairing correlations and thereby superfluidity/superconductivity in fermionic systems.

Exercise 3

Calculate the matrix elements

$$\langle \alpha_1 \alpha_2 | \hat{F} | \alpha_1 \alpha_2 \rangle$$

and

$$\langle \alpha_1 \alpha_2 | \hat{G} | \alpha_1 \alpha_2 \rangle$$

with

$$|\alpha_1 \alpha_2\rangle = a^\dagger_{\alpha_1} a^\dagger_{\alpha_2} |0\rangle ,$$

$$\hat{F} = \sum_{\alpha\beta} \langle \alpha | f | \beta \rangle \, a^\dagger_\alpha a_\beta,$$

$$\langle \alpha | f | \beta \rangle = \int \psi^*_\alpha(x) f(x) \psi_\beta(x) dx,$$

$$\hat{G} = \frac{1}{2}\sum_{\alpha\beta\gamma\delta} \langle\alpha\beta|\, g\, |\gamma\delta\rangle\, a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma,$$

and

$$\langle\alpha\beta|\, g\, |\gamma\delta\rangle = \int\int \psi^*_\alpha(x_1)\psi^*_\beta(x_2) g(x_1,x_2)\psi_\gamma(x_1)\psi_\delta(x_2) dx_1 dx_2$$

Compare these results with those from exercise 1c).

Exercise 4

We define the one-particle operator

$$\hat{T} = \sum_{\alpha\beta} \langle\alpha|\, t\, |\beta\rangle\, a^\dagger_\alpha a_\beta,$$

and the two-particle operator

$$\hat{V} = \frac{1}{2}\sum_{\alpha\beta\gamma\delta} \langle\alpha\beta|\, v\, |\gamma\delta\rangle\, a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma.$$

We have defined a single-particle basis with quantum numbers given by the set of greek letters $\alpha, \beta, \gamma, \ldots$ Show that the form of these operators remain unchanged under a transformation of the single-particle basis given by

$$|i\rangle = \sum_\lambda |\lambda\rangle\, \langle\lambda|i\rangle\,,$$

with $\lambda \in \{\alpha, \beta, \gamma, \ldots\}$. Show also that $a^\dagger_i a_i$ is the number operator for the orbital $|i\rangle$.

Find also the expressions for the operators T and V when T is diagonal in the representation i.

Show also that the operator

$$\hat{N}_p = \frac{1}{2}\sum_{\alpha\neq\beta} a^\dagger_\alpha a^\dagger_\beta a_\beta a_\alpha,$$

is an operator that represents the number of pairs. Can you rewrite the operators for $\hat{T}$ and $\hat{V}$ in terms of the above number operator?

Exercise 5

Consider the Hamilton operator for a harmonic oscillator ($c = \hbar = 1$)

$$\hat{H} = \frac{1}{2m}p^2 + \frac{1}{2}kx^2, \qquad k = m\omega^2$$

a) Define the operators

$$a^\dagger = \frac{1}{\sqrt{2m\omega}}(p + im\omega x), \qquad a = \frac{1}{\sqrt{2m\omega}}(p - im\omega x)$$

and find the commutation relations for these operators by using the corresponding relations for p and x.

b) Show that

$$H = \omega(a^\dagger a + \frac{1}{2})$$

c) Show that if for a state $|0\rangle$ which satisfies $\hat{H}\,|0\rangle = \frac{1}{2}\omega\,|0\rangle$, then we have

$$\hat{H}\,|n\rangle = \hat{H}(a^\dagger)^n\,|0\rangle = (n+\frac{1}{2})\omega\,|n\rangle$$

d) Show that the state $|0\rangle$ from c), with the property $a\,|0\rangle = 0$, must exist.

e) Find the coordinate-space representation of $|0\rangle$ and explain how you would construct the wave functions for excited states based on this state.

Exercise 6

Starting with the Slater determinant

$$\Phi_0 = \prod_{i=1}^{n} a^\dagger_{\alpha_i}\,|0\rangle\,,$$

use Wick's theorem to compute the normalization integral $<\Phi_0|\Phi_0>$.

Exercise 7

Compute the matrix element

$$\langle\alpha_1\alpha_2\alpha_3|\,G\,|\alpha'_1\alpha'_2\alpha'_3\rangle$$

using Wick's theorem and express the two-body operator G (from exercise 1) in the occupation number (second quantization) representation.

Exercise 8

Write the two-particle operator

$$G = \frac{1}{4}\sum_{\alpha\beta\gamma\delta}\langle\alpha\beta|\,g\,|\gamma\delta\rangle\,a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma$$

in the quasi-particle representation for particles and holes

$$b^\dagger_\alpha = \begin{cases} a^\dagger_\alpha \\ a_\alpha \end{cases} \qquad b_\alpha = \begin{cases} a_\alpha & \alpha > \alpha_F \\ a^\dagger_\alpha & \alpha \le \alpha_F \end{cases}$$

The two-body matrix elements are antisymmetric.

Exercise 9

Use the results from exercise 8 and Wick's theorem to calculate

$$\left\langle\beta_1\gamma_1^{-1}\right|\,G\,\left|\beta_2\gamma_2^{-1}\right\rangle$$

You need to consider that case that β_1 be equal β_2 and that γ_1 be equal γ_2.

Exercise 10

Show that the onebody part of the Hamiltonian

$$\hat{H}_0 = \sum_{pq} \langle p| \hat{h}_0 |q\rangle \, a_p^\dagger a_q$$

can be written, using standard annihilation and creation operators, in normal-ordered form as

$$\begin{aligned}\hat{H}_0 &= \sum_{pq} \langle p| \hat{h}_0 |q\rangle \, a_p^\dagger a_q \\ &= \sum_{pq} \langle p| \hat{h}_0 |q\rangle \left\{a_p^\dagger a_q\right\} + \delta_{pq\in i} \sum_{pq} \langle p| \hat{h}_0 |q\rangle \\ &= \sum_{pq} \langle p| \hat{h}_0 |q\rangle \left\{a_p^\dagger a_q\right\} + \sum_{i} \langle i| \hat{h}_0 |i\rangle\end{aligned}$$

Explain the meaning of the various symbols. Which reference vacuum has been used?

Exercise 11

Show that the twobody part of the Hamiltonian

$$\hat{H}_I = \frac{1}{4} \sum_{pqrs} \langle pq| \hat{v} |rs\rangle \, a_p^\dagger a_q^\dagger a_s a_r$$

can be written, using standard annihilation and creation operators, in normal-ordered form as

$$\begin{aligned}\hat{H}_I &= \frac{1}{4} \sum_{pqrs} \langle pq| \hat{v} |rs\rangle \, a_p^\dagger a_q^\dagger a_s a_r \\ &= \frac{1}{4} \sum_{pqrs} \langle pq| \hat{v} |rs\rangle \left\{a_p^\dagger a_q^\dagger a_s a_r\right\} + \sum_{pqi} \langle pi| \hat{v} |qi\rangle \left\{a_p^\dagger a_q\right\} + \frac{1}{2} \sum_{ij} \langle ij| \hat{v} |ij\rangle\end{aligned}$$

Explain again the meaning of the various symbols.

Derive the normal-ordered form of the threebody part of the Hamiltonian.

$$\hat{H}_3 = \frac{1}{36} \sum_{\substack{pqr \\ stu}} \langle pqr| \hat{v}_3 |stu\rangle \, a_p^\dagger a_q^\dagger a_r^\dagger a_u a_t a_s$$

and specify the contributions to the twobody, onebody and the scalar part.

Exercise 12

a) Place indices and write the algebraic expressions and discuss the physical meaning of the following diagrams:

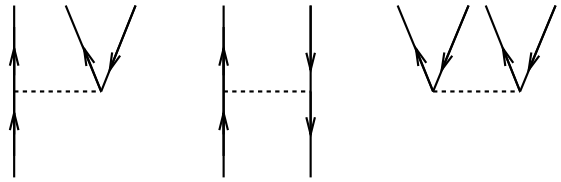


FIG. 2: Examples of diagrams.

b) Can you find the diagrammatic expression for $\langle c| \hat{H}_I |c\rangle$ using the normal-ordered form from the previous exercise?

Exercise 13

In this exercise we will develop two simple models for studying the helium atom (with two electrons) and the beryllium atom with four electrons.

After having introduced the Born-Oppenheimer approximation which effectively freezes out the nucleonic degrees of freedom, the Hamiltonian for N electrons takes the following form

$$\hat{H} = \sum_{i=1}^{N} t(x_i) - \sum_{i=1}^{N} k\frac{Ze^2}{r_i} + \sum_{i<j}^{N} \frac{ke^2}{r_{ij}},$$

with $k = 1.44$ eVnm. We will use atomic units, this means that $\hbar = c = e = m_e = 1$. The constant k becomes also equal 1. The resulting energies have to be multiplied by 2×13.6 eV in order to obtain energies in eletronvolts.

We can rewrite our Hamiltonians as

$$\hat{H} = \hat{H}_0 + \hat{H}_I = \sum_{i=1}^{N} \hat{h}_0(x_i) + \sum_{i<j}^{N} \frac{1}{r_{ij}}, \tag{1}$$

where we have defined $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$ and $\hat{h}_0(x_i) = \hat{t}(x_i) - \frac{Z}{r_i}$ The variable x contains both the spatial coordinates and the spin values. The first term of Eq. (1), H_0, is the sum of the N *one-body* Hamiltonians $\hat{h}_0$. Each individual Hamiltonian $\hat{h}_0$ contains the kinetic energy operator of an electron and its potential energy due to the attraction of the nucleus. The second term, H_I, is the sum of the $N(N-1)/2$ two-body interactions between each pair of electrons. Note that the double sum carries a restriction $i < j$.

As basis functions for our calculations we will use hydrogen-like single-particle functions. This means the onebody operator is diagonal in this basis for states i, j with quantum numbers $nlm_l sm_s$ with energies

$$\langle i|\hat{h}_0|j\rangle = -Z^2/2n^2\delta_{i,j}.$$

The quantum number n refers to the number of nodes of the wave function. Observe that this expectation value is independent of spin.

We will in all calculations here restrict ourselves to only so-called s -waves, that is the orbital momentum l is zero. We will also limit the quantum number n to $n \leq 3$. It means that every ns state can accomodate two electrons due to the spin degeneracy. This is illustrated in Fig. 3 here.

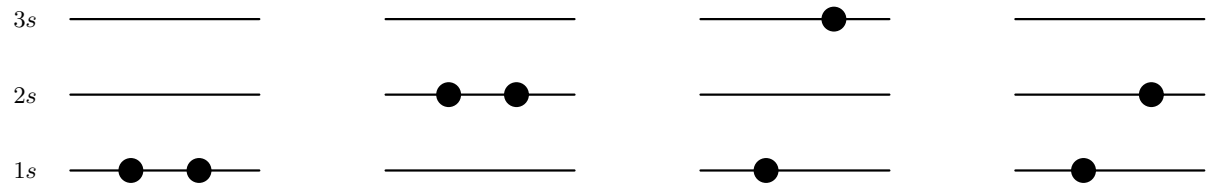


FIG. 3: Schematic plot of the possible single-particle levels with double degeneracy. The filled circles indicate occupied particle states. We show some possible two-particle states which can describe states in the helium atom.

In the calculations you will need the Coulomb interaction with matrix elements involving single-particle wave functions with $l = 0$ only, the so-called s-waves. We need only the radial part since the spherical harmonics for the s-waves are rather simple. We omit single-particle states with $l > 0$. Our radial wave functions are

$$R_{n0}(r) = \left(\frac{2Z}{n}\right)^{3/2} \sqrt{\frac{(n-1)!}{2n \times n!}} L^1_{n-1}(\frac{2Zr}{n}) \exp{(-\frac{Zr}{n})},$$

where $L^1_{n-1}(r)$ are the so-called Laguerre polynomials. These wave functions can then be used to compute the direct part of the Coulomb interaction

$$\langle\alpha\beta|V|\gamma\delta\rangle = \int r_1^2 dr_1 \int r_2^2 dr_2 R^*_{n_\alpha 0}(r_1) R^*_{n_\beta 0}(r_2) \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} R_{n_\gamma 0}(r_1) R_{n_\delta 0}(r_2)$$

Observe that this is only the radial integral and that the labels $\alpha\beta\gamma\delta$ refer only to the quantum numbers nlm_l, with m_l the projection of the orbital momentum l. A similar expression can be found for the exchange part. Since we have restricted ourselves to only s-waves, these integrals are straightforward but tedious to calculate. As an addendum to this exercise we list all closed-form expressions for the relevant matrix elements. Note well that these matrix elements do not include spin. When setting up the final antisymmetrized matrix elements you need to consider the spin degrees of freedom as well. Please pay in particular special attention to the exchange part and the pertinent spin values of the single-particle states.

We will also, for both helium and beryllium assume that the many-particle states we construct have always the same total spin projection $M_S = 0$. This means that if we excite one or two particles from the ground state, the spins of the various single-particle states should always sum up to zero.

a) We start with the helium atom and define our single-particle Hilbert space to consist of the single-particle orbits $1s$, $2s$ and $3s$, with their corresponding spin degeneracies, see Fig. 3.

   Set up the ansatz for the ground state $|c\rangle = |\Phi_0\rangle$ in second quantization and define a table of single-particle states. Construct thereafter all possible one-particle-one-hole excitations $|\Phi_i^a\rangle$ where i refer to levels below the Fermi level (define this level) and a refers to particle states. Define particles and holes. The Slater determinants have to be written in terms of the respective creation and annihilation operators. The states you construct should all have total spin projection $M_S = 0$. Construct also all possible two-particle-two-hole states $|\Phi_{ij}^{ab}\rangle$ in a second quantization representation.

b) Define the Hamiltonian in a second-quantized form and use this to compute the expectation value of the ground state (defining the so-called reference energy of the helium atom. Show that it is given by

$$E[\Phi_0] = \langle c|\hat{H}|c\rangle = \sum_i \langle i|\hat{h}_0|i\rangle + \frac{1}{2}\sum_{ij}\left[\langle ij|\frac{1}{r}|ij\rangle - \langle ij|\frac{1}{r}|ji\rangle\right].$$

   Define properly the sums keeping in mind that the states ij refer to all quantum numbers nlm_lsm_s. Use the values for the various matrix elements listed at the end of the exercise to find the value of E as function of $Z = 2$. Be careful when you set up the matrix elements. Pay in particular attention to the spin values.

c) Hereafter we will limit ourselves to a system which now contains only one-particle-one-hole excitations beyond the chosen state $|c\rangle$. Using the possible Slater determinants from exercise a) for the helium atom, compute also the expectation values (without inserting the explicit values for the matrix elements first) of

$$\langle c|\hat{H}|\Phi_i^a\rangle,$$

   and

$$\langle \Phi_i^a|\hat{H}|\Phi_j^b\rangle.$$

   Represent these expectation values in a diagrammatic form, both for the onebody part and the two-body part of the Hamiltonian.

   Insert then the explicit values for the various matrix elements and set up the final Hamiltonian matrix and diagonalize it using for example Octave, Matlab, Python, C++ or Fortran as programming tools.

   Compare your results from those of exercise b) and comment your results. The exact energy with our Hamiltonian is -2.9037 atomic units for helium. This value is also close to the experimental energy.

d) We repeat exercises b) and c) but now for the beryllium atom. Define the ansatz for $|c\rangle$ and limit yourself again to one-particle-one-hole excitations. Compute the reference energy $\langle c|\hat{H}|c\rangle$ for $Z = 4$. Thereafter you will need to set up the appropriate Hamiltonian matrix which involves also one-particle-one-hole excitations. Diagonalize this matrix and compare your eigenvalues with $\langle c|\hat{H}|c\rangle$ for $Z = 4$ and comment your results. The exact energy with our Hamiltonian is -14.6674 atomic units for beryllium. This value is again close to the experimental energy.

We conclude by listing in Table I the matrix elements for the radial integrals to be used for the direct part and the exchange part. Note again that these integrals do not include spin.

TABLE I: Closed form expressions for the Coulomb matrix elements. The nomenclature is $1 = 1s$, $2 = 2s$ and $3 = 3s$, with no spin degrees of freedom.

$\langle 11\|V\|11\rangle =$	$(5Z)/8$	$\langle 11\|V\|12\rangle =$	$(4096\sqrt{2}Z)/64827$
$\langle 11\|V\|13\rangle =$	$(1269\sqrt{3}Z)/50000$	$\langle 11\|V\|21\rangle =$	$(4096\sqrt{2}Z)/64827$
$\langle 11\|V\|22\rangle =$	$(16Z)/729$	$\langle 11\|V\|23\rangle =$	$(110592\sqrt{6}Z)/24137569$
$\langle 11\|V\|31\rangle =$	$(1269\sqrt{3}Z)/50000$	$\langle 11\|V\|32\rangle =$	$(110592\sqrt{6}Z)/24137569$
$\langle 11\|V\|33\rangle =$	$(189Z)/32768$	$\langle 12\|V\|11\rangle =$	$(4096\sqrt{2}Z)/64827$
$\langle 12\|V\|12\rangle =$	$(17Z)/81$	$\langle 12\|V\|13\rangle =$	$(1555918848\sqrt{6}Z)/75429903125$
$\langle 12\|V\|21\rangle =$	$(16Z)/729$	$\langle 12\|V\|22\rangle =$	$(512\sqrt{2}Z)/84375$
$\langle 12\|V\|23\rangle =$	$(2160\sqrt{3}Z)/823543$	$\langle 12\|V\|31\rangle =$	$(110592\sqrt{6}Z)/24137569$
$\langle 12\|V\|32\rangle =$	$(29943\sqrt{3}Z)/13176688$	$\langle 12\|V\|33\rangle =$	$(1216512\sqrt{2}Z)/815730721$
$\langle 13\|V\|11\rangle =$	$(1269\sqrt{3}Z)/50000$	$\langle 13\|V\|12\rangle =$	$(1555918848\sqrt{6}Z)/75429903125$
$\langle 13\|V\|13\rangle =$	$(815Z)/8192$	$\langle 13\|V\|21\rangle =$	$(110592\sqrt{6}Z)/24137569$
$\langle 13\|V\|22\rangle =$	$(2160\sqrt{3}Z)/823543$	$\langle 13\|V\|23\rangle =$	$(37826560\sqrt{2}Z)/22024729467$
$\langle 13\|V\|31\rangle =$	$(189Z)/32768$	$\langle 13\|V\|32\rangle =$	$(1216512\sqrt{2}Z)/815730721$
$\langle 13\|V\|33\rangle =$	$(617Z)/(314928\sqrt{3})$	$\langle 21\|V\|11\rangle =$	$(4096\sqrt{2}Z)/64827$
$\langle 21\|V\|12\rangle =$	$(16Z)/729$	$\langle 21\|V\|13\rangle =$	$(110592\sqrt{6}Z)/24137569$
$\langle 21\|V\|21\rangle =$	$(17Z)/81$	$\langle 21\|V\|22\rangle =$	$(512\sqrt{2}Z)/84375$
$\langle 21\|V\|23\rangle =$	$(29943\sqrt{3}Z)/13176688$	$\langle 21\|V\|31\rangle =$	$(1555918848\sqrt{6}Z)/75429903125$
$\langle 21\|V\|32\rangle =$	$(2160\sqrt{3}Z)/823543$	$\langle 21\|V\|33\rangle =$	$(1216512\sqrt{2}Z)/815730721$
$\langle 22\|V\|11\rangle =$	$(16Z)/729$	$\langle 22\|V\|12\rangle =$	$(512\sqrt{2}Z)/84375$
$\langle 22\|V\|13\rangle =$	$(2160\sqrt{3}Z)/823543$	$\langle 22\|V\|21\rangle =$	$(512\sqrt{2}Z)/84375$
$\langle 22\|V\|22\rangle =$	$(77Z)/512$	$\langle 22\|V\|23\rangle =$	$(5870679552\sqrt{6}Z)/669871503125$
$\langle 22\|V\|31\rangle =$	$(2160\sqrt{3}Z)/823543$	$\langle 22\|V\|32\rangle =$	$(5870679552\sqrt{6}Z)/669871503125$
$\langle 22\|V\|33\rangle =$	$(73008Z)/9765625$	$\langle 23\|V\|11\rangle =$	$(110592\sqrt{6}Z)/24137569$
$\langle 23\|V\|12\rangle =$	$(2160\sqrt{3}Z)/823543$	$\langle 23\|V\|13\rangle =$	$(37826560\sqrt{2}Z)/22024729467$
$\langle 23\|V\|21\rangle =$	$(29943\sqrt{3}Z)/13176688$	$\langle 23\|V\|22\rangle =$	$(5870679552\sqrt{6}Z)/669871503125$
$\langle 23\|V\|23\rangle =$	$(32857Z)/390625$	$\langle 23\|V\|31\rangle =$	$(1216512\sqrt{2}Z)/815730721$
$\langle 23\|V\|32\rangle =$	$(73008Z)/9765625$	$\langle 23\|V\|33\rangle =$	$(6890942464\sqrt{2/3}Z)/1210689028125$
$\langle 31\|V\|11\rangle =$	$(1269\sqrt{3}Z)/50000$	$\langle 31\|V\|12\rangle =$	$(110592\sqrt{6}Z)/24137569$
$\langle 31\|V\|13\rangle =$	$(189Z)/32768$	$\langle 31\|V\|21\rangle =$	$(1555918848\sqrt{6}Z)/75429903125$
$\langle 31\|V\|22\rangle =$	$(2160\sqrt{3}Z)/823543$	$\langle 31\|V\|23\rangle =$	$(1216512\sqrt{2}Z)/815730721$
$\langle 31\|V\|31\rangle =$	$(815Z)/8192$	$\langle 31\|V\|32\rangle =$	$(37826560\sqrt{2}Z)/22024729467$
$\langle 31\|V\|33\rangle =$	$(617Z)/(314928\sqrt{3})$	$\langle 32\|V\|11\rangle =$	$(110592\sqrt{6}Z)/24137569$
$\langle 32\|V\|12\rangle =$	$(29943\sqrt{3}Z)/13176688$	$\langle 32\|V\|13\rangle =$	$(1216512\sqrt{2}Z)/815730721$
$\langle 32\|V\|21\rangle =$	$(2160\sqrt{3}Z)/823543$	$\langle 32\|V\|22\rangle =$	$(5870679552\sqrt{6}Z)/669871503125$
$\langle 32\|V\|23\rangle =$	$(73008Z)/9765625$	$\langle 32\|V\|31\rangle =$	$(37826560\sqrt{2}Z)/22024729467$
$\langle 32\|V\|32\rangle =$	$(32857Z)/390625$	$\langle 32\|V\|33\rangle =$	$(6890942464\sqrt{2/3}Z)/1210689028125$
$\langle 33\|V\|11\rangle =$	$(189Z)/32768$	$\langle 33\|V\|12\rangle =$	$(1216512\sqrt{2}Z)/815730721$
$\langle 33\|V\|13\rangle =$	$(617Z)/(314928\sqrt{3})$	$\langle 33\|V\|21\rangle =$	$(1216512\sqrt{2}Z)/815730721$
$\langle 33\|V\|22\rangle =$	$(73008Z)/9765625$	$\langle 33\|V\|23\rangle =$	$(6890942464\sqrt{2/3}Z)/1210689028125$
$\langle 33\|V\|31\rangle =$	$(617Z)/(314928\sqrt{3})$	$\langle 33\|V\|32\rangle =$	$(6890942464\sqrt{2/3}Z)/1210689028125$
$\langle 33\|V\|33\rangle =$	$(17Z)/256$		

Exercise 14

Consider a Slater determinant built up of single-particle orbitals ψ_λ, with $\lambda = 1, 2, \ldots, N$.
The unitary transformation

$$\psi_a = \sum_\lambda C_{a\lambda}\phi_\lambda,$$

brings us into the new basis. The new basis has quantum numbers $a = 1, 2, \ldots, N$. Show that the new basis is orthonormal. Show that the new Slater determinant constructed from the new single-particle wave functions can be written as the determinant based on the previous basis and the determinant of the matrix C. Show that the old and the new Slater determinants are equal up to a complex constant with absolute value unity. (Hint, C is a unitary matrix).

Exercise 15

Consider the Slater determinant

$$\Phi_0 = \frac{1}{\sqrt{n!}} \sum_p (-)^p P \prod_{i=1}^{n} \psi_{\alpha_i}(x_i).$$

A small variation in this function is given by

$$\delta\Phi_0 = \frac{1}{\sqrt{n!}} \sum_p (-)^p P \psi_{\alpha_1}(x_1)\psi_{\alpha_2}(x_2)\dots\psi_{\alpha_{i-1}}(x_{i-1})(\delta\psi_{\alpha_i}(x_i))\psi_{\alpha_{i+1}}(x_{i+1})\dots\psi_{\alpha_n}(x_n).$$

Show that

$$\langle\delta\Phi_0| \sum_{i=1}^{n} \{t(x_i) + u(x_i)\} + \frac{1}{2} \sum_{i\neq j=1}^{n} v(x_i, x_j) |\Phi_0\rangle =$$

$$\sum_{i=1}^{n} \langle\delta\psi_{\alpha_i}| t + u |\phi_{\alpha_i}\rangle + \sum_{i\neq j=1}^{n} \left\{ \left\langle \delta\psi_{\alpha_i}\psi_{\alpha_j} \right| v \left| \psi_{\alpha_i}\psi_{\alpha_j} \right\rangle - \left\langle \delta\psi_{\alpha_i}\psi_{\alpha_j} \right| v \left| \psi_{\alpha_j}\psi_{\alpha_i} \right\rangle \right\}$$

Exercise 16

What is the diagrammatic representation of the HF equation?

$$-\langle\alpha_k| u^{HF} |\alpha_i\rangle + \sum_{j=1}^{n} [\langle\alpha_k\alpha_j| v |\alpha_i\alpha_j\rangle - \langle\alpha_k\alpha_j| v |\alpha_j\alpha_i\rangle] = 0 \quad ?$$

(Represent $(-u^{HF})$ by the symbol $---$X .)

Exercise 17

Consider the ground state $|\Phi\rangle$ of a bound many-particle system of fermions. Assume that we remove one particle from the single-particle state λ and that our system ends in a new state $|\Phi_n\rangle$. Define the energy needed to remove this particle as

$$\mathcal{E}_\lambda = \sum_n |\langle\Phi_n| a_\lambda |\Phi\rangle|^2 (E_0 - E_n),$$

where E_0 and E_n are the ground state energies of the states $|\Phi\rangle$ and $|\Phi_n\rangle$, respectively.
a) Show that

$$\mathcal{E}_\lambda = \langle\Phi| a_\lambda^\dagger [a_\lambda, H] |\Phi\rangle,$$

where H is the Hamiltonian of this system.
b) If we assume that Φ is the Hartree-Fock result, find the relation between $\mathcal{E}_\lambda$ and the single-particle energy ε_λ for states $\lambda \leq F$ and $\lambda > F$, with

$$\varepsilon_\lambda = \langle\lambda| (t + u) |\lambda\rangle$$

and

$$\langle\lambda| u |\lambda\rangle = \sum_{\beta\leq F} \langle\lambda\beta| v |\lambda\beta\rangle.$$

We have assumed an antisymmetrized matrix element here. Discuss the result.

The Hamiltonian operator is defined as

$$H = \sum_{\alpha\beta} \langle\alpha| t |\beta\rangle a_\alpha^\dagger a_\beta + \frac{1}{2} \sum_{\alpha\beta\gamma\delta} \langle\alpha\beta| v |\gamma\delta\rangle a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma.$$

Exercise 18

The electron gas model allows closed form solutions for quantities like the single-particle Hartree-Fock energy. The latter quantity is given by the following expression

$$\varepsilon_k^{HF} = \frac{\hbar^2 k^2}{2m} - \frac{e^2}{V^2} \sum_{k' \leq k_F} \int d\vec{r} e^{i(\vec{k'}-\vec{k})\vec{r}} \int d\vec{r'} \frac{e^{i(\vec{k}-\vec{k'})\vec{r'}}}{|\vec{r}-\vec{r'}|}$$

a) Show that

$$\varepsilon_k^{HF} = \frac{\hbar^2 k^2}{2m} - \frac{e^2 k_F}{2\pi} \left[2 + \frac{k_F^2 - k^2}{k k_F} ln \left| \frac{k+k_F}{k-k_F} \right| \right]$$

(Hint: Introduce the convergence factor $e^{-\mu|\vec{r}-\vec{r'}|}$ in the potential and use $\sum_{\vec{k}} \rightarrow \frac{V}{(2\pi)^3} \int d\vec{k}$)
b) Rewrite the above result as a function of the density

$$n = \frac{k_F^3}{3\pi^2} = \frac{3}{4\pi r_s^3},$$

where $n = N/V$, N being the number of particles, and r_s is the radius of a sphere which represents the volum per conducting electron. It can be convenient to use the Bohr radius $a_0 = \hbar^2/e^2 m$.

For most metals we have a relation $r_s/a_0 \sim 2-6$.

Make a plot of the free electron energy and the Hartree-Fock energy and discuss the behavior around the Fermi surface. Extract also the Hartree-Fock band width $\Delta\varepsilon^{HF}$ defined as

$$\Delta\varepsilon^{HF} = \varepsilon_{k_F}^{HF} - \varepsilon_0^{HF}.$$

Compare this results with the corresponding one for a free electron and comment your results. How large is the contribution due to the exchange term in the Hartree-Fock equation?
c) We will now define a quantity called the effective mass. For $|\vec{k}|$ near k_F, we can Taylor expand the Hartree-Fock energy as

$$\varepsilon_k^{HF} = \varepsilon_{k_F}^{HF} + \left(\frac{\partial \varepsilon_k^{HF}}{\partial k} \right)_{k_F} (k - k_F) + \ldots$$

If we compare the latter with the corresponding expressiyon for the non-interacting system

$$\varepsilon_k^{(0)} = \frac{\hbar^2 k_F^2}{2m} + \frac{\hbar^2 k_F}{m} (k - k_F) + \ldots,$$

we can define the so-called effective Hartree-Fock mass as

$$m_{HF}^* \equiv \hbar^2 k_F \left(\frac{\partial \varepsilon_k^{HF}}{\partial k} \right)_{k_F}^{-1}$$

Compute m_{HF}^* and comment your results after you have done point d).
d) Show that the level density (the number of single-electron states per unit energy) can be written as

$$n(\varepsilon) = \frac{V k^2}{2\pi^2} \left(\frac{\partial \varepsilon}{\partial k} \right)^{-1}$$

Calculate $n(\varepsilon_F^{HF})$ and comment the results from c) and d).

Exercise 19

We consider a system of electrons in infinite matter, the so-called electron gas. This is a homogeneous system and the one-particle states are given by plane wave function normalized to a volume Ω for a box with length L (the limit $L \rightarrow \infty$ is to be taken after we have computed various expectation values)

$$\psi_{\mathbf{k}\sigma}(\mathbf{r}) = \frac{1}{\sqrt{\Omega}} \exp(i\mathbf{k}\mathbf{r}) \xi_\sigma$$

where $\mathbf{k}$ is the wave number and ξ_σ is a spin function for either spin up or down

$$\xi_{\sigma=+1/2} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad \xi_{\sigma=-1/2} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

We assume that we have periodic boundary conditions which limit the allowed wave numbers to

$$k_i = \frac{2\pi n_i}{L} \qquad i = x, y, z \qquad n_i = 0, \pm 1, \pm 2, \ldots$$

We assume first that the particles interact via a central, symmetric and translationally invariant interaction $V(r_{12})$ with $r_{12} = |\mathbf{r}_1 - \mathbf{r}_2|$. The interaction is spin independent.

The total Hamiltonian consists then of kinetic and potential energy

$$\hat{H} = \hat{T} + \hat{V}.$$

a) Show that the operator for the kinetic energy can be written as

$$\hat{T} = \sum_{\mathbf{k}\sigma} \frac{\hbar^2 k^2}{2m} a^\dagger_{\mathbf{k}\sigma} a_{\mathbf{k}\sigma}.$$

Find also the number operator $\hat{N}$ and find a corresponding expression for the interaction $\hat{V}$ expressed with creation and annihilation operators. The expression for the interaction has to be written in k space, even though V depends only on the relative distance. It means that you ned to set up the Fourier transform $\langle \mathbf{k}_i \mathbf{k}_j | V | \mathbf{k}_m \mathbf{k}_n \rangle$.

b) We assume that $V(r_{12}) < 0$ kand that the integral $\int |V(x)| d^3x < \infty$.

Use the operator form for $\hat{H}$ from the previous exercise and calculate $E_0 = \langle \Phi_0 | H | \Phi_0 \rangle$ for this system to first order in perturbation theory and express the result as a function of the density $\rho = N/\Omega$. The state $|\Phi_0\rangle$ is a Slater determinant determined by filling all states up to Fermi level. Show that the system will collapse (you wil not be able to find an energy minimum). Comment your results.

c) We will now study the electron gas. The Hamilton operator is given by

$$\hat{H} = \hat{H}_{el} + \hat{H}_b + \hat{H}_{el-b},$$

with the electronic part

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

where we have introduced an explicit convergence factor (the limit $\mu \to 0$ is performed after having calculated the various integrals). Correspondingly, we have

$$\hat{H}_b = \frac{e^2}{2} \int\int d\mathbf{r} d\mathbf{r}' \frac{n(\mathbf{r}) n(\mathbf{r}') e^{-\mu|\mathbf{r} - \mathbf{r}'|}}{|\mathbf{r} - \mathbf{r}'|},$$

which is the energy contribution from the positive background charge with density $n(\mathbf{r}) = N/\Omega$. Finally,

$$\hat{H}_{el-b} = -\frac{e^2}{2} \sum_{i=1}^{N} \int d\mathbf{r} \frac{n(\mathbf{r}) e^{-\mu|\mathbf{r} - \mathbf{x}_i|}}{|\mathbf{r} - \mathbf{x}_i|},$$

is the interaction between the electrons and the positive background.

Show that

$$\hat{H}_b = \frac{e^2}{2} \frac{N^2}{\Omega} \frac{4\pi}{\mu^2},$$

and

$$\hat{H}_{el-b} = -e^2 \frac{N^2}{\Omega} \frac{4\pi}{\mu^2}.$$

Show thereafter that the final Hamiltonian can be written as

$$H = H_0 + H_I,$$

with

$$H_0 = \sum_{\mathbf{k}\sigma} \frac{\hbar^2 k^2}{2m} a^\dagger_{\mathbf{k}\sigma} a_{\mathbf{k}\sigma},$$

and

$$H_I = \frac{e^2}{2\Omega} \sum_{\sigma_1\sigma_2} \sum_{\mathbf{q}\neq 0,\mathbf{k},\mathbf{p}} \frac{4\pi}{q^2} a^\dagger_{\mathbf{k}+\mathbf{q},\sigma_1} a^\dagger_{\mathbf{p}-\mathbf{q},\sigma_2} a_{\mathbf{p}\sigma_2} a_{\mathbf{k}\sigma_1}.$$

d) Calculate $E_0/N = \langle \Phi_0 | H | \Phi_0 \rangle / N$ for for this system to first order in the interaction. Show that, by using

$$\rho = \frac{k_F^3}{3\pi^2} = \frac{3}{4\pi r_0^3},$$

with $\rho = N/\Omega$, r_0 being the radius of a sphere representing the volume an electron occupies and the Bohr radius $a_0 = \hbar^2/e^2 m$, that the energy per electron can be written as

$$E_0/N = \frac{e^2}{2a_0}\left[\frac{2.21}{r_s^2} - \frac{0.916}{r_s}\right].$$

Here we have defined $r_s = r_0/a_0$ to be a dimensionless quantity.

Plot your results and link your discussion to the result in exercise b). Why is this system stable?

e) Calculate thermodynamical quantities like the pressure, given by

$$P = -\left(\frac{\partial E}{\partial \Omega}\right)_N,$$

and the bulk modulus

$$B = -\Omega\left(\frac{\partial P}{\partial \Omega}\right)_N,$$

and comment your results.

f) The single-particle Hartree-Fock energies are given by the expression

$$\varepsilon_k^{HF} = \frac{\hbar^2 k^2}{2m} - \frac{e^2 k_F}{2\pi}\left[2 + \frac{k_F^2 - k^2}{k k_F} ln\left|\frac{k + k_F}{k - k_F}\right|\right].$$

(You don't need to calculate this quantity). How can you use the Hartree-Fock energy to find the ground state energy? Are there differences between the Hartree-Fock results and those you found in exercise d)? Comment your results.

Exercise 20

Show Thouless' theorem: An arbitrary Slater determinant $|c'\rangle$ which is not orthogonal to a determinant $|c\rangle = \prod_{i=1}^{n} a^\dagger_{\alpha_i} |0\rangle$, can be written as

$$|c'\rangle = exp\left\{\sum_{p=\alpha_{n+1}}^{\infty} \sum_{h=\alpha_1}^{\alpha_n} C_{ph} a_p^\dagger a_h\right\} |c\rangle$$

Exercise 21

We have

$$|c\rangle = \prod_{k>0}(u_k + v_k a_k^\dagger a_{-k}^\dagger)\,|0\rangle$$

with $u_k^2 + v_k^2 = 1$, $\hat{N} = \sum_\nu a_\nu^\dagger a_\nu$ and $\hat{H} = -|G| \sum_{\nu,\nu'>0} a_\nu^\dagger a_{-\nu}^\dagger a_{-\nu'} a_{\nu'}$. Show that

a)

$$\langle c|c\rangle = \prod_{k>0}(u_k^2 + v_k^2)$$

b)

$$\langle c|\,\hat{N}\,|c\rangle = 2\sum_{\nu>0} v_\nu^2$$

c)

$$\langle c|\,\hat{N}^2\,|c\rangle = 4\sum_{\nu>0} v_\nu^2 + 4\sum_{\nu\neq\nu'>0} v_\nu^2 v_{\nu'}^2$$

d)

$$(\Delta N)^2 = \langle c|\,\hat{N}^2\,|c\rangle - (\langle c|\,\hat{N}\,|c\rangle)^2 = 4\sum_{\nu>0} u_\nu^2 v_\nu^2$$

e)

$$\langle c|\,\hat{H}\,|c\rangle = -|G|\left[\sum_{\nu>0} u_\nu v_\nu\right]^2 - |G|\sum_{\nu>0} v_\nu^4$$

Exercise 22

Show that

$$\left\{\alpha_k, \alpha_l^\dagger\right\} = \delta_{kl}, \qquad \{\alpha_k, \alpha_l\} = 0, \qquad \left\{\alpha_k^\dagger, \alpha_l^\dagger\right\} = 0$$

is fulfilled

$$u_k^2 + v_k^2 = 1, \qquad u_k = u_{-k}, \qquad v_k = v_{-k}$$

(Recall that $\alpha_k^\dagger = u_k a_k^\dagger + v_{-k} a_{-k}$)

Exercise 23

Apply the Bogoliubov transformation on

$$H' = \sum_{k>0} \varepsilon_k a_k^\dagger a_k - |G| \sum_{k,k'>0} a_k^\dagger a_{-k}^\dagger a_{-k'} a_{k'}$$

and show that in the resulting

$$H' = U + H_{11} + H_{20} + H(4operatorer)$$

we have

$$U = 2\sum_{k>0} \varepsilon_k v_k^2 - |G| \left[\sum_{k>0} u_k v_k\right]^2 - |G| \sum_{k>0} v_k^4$$

$$H_{11} = \sum_{k>0} \left\{ (u_k^2 - v_k^2)(\varepsilon_k - |G| v_k^2) + 2u_k v_k |G| \sum_{k'>0} u_{k'} v_{k'} \right\} (\alpha_k^\dagger \alpha_k + \alpha_{-k}^\dagger \alpha_{-k})$$

$$H_{20} = \sum_{k>0} \left\{ 2u_k v_k (\varepsilon_k - |G| v_k^2) - (u_k^2 - v_k^2)|G| \sum_{k'>0} u_{k'} v_{k'} \right\} (\alpha_k^\dagger \alpha_{-k}^\dagger + \alpha_{-k} \alpha_k)$$

Exercise 24

Let $H = H_0 + V$ and $|\phi_n\rangle$ be the eigenstates of H_0 and that $|\psi_n\rangle$ are the corresponding ones for H. Assume that the ground states $|\phi_0\rangle$ and $|\psi_0\rangle$ are not degenerate. Show that

$$E_0 - \varepsilon_0 = \frac{\langle \phi_0 | V | \psi_0 \rangle}{\langle \phi_0 | \psi_0 \rangle},$$

with $H|\psi_0\rangle = E|\psi_0\rangle$ and $H_0|\phi_0\rangle = \varepsilon_0|\phi_0\rangle$.

a) Define the new operators $P = |\phi_0\rangle\langle\phi_0|$ and $Q = 1 - P$. Show that these operators are idempotent.

b) Show that for any z we have

$$|\psi_0\rangle = \langle \phi_0 | \psi_0 \rangle \sum_{n=0}^{\infty} \left(\frac{Q}{z - H_0} (z - E_0 + V) \right)^n |\phi_0\rangle,$$

and

$$E_0 = \varepsilon_0 + \sum_{n=0}^{\infty} \langle \phi_0 | V \left(\frac{Q}{z - H_0} (z - E_0 + V) \right)^n |\phi_0\rangle.$$

c) Discuss these results for $z = E_0$ (Brillouin-Wigner perturbation theory) and $z = \varepsilon_0$ (Rayleigh-Schrödinger perturbation theory). Compare the first few terms in these expansions.

Exercise 25

Consider a system of two fermions in the pair-orbitals $|m_0\rangle$ and $|-m_0\rangle$ in a single shell j with $2j + 1 > 2$. Assume that the matrix elements for the interaction between the particles takes the form

$$\langle m, -m | v | m', -m' \rangle = -G.$$

a) Show that the Brillouin-Wigner expansion from the previous exercise can be used to give

$$E_0 = -(j + 1/2)G.$$

b) Show thereafter by direct diagonalization of the Hamiltonian matrix that this is the exact energy. Use thereafter Rayleigh-Schrödinger perturbation theory and discuss the differences.

Exercise 26

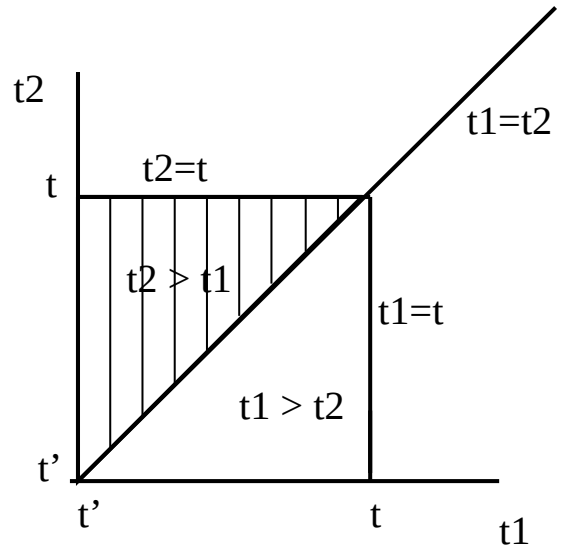
Show that

$$\int_{t'}^{t} dt_1 \int_{t'}^{t_1} dt_2 H_1(t_1) H_1(t_2) = \frac{1}{2} \int_{t'}^{t} dt_1 \int_{t'}^{t} dt_2 T\left[H_1(t_1) H_1(t_2)\right]$$

Hint: Use the definition of T in order to distinguish between $t_1 > t_2$ and $t_1 < t_2$;

$$\int_{t'}^{t} dt_1 \int_{t'}^{t} dt_2 T\left[H_1(t_1) H_1(t_2)\right] = \int_{t'}^{t} dt_1 \left\{ \int_{t'}^{t_1} dt_2 H_1(t_1) H_1(t_2) + \int_{t_1}^{t} dt_2 H_1(t_2) H_1(t_1) \right\}$$

Show that the last term on the right-hand side equals the first term (change the order of the integrations and thereafter integration variables). The area of integration for the first term is shown in the figure below.



Exercise 27

In exercise 19 you found an expression for the interaction part of the Hamiltonian for the electron gas given by

$$H_I = \frac{e^2}{2V} \sum_{\sigma_1 \sigma_2} \sum_{\vec{q} \neq 0, \vec{k}, \vec{p}} \frac{4\pi}{q^2} a^{\dagger}_{\vec{k}+\vec{q},\sigma_1} a^{\dagger}_{\vec{p}-\vec{q},\sigma_2} a_{\vec{p}\sigma_2} a_{\vec{k}\sigma_1}$$

a) Find all diagrams to second order in perturbation theory. Set up the corresponding expressions and discuss their behavior.

b) What happens in case you keep the convergence factor μ finite?

Exercise 28

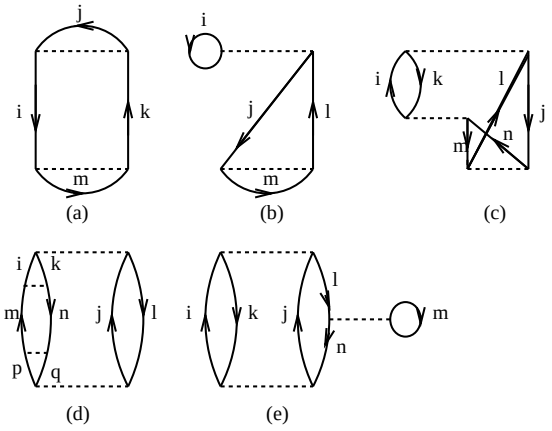
Consider the following diagrams:

a) Set up the expressions for diagrams (a)-(e).

b) Diagram (b) does not give a contribution for a uniform and degenerate electron gas (or any uniform degenerate infinite system). Explain why. What about diagram (a)?

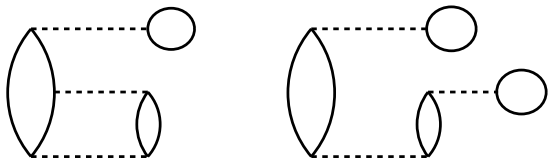
c) Diagram (c) is a so-called exchange diagram. Can you find the corresponding direct diagram?

d) Can you find the exchange diagram of diagram (e) under the assumption that the exchange takes place at the middle vertex?

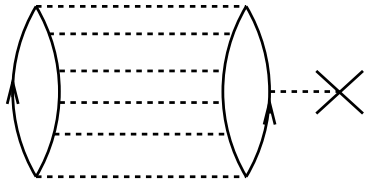


Exercise 29

Explain how the Hartree-Fock approximation can be used to cancel the diagrams of (a) in the figure. Set up their corresponding expressions. Find thereafter the expression for the diagram in (b).



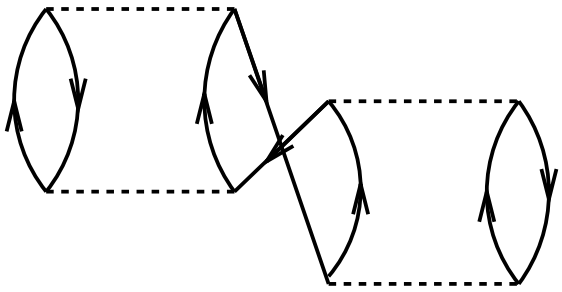
(a)



(b)

Exercise 23

Compute the contribution to ΔE_0 for the diagram shown here. Can the crossing hole lines have the same quantum



numbers?

Exercise 30

We consider a one-particle system with the following Hamiltonian $H = H_0 + H_1$ where

$$H_0 = \sum_{i=1,2} \varepsilon_i a_i^\dagger a_i$$

$$H_1 = \lambda \sum_{i \neq j=1,2} a_i^\dagger a_j$$

a) Find the ground state energy to third order in perturbation theory using both Brillouin-Wigner and Rayleigh-Schödinger perturbation theory.

b) Write down the corresponding diagrams in the particle picture (using the true vacuum).

c) Find the exact energy and expand the exact results in terms of the parameter λ and compare with the results obtained with the above two expansions. Discuss the eventual differences.

d) Rewrite the unperturbed ground state in the particle-hole representation

$$|c\rangle = |\Phi_1\rangle = a_1^\dagger |0\rangle ,$$

and write down the corresponding diagrams

e) To fourth order in perturbation theory we have unlinked diagrams. Give examples of these and show how they can be cancelled.

Exercise 31

We present a simplified Hamiltonian consisting of an unperturbed Hamiltonian and a so-called pairing interaction term. It is a model which to a large extent mimicks some central features of atomic nuclei, certain atoms and systems which exhibit superfluiditity or superconductivity. To study this system, we will use a mix of many-body perturbation theory, Hartree-Fock theory and the configuration interaction method. The latter will also provide us with the exact answer. When setting up the Hamiltonian matrix you will need to solve an eigenvalue problem. This can easily be done with either octave or Matlab or writing your own program.

We define first the Hamiltonian, with a definition of the model space and the single-particle basis. Thereafter, we present the various exercises.

The Hamiltonian acting in the complete Hilbert space (usually infinite dimensional) consists of an unperturbed one-body part, $\hat{H}_0$, and a perturbation $\hat{V}$.

We limit ourselves to at most two-body interactions, our Hamiltonian is then represented by the following operators

$$\hat{H} = \sum_{\alpha\beta} \langle \alpha | h_0 | \beta \rangle a_\alpha^\dagger a_\beta + \frac{1}{4} \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta | V | \gamma\delta \rangle a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma,$$

where $a_\alpha^\dagger$ and a_α etc. are standard fermion creation and annihilation operators, respectively, and $\alpha\beta\gamma\delta$ represent all possible single-particle quantum numbers. The full single-particle space is defined by the completeness relation $\hat{\mathbf{1}} = \sum_{\alpha=1}^{\infty} |\alpha\rangle\langle\alpha|$. In our calculations we will let the single-particle states $|\alpha\rangle$ be eigenfunctions of the one-particle operator $\hat{h}_0$.

The above Hamiltonian acts in turn on various many-body Slater determinants constructed from the single-basis defined by the one-body operator $\hat{h}_0$. As an example, the two-particle model space $\mathcal{P}$ is defined by an operator

$$\hat{P} = \sum_{\alpha\beta=1}^{m} |\alpha\beta\rangle\langle\alpha\beta|,$$

where we assume that $m = \dim(\mathcal{P})$ and the full space is defined by

$$\hat{P} + \hat{Q} = \hat{\mathbf{1}},$$

with the projection operator

$$\hat{Q} = \sum_{\alpha\beta=m+1}^{\infty} |\alpha\beta\rangle\langle\alpha\beta|,$$

being the complement of $\hat{P}$.

Our specific model consists of N doubly-degenerate and equally spaced single-particle levels labelled by $p = 1, 2, \ldots$ and spin $\sigma = \pm 1$. These states are schematically portrayed in Fig. 4. The first two single-particle levels define a possible model space, indicated by the label $\mathcal{P}$. The remaining states span the excluded space $\mathcal{Q}$.

We write the Hamiltonian as

$$\hat{H} = \hat{H}_0 + \hat{V},$$

where

$$\hat{H}_0 = \xi \sum_{p\sigma} (p-1) a^\dagger_{p\sigma} a_{p\sigma}$$

and

$$\hat{V} = -\frac{1}{2} g \sum_{pq} a^\dagger_{p+} a^\dagger_{p-} a_{q-} a_{q+}.$$

Here, H_0 is the unperturbed Hamiltonian with a spacing between successive single-particle states given by ξ, which we will set to a constant value $\xi = 1$ without loss of generality. The two-body operator $\hat{V}$ has one term only. It represents the pairing contribution and carries a constant strength g. The indices $\sigma = \pm$ represent the two possible spin values. The interaction can only couple pairs and excites therefore only two particles at the time, as indicated by the rightmost four-particle state in Fig. 4. There one of the pairs is excited to the state with $p = 9$ and the other to the state $p = 7$. The two middle possibilities are not possible with the present model. We label single-particle states within the model space as hole-states. The single-particle states outside the model space are then particle states.

In our model we have kept both the interaction strength and the single-particle level as constants. In a realistic system like an atom or the atomic nucleus this is not the case.

a) Show that the unperturbed Hamiltonian $\hat{H}_0$ and $\hat{V}$ commute with both the spin projection $\hat{S}_z$ and the total spin $\hat{S}^2$, given by

$$\hat{S}_z := \frac{1}{2} \sum_{p\sigma} \sigma a^\dagger_{p\sigma} a_{p\sigma}$$

and

$$\hat{S}^2 := \hat{S}_z^2 + \frac{1}{2}(\hat{S}_+ \hat{S}_- + \hat{S}_- \hat{S}_+),$$

where

$$\hat{S}_\pm := \sum_p a^\dagger_{p\pm} a_{p\mp}.$$

This is an important feature of our system that allows us to block-diagonalize the full Hamiltonian. We will focus on total spin $S = 0$. In this case, it is convenient to define the so-called pair creation and pair annihilation operators

$$\hat{P}^+_p = a^\dagger_{p+} a^\dagger_{p-},$$

and

$$\hat{P}^-_p = a_{p-} a_{p+},$$

respectively.

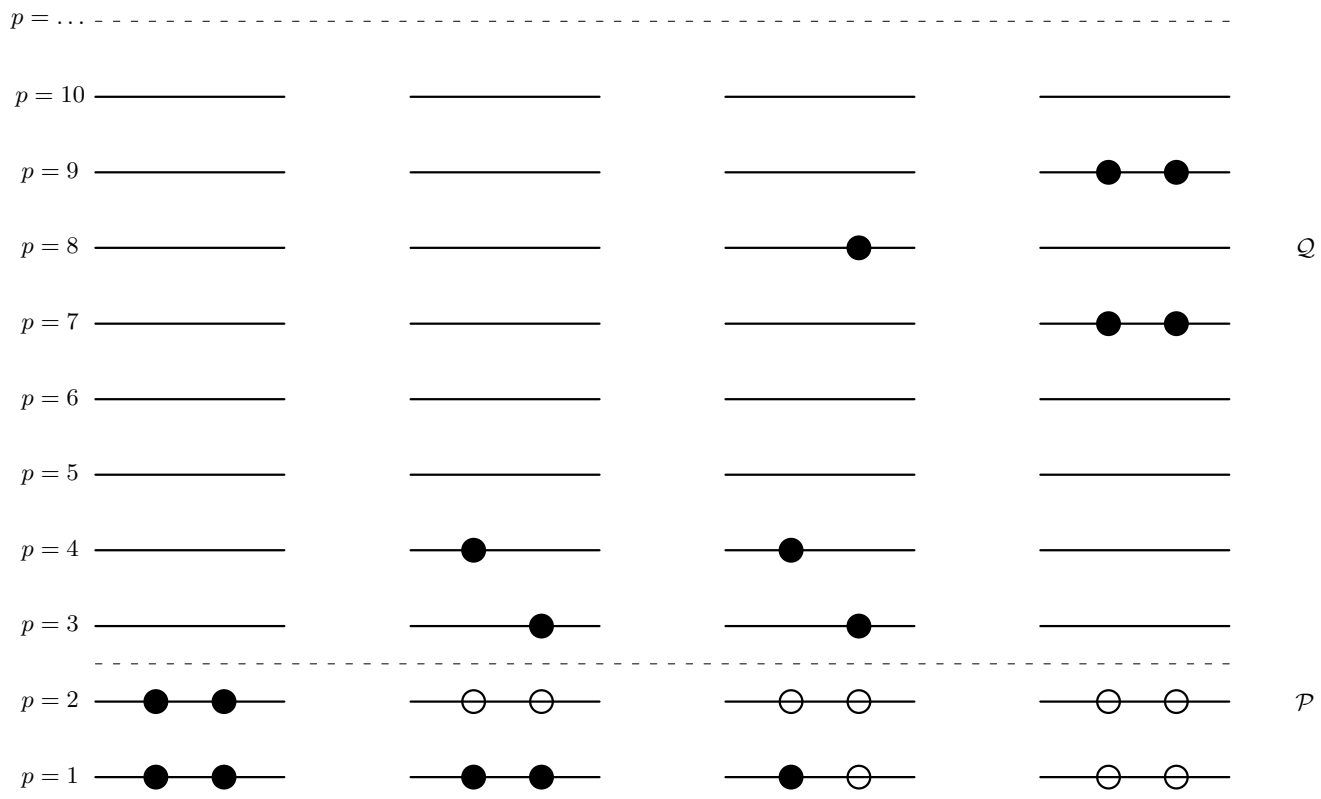


FIG. 4: Schematic plot of the possible single-particle levels with double degeneracy. The filled circles indicate occupied particle states while the empty circles represent vacant particle(hole) states. The spacing between each level p is constant in this picture. The first two single-particle levels define our possible model space, indicated by the label $\mathcal{P}$. The remaining states span the excluded space $\mathcal{Q}$. The first state to the left represents a possible ground state representation for a four-fermion system. In the second state to the left, one pair is broken. This possibility is however not included in our interaction.

Show that you can rewrite the Hamiltonian (with $\xi = 1$) as

$$\hat{H} = \sum_{p\sigma}(p-1)a^{\dagger}_{p\sigma}a_{p\sigma} - \frac{1}{2}g\sum_{pq}\hat{P}^{+}_{p}\hat{P}^{-}_{q}.$$

Show also that Hamiltonian commutes with the product of the pair creation and annihilation operators. This model corresponds to a system with no broken pairs. This means that the Hamiltonian can only link two-particle states in so-called spin-reversed states.

b) Construct thereafter the Hamiltonian matrix for a system with no broken pairs and spin $S = 0$ for the case of the four lowest single-particle levels indicated in the Fig. 4. Our system consists of four particles only. Our single-particle space consists of only the four lowest levels $p = 1, 2, 3, 4$. You need to set up all possible Slater determinants. Find all eigenvalues by diagonalizing the Hamiltonian matrix. Vary your results for values of $g \in [-1, 1]$. We refer to this as the exact calculation. Comment the behavior of the ground state as function of g.

c) Instead of setting up all possible Slater determinants, construct only an approximation to the ground state (where we assume that the four particles are in the two lowest single-particle orbits only) which includes at most two-particle-two-hole excitations. Diagonalize this matrix and compare with the exact calculation and comment your results. Can you set up which diagrams this approximation corresponds to?

d) Hereafter we will define our model space to consist of the single-particle levels $p = 1, 2$. The remaining levels $p = 3, 4$ define our excluded space. This means that our ground state Slater determinant consists of four particles which can be placed in the doubly degenerate orbits $p = 1$ and $p = 2$.

We will now study the system using non-degenerate Rayleigh-Schrödinger perturbation theory to third order in the interaction. If we exclude the first order contribution, all possible diagrams (Hugenholz diagrams where the vertices have been opened) are shown in Fig. 5.

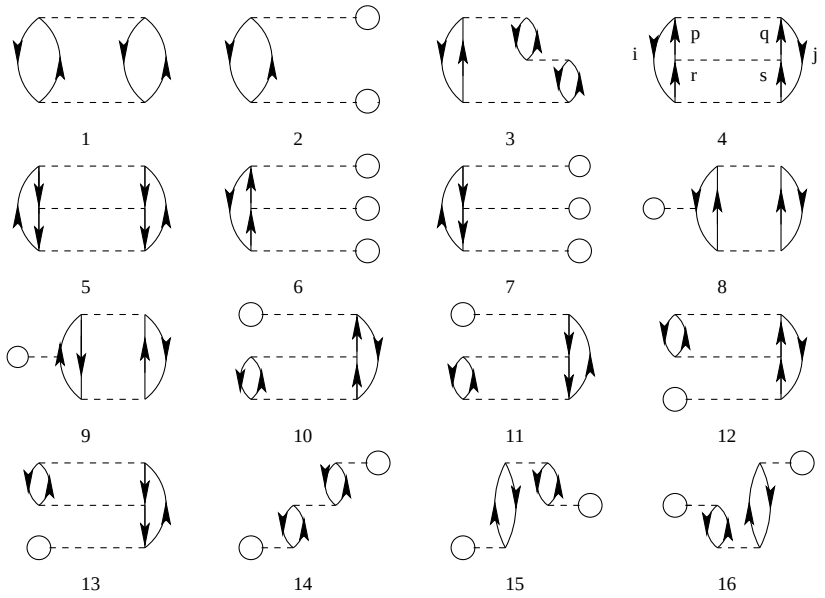


FIG. 5: Diagrams to third order in the interaction. The first order term is excluded.

Based on the form of the interaction, which diagrams contribute to the binding energy of the ground state? Write down the expressions for the diagrams that contribute and find the contribution to the ground state energy as function $g \in [-1, 1]$. Comment your results. Compare these results with those you obtained in 2) and 3).

e) The diagrams with only two single particle states as intermediate states (for example diagrams 1 and 4 in Fig. 5) can be summed to infinite order since they can be expressed as a geometric series. Find this contribution and compare the final energy with the results from 2) and 3). Comment your results. You can also perform a resummation of diagrams like diagram 5 with hole lines as intermediate states only between various vertices. Can you find this result as well? Compare now the final results with the resummed two-particle and two-hole diagrams with the results from 2) and 3).

f) We will now set up the Hartree-Fock equations by varying the coefficients of the single-particle functions. The single-particle basis functions are defined as

$$\psi_p = \sum_\lambda C_{p\lambda}\psi_\lambda.$$

where in our case $p = 1, 2, 3, 4$ and $\lambda = 1, 2, 3, 4$, that is the first four lowest single-particle orbits of Fig. 4. Set up the Hartree-Fock equations for this system by varying the coefficients $C_{p\lambda}$ and solve them for values of $g \in [-1, 1]$. Comment your results and compare with the exact solution. Discuss also which diagrams in Fig. 5 that can be affected by a Hartree-Fock basis. Compute the total binding energy using a Hartree-Fock basis and comment your results.

g) To fourth order in perturbation theory we can produce diagrams with so-called four-particle-four-hole excitations. An example is given in Fig. 6. Find the contribution to the binding energy of the ground state from this type

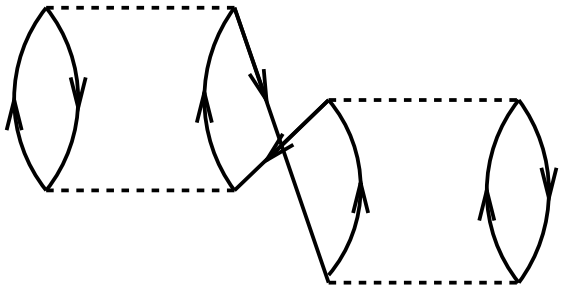


FIG. 6: An example of a fourth-order diagram with an intermediate state involving four-particle-four-hole excitations.

of contributions and compare with your previous results with and without a Hartree-Fock basis. Discuss in particular the connection with the results for the full diagonalization where Slater determinants involving four-particle-four-hole excitations are involved.

h) When summing over all intermediate states in diagram 1 or 4 of Fig. 5, we have limited the sum over intermediate particle states to include the states $p = 3$ and $p = 4$ only. Compute this sum by taking the limit $p = \infty$. Comment your results.

Exercise 32

We will study a schematic model (the Lipkin model, Nucl. Phys. **62** (1965) 188) for the interaction among 4 fermions that can occupy two different energy levels. Each levels has degeneration $d = 4$. The two levels have quantum numbers $\sigma = \pm 1$, with the upper level having $\sigma = +1$ and energy $\varepsilon_1 = \varepsilon/2$. The lower level has $\sigma = -1$ and energy $\varepsilon_2 = -\varepsilon/2$. In addition, the substates of each level are characterized by the quantum numbers $p = 1, 2, 3, 4$.

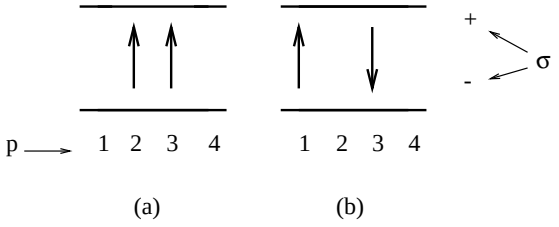
We define the single-particle states

$$|u_{\sigma=-1,p}\rangle = a^\dagger_{-p}\,|0\rangle \qquad |u_{\sigma=1,p}\rangle = a^\dagger_{+p}\,|0\rangle\,.$$

The single-particle states span an orthonormal basis. The Hamiltonian of the system is given by

$$\begin{aligned} H &= H_0 + H_1 + H_2 \\ H_0 &= \tfrac{1}{2}\varepsilon \textstyle\sum_{\sigma,p} \sigma a^\dagger_{\sigma,p} a_{\sigma,p} \\ H_1 &= \tfrac{1}{2} V \textstyle\sum_{\sigma,p,p'} a^\dagger_{\sigma,p} a^\dagger_{\sigma,p'} a_{-\sigma,p'} a_{-\sigma,p} \\ H_2 &= \tfrac{1}{2} W \textstyle\sum_{\sigma,p,p'} a^\dagger_{\sigma,p} a^\dagger_{-\sigma,p'} a_{\sigma,p'} a_{-\sigma,p} \end{aligned}$$

where V and W are constants. The operator H_1 can move pairs of fermions as shown in Fig. (a) while H_2 is a spin-exchange term. As shown in Fig. (b), H_2 moves a pair of fermions from a state $(p\sigma, p' - \sigma)$ to a state $(p - \sigma, p'\sigma)$.



a) Introduce the quasispin operators

$$\begin{aligned} J_+ &= \sum_p a^\dagger_{p+} a_{p-} \\ J_- &= \sum_p a^\dagger_{p-} a_{p+} \\ J_z &= \tfrac{1}{2}\sum_{p\sigma} \sigma a^\dagger_{p\sigma} a_{p\sigma} \\ J^2 &= J_+ J_- + J_z^2 - J_z \end{aligned}$$

Show that these operators obey the commutation relations for angular momentum.
b) Express H in terms of the above quasispin operators and the number operator

$$N = \sum_{p\sigma} a^\dagger_{p\sigma} a_{p\sigma}.$$

c) Show that H commutes with J^2, viz., J is a good quantum number.
d) Consider thereafter a state with all four fermions in the lowest level (see the above figure). We can write this state as

$$|\Phi_{J_z=-2}\rangle = a^\dagger_{1-} a^\dagger_{2-} a^\dagger_{3-} a^\dagger_{4-} |0\rangle .$$

This state has $J_z = -2$ and belongs to the set of possible projections of $J = 2$. We introduce the shorthand notation $|J, J_z\rangle$ for states with different values of spin J and its projection J_z.

The other possible values are $J_z = -1$, $J_z = 0$, $J_z = 1$ and $J_z = 2$. Use the ladder operators J_+ and J_- to set up the states with spin $J_z = -1$ $J_z = 0$, $J_z = 1$ and $J_z = 2$. The action of these operators on a state with given spin J and J_z is (with $\hbar = 1$) $J_+ |J, J_z\rangle = \sqrt{J(J+1) - J_z(J_z+1)}\, |J, J_z + 1\rangle$ and $J_- |J, J_z\rangle = \sqrt{J(J+1) - J_z(J_z-1)}\, |J, J_z - 1\rangle$, respectively.
e) use thereafter the quasispin operators to construct the Hamiltonian matrix H for this five-dimensional space. Find thereafter the eigenvalues (numerically using for example Octave or Matlab or python) for the following parameter sets: sett av verdier:

$$\begin{aligned} &(1)\ \ \varepsilon = 2,\ \ V = -1/3,\ \ W = -1/4 \\ &(2)\ \ \varepsilon = 2,\ \ V = -4/3,\quad W = -1 \end{aligned}$$

Which state is the ground state? Comment your results.
f) The single-particle states for the Lipkin model

$$|u_{\sigma=-1,p}\rangle = a^\dagger_{-p} |0\rangle \qquad |u_{\sigma=1,p}\rangle = a^\dagger_{+p} |0\rangle$$

can now be used as basis for a new single-particle state $|\phi_{\alpha,p}\rangle$ via a unitary transformation

$$|\phi_{\alpha,p}\rangle = \sum_{\sigma=\pm 1} C_{\alpha\sigma} |u_{\sigma,p}\rangle$$

with $\alpha = \pm 1$ og $p = 1, 2, 3, 4$. Why is p the same in $|\phi\rangle$ as in $|u\rangle$? Show that the new basis is orthonormal.
g) With the new basis we can construct a new Slater determinant given by $|\Psi\rangle$

$$|\Psi\rangle = \prod_{p=1}^{4} b^\dagger_{\alpha,p} |0\rangle$$

with $b^\dagger_{\alpha,p} |0\rangle = |\phi_{\alpha,p}\rangle$. h) Use the Slater determinanten from the previous exercise to calculate

$$E = \langle\Psi| H |\Psi\rangle ,$$

as a function of the coefficients $C_{\sigma\alpha}$. We assume the coefficients to be real.
i) Show that

$$\frac{\epsilon}{3} > V + W,$$

has to be fulfilled in order to find a minimum in the energy.

Hint: calculate the functional derivative of the energy with respect to the coefficients $C_{\sigma\alpha}$.

Exercise 33, Exam Fall semester 2011

Let $\hat{H} = \hat{H}_0 + \hat{H}_I$ and $|\Phi_n\rangle$ be the eigenstates of $\hat{H}_0$ and that $|\Psi_n\rangle$ are the corresponding ones for $\hat{H}$. Assume that the ground states $|\Phi_0\rangle$ and $|\Psi_0\rangle$ are not degenerate. We can then write the energy of the ground state as

$$E_0 - \varepsilon_0 = \frac{\langle\Phi_0|\,\hat{H}_I\,|\Psi_0\rangle}{\langle\Phi_0|\Psi_0\rangle},$$

with $\hat{H}\,|\Psi_0\rangle = E_0\,|\Psi_0\rangle$ and $H_0\,|\Phi_0\rangle = \varepsilon_0\,|\Phi_0\rangle$. We define also the projection operators $\hat{P} = |\Phi_0\rangle\langle\Phi_0|$ and $\hat{Q} = 1 - \hat{P}$. These operators satisfy $\hat{P}^2 = \hat{P}$, $\hat{Q}^2 = \hat{Q}$ and $\hat{P}\hat{Q} = 0$.

a) Show that for any ω we have can write the ground state energy as

$$E_0 = \varepsilon_0 + \sum_{n=0}^{\infty} \langle\Phi_0|\,\hat{H}_I \left(\frac{\hat{Q}}{\omega - \hat{H}_0}(\omega - E_0 + \hat{H}_I)\right)^n |\Phi_0\rangle\,.$$

b) Discuss these results for $\omega = E_0$ (Brillouin-Wigner perturbation theory) and $\omega = \varepsilon_0$ (Rayleigh-Schrödinger perturbation theory). Compare the first few terms in these expansions and discuss the differences.

c) Show that the onebody part of the Hamiltonian

$$\hat{H}_0 = \sum_{pq} \langle p|\,\hat{h}_0\,|q\rangle\, a_p^\dagger a_q$$

can be written, using standard annihilation and creation operators, in normal-ordered form as

$$\hat{H}_0 = \sum_{pq} \langle p|\,\hat{h}_0\,|q\rangle\, a_p^\dagger a_q = \sum_{pq} \langle p|\,\hat{h}_0\,|q\rangle\, \{a_p^\dagger a_q\} + \sum_i \langle i|\,\hat{h}_0\,|i\rangle\,,$$

and that the two-body Hamiltonian

$$\hat{H}_I = \frac{1}{4}\sum_{pqrs} \langle pq|\,\hat{v}\,|rs\rangle\, a_p^\dagger a_q^\dagger a_s a_r,$$

can be written

$$\hat{H}_I = \frac{1}{4}\sum_{pqrs} \langle pq|\,\hat{v}\,|rs\rangle\, \{a_p^\dagger a_q^\dagger a_s a_r\} + \sum_{pqi} \langle pi|\,\hat{v}\,|qi\rangle\, \{a_p^\dagger a_q\} + \frac{1}{2}\sum_{ij} \langle ij|\,\hat{v}\,|ij\rangle$$

Explain the meaning of the various symbols. Which reference vacuum has been used? Write down the diagrammatic representation of all these terms.

d) Use the diagrammatic representation of the Hamiltonian operator from the previous exercise to set up all diagrams (use either anti-symmetrized Goldstone diagrams or Hugenholz diagrams) to second order (including the reference energy) in Rayleigh Schrödinger perturbation theory that contribute to the expectation value of E_0.

Use the diagram rules to write down their closed-form expressions. If a Hartree-Fock basis is used, which diagrams remain?

We consider now a one-particle system with the following Hamiltonian $\hat{H} = \hat{H}_0 + \hat{H}_I$ where

$$\hat{H}_0 = \sum_p \varepsilon_p a_p^\dagger a_p,$$

and

$$\hat{H}_I = g\sum_{pq} a_p^\dagger a_q.$$

The strength parameter g is a real constant. The first part of the Hamiltonian plays the role of the unperturbed part, with

$$\langle p|\,\hat{h}_0\,|q\rangle = \delta_{p,q}\varepsilon_p.$$

We have only two one-particle states, with $\varepsilon_1 < \varepsilon_2$, and we will let the first state $p = 1$ correspond to the model space and the other, $p = 2$, correspond to the excluded space. Use labels $ijk\ldots$ for hole states (below the Fermi level) and labels $abc\ldots$ for particle (virtual) states (above the Fermi level).

e) Use the results from exercise c) to write down the above Hamiltonian in a normal-ordered form and set up all diagrams. Use an X to indicate the interaction part H_I.

f) Define the ground state (which is our model space) as

$$|\Phi_0\rangle = a_i^\dagger\,|0\rangle = a_1^\dagger\,|0\rangle\,,$$

and the excited state as

$$|\Phi_i^a\rangle = a_a^\dagger a_i\,|\Phi_0\rangle\,,$$

where $a = 2$ and $i = 1$. Set up the Hamiltonian matrix (a 2×2 matrix) and find the exact energy and expand the exact result for the ground state in terms of the parameter g.

g) Find the ground state energy to third order in Rayleigh-Schödinger perturbation theory and compare the results with the expansion of the exact energy from the previous exercise. Write down all diagrams which contribute and comment your results.

The final part deals with coupled-cluster theory. Since we have only a one-body problem, coupled-cluster theory truncated at the level of T_1 is exact. The similarity transformed normal-ordered Hamiltonian can then be written out as

$$\bar{H} = \hat{H}_N + \left(\hat{H}_N\hat{T}\right)_c + \frac{1}{2}\left(\hat{H}_N\hat{T}^2\right)_c + \cdots +,$$

where only linked diagrams appear. The expectation value of the ground state energy (beyond the reference energy is)

$$\mathrm{E_{CCS}} = \langle\Phi_0|\,\bar{H}\,|\Phi_0\rangle\,,$$

and the amplitudes t_i^a are determined from the equation

$$0 = \langle\Phi_i^a|\,\bar{H}\,|\Phi_0\rangle\,.$$

For the latter we need to take into account diagrams which lead to a final excitation level of +1 only.

h) Set up the definition of the operator $\hat{T} = \hat{T}_1$. We will use a diagrammatic approach only to find the diagrammatic contribution to the ground state beyond the reference energy. Show that the only possibility is

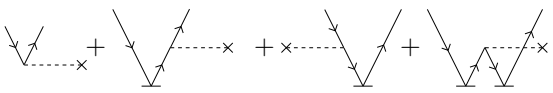
$E_{CCS} =$ 

Find the closed form expression.

i) Show, using a diagrammatic approach and keeping in mind the final excitation level, that the only diagrams that lead to

$$0 = \langle\Phi_i^a|\,\bar{H}\,|\Phi_0\rangle\,,$$

are

$0 =$ 

Set up the final closed form expressions and the algorithm for finding the amplitudes t_i^a. Can you solve the problem?