Exercises FYS-KJM4480, Fall semester 2009

Exercises week 35, August 24-28 2009

Exercise 1

Consider the Slater determinant

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

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 can be written as

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

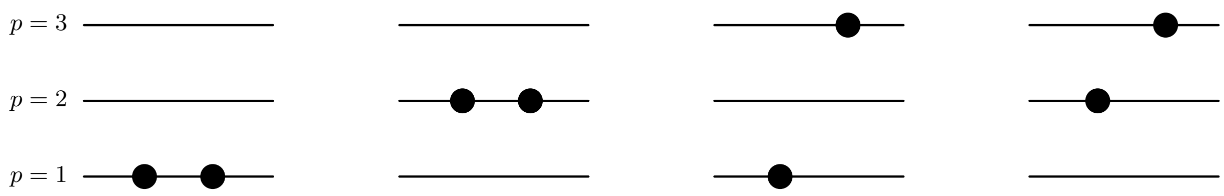


FIG. 1: Schematic plot of the possible single-particle levels with double degeneracy. The filled circles indicate occupied particle states. The spacing between each level p is constant in this picture. We show some possible two-particle states.

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.

Exercises week 36, August 31- September 4 2009

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

$$\langle \alpha\beta| g |\gamma\delta\rangle = \int\int \psi^*_\alpha(x_1)\psi^*_\beta(x_2)g(x_1,x_2)\psi_\gamma(x_1)\psi_\delta(x_2)dx_1dx_2$$

Compare these results with those from exercise 1c).

Exercise 4

We define the two-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 $\alpha, \beta, \gamma, \dots$ 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 $\lambda \in \{\alpha, \beta, \gamma, \dots\}$. 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 and find an expression $\hat{T}$ and $\hat{V}$ when v is diagonal in α, β.

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.

Exercises week 37, September 7-11 2009

Exercise 6

Write the two-particle operator

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

in the quasi-particle representation for particles and holes

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

You can use Wick's theorem.

Exercise 7

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 8

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.

Exercises week 38, September 14-18 2009

Exercise 9

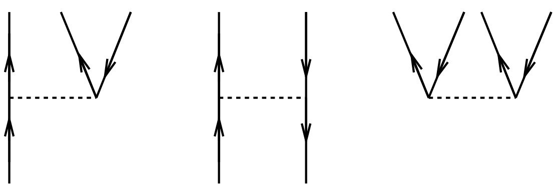
Use the results from exercise 6 and Wick's theorem to calculate

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

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

Exercise 10

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



What is the diagram for $\langle c | \, G \, | c \rangle$? The operator G is the same as the one discussed in the previous exercises. Use the diagrammatic rules to write down the algebraic expression.

Exercise 11

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 12

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

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

Show that

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

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

Exercises week 39, September 21-25 2009

No exercises this week due to project work.

Exercises week 39, September 28- October 2 2009

Exercise 13

What is the diagrammatic representation of the HF equation?

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

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

Exercise 14

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

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