Exercises FYS-KJM4480, Fall semester 2010

Exercises week 35, August 30- September 3 2010

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 can be written as

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

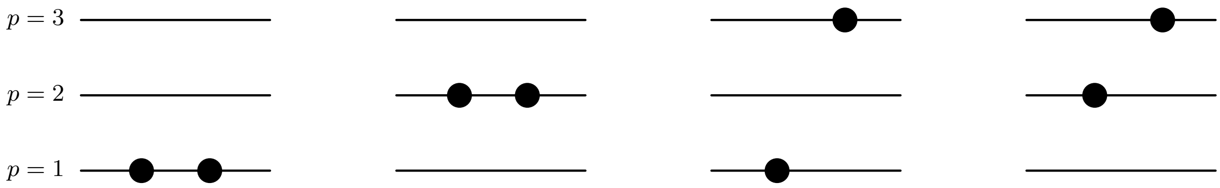

FIG. 1: Schematic plot of the possible single-particle levels with double degeneracy. The filled circles indicate occupied particle states. The spacing between each level p is constant in this picture. We show some possible two-particle states.

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, September 6-10 2010

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 13-17 2010

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

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

in the quasi-particle representation for particles and holes

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