

Exercises FYS-KJM4480, Fall semester 2010

Exercises week 35, August 30- September 3 2010

Exercise 1

Consider the Slater determinant

$$\Phi_{\lambda}^{AS}(x_1 x_2 \dots x_N; \alpha_1 \alpha_2 \dots \alpha_N) = \frac{1}{\sqrt{N!}} \sum_p (-1)^p P \prod_{i=1}^N \psi_{\alpha_i}(x_i).$$

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

$$\int dx_1 dx_2 \dots dx_N |\Phi_{\lambda}^{AS}(x_1 x_2 \dots x_N; \alpha_1 \alpha_2 \dots \alpha_N)|^2 = 1.$$

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

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

and

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

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

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

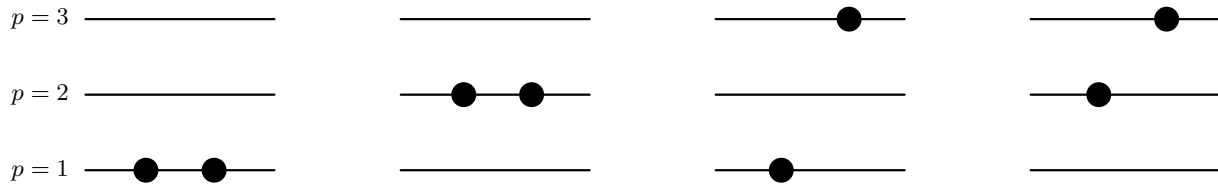


FIG. 1: Schematic plot of the possible single-particle levels with double degeneracy. The filled circles indicate occupied particle states. The spacing between each level p is constant in this picture. We show some possible two-particle states.

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

$$|\alpha_1 \alpha_2\rangle = a_{\alpha_1}^\dagger a_{\alpha_2}^\dagger |0\rangle,$$

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

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

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

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 two-particle operator

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

and the two-particle operator

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

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 $a_i^\dagger a_i$ 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

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

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 ($c = \hbar = 1$)

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

(a) Define the operators

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

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

(b) Show that

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

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

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

(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.