Exercises FYS4480/9480, week 35, August 25-29, 2025

Exercise 1

Consider the fermion Slater determinant as ansatz for a quantum mechanical state function,

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

where P is an operator which allows for all possible permutations among the particles that are present. The sum over p runs over all possible permutations. 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 $\alpha_1\alpha_2\dots\alpha_N$. We assume that the single-particle basis $\psi_{\alpha_i}(x_i)$ is a so-called orthonormal basis.

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

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

and

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

Which properties do you expect these operators to have in addition to an eventual permutation symmetry?

Exercise 2

We will now consider a simple three-level problem, depicted in the figure below. This is our first and very simple model of a possible many-fermion problem and what we later will call full configuration interaction theory (dubbed FCI). We will assume the particles are fermions. 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

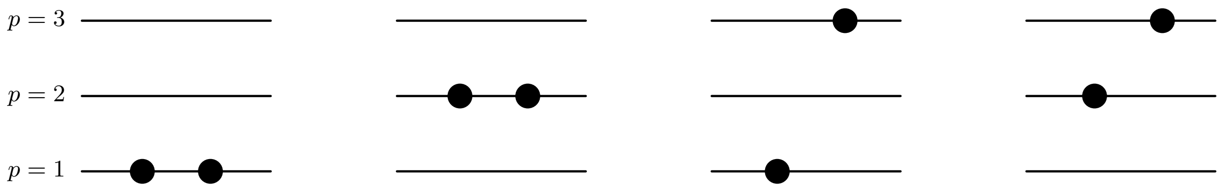

FIG. 1: Schematic plot of the possible single-particle levels with double degeneracy. The filled circles indicate occupied particle states. The spacing between each level p is constant in this picture. We show some possible two-particle states.

can be written as

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

and find the eigenvalues and eigenvectors. What is the 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.