Exercises FYS4480, week 35, August 29-September 2, 2022

Exercise 1

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

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

where P is an operator which permutes the coordinates of two particles. It acts on pairs of 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 $\alpha_1\alpha_2\dots\alpha_N$. 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

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

and

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

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

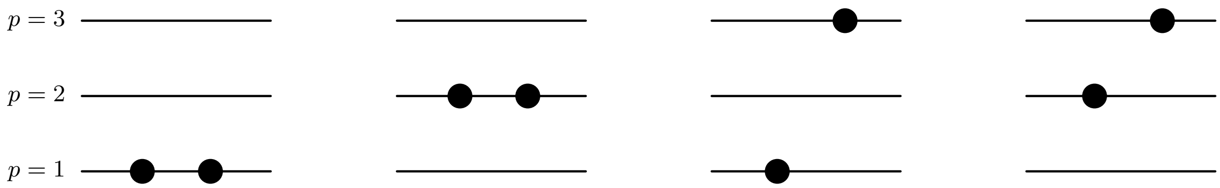

FIG. 1: Schematic plot of the possible single-particle levels with double degeneracy. The filled circles indicate occupied particle states. The spacing between each level p is constant in this picture. We show some possible two-particle states.

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.