UNIVERSITY
OF OSLO

FYS4480 Oral Exam

Quantum mechanics for
many-particle systems

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Notation

Here, we follow the notation of having states $ijk\ldots$ refer to occupied states, and $abc\ldots$ refer to unoccupied states, typically below and above the Fermi level, respectively. From a reference state $|\Phi_0\rangle$ with N particles, we write a 1-particle-1-hole (1p1h) excitation as

$$|\Phi_i^a\rangle = a_a^\dagger a_i |\Phi_0\rangle, \tag{1}$$

and similarly for 2p2h, 3p3h, etc.

Motivation

We are, in essence, interested in finding the ground state energy of a many-body system, that is, solving the eigenvalue problem

$$\hat{H}|\Psi_0\rangle = E_0|\Psi_0\rangle, \tag{2}$$

where $\hat{H}$ is the Hamiltonian operator and $|\Psi_0\rangle$ is the ground state wave function, such that the ground state energy E_0 is minimized.

The complexity arises from the fact that the exact solution cannot typically be found for systems with more than a few particles, and we must resort to approximations.

Full configuration interaction theory

In full configuration interaction (FCI) theory, we seek to write the wave function as a linear combination of all possible Slater determinants, that is, all possible configurations of the system, truncated at some level.

That is, we with to write the wave function as

$$|\Psi_0\rangle = C_0|\Phi_0\rangle + \sum_{ia} C_i^a|\Phi_i^a\rangle + \sum_{ijab} C_{ij}^{ab}|\Phi_{ij}^{ab}\rangle + \dots, \tag{3}$$

where the coefficients C are determined by solving the eigenvalue problem.

Slater determinants for pairing model

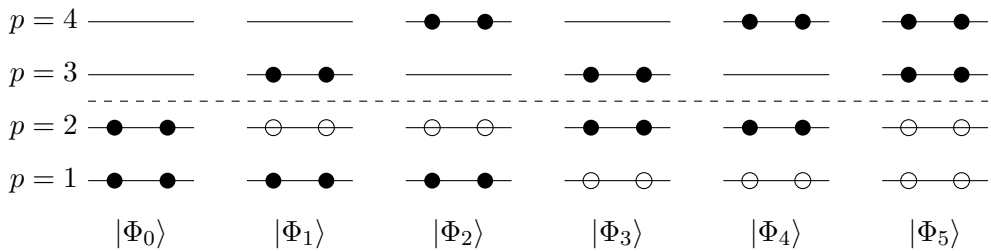

Figure: Schematic representation of the six possible Slater determinants for a system with four particles, under the constraint of no broken pairs, total spin $S = 0$, considering only the four lowest levels $p = 1, 2, 3, 4$.

Solving the problem

In solving the system, one first has to set up the Hamiltonian matrix, with elements

$$H_{i,j} = \langle \Phi_i | \hat{H} | \Phi_j \rangle, \tag{4}$$

and then diagonalize the matrix to find the eigenvalues and eigenvectors. The ground state energy can then be found as the lowest eigenvalue, with the corresponding eigenvector giving the coefficients C.

FCI is exact, but computationally expensive, as the number of configurations grows factorially with the number of energy levels included. Approximative methods are therefore required.

Hatree-Fock theory

In Hatree-Fock theory, we seek to write the wave function as a single Slater determinant, that is, a single configuration of the system.

The wave function is then written as

$$|\Psi_0\rangle = |\Phi_0\rangle, \tag{5}$$

where $|\Phi_0\rangle$ is the Slater determinant that minimizes the energy.

The Hatree-Fock method is a variational method, and the energy is minimized by varying the coefficients in the Slater determinant.