Exercise No. 12: Second Quantization III

1. Two electrons are in plane wave states in a box. Calculate to first order in the Coulomb interaction the energy difference of parallel and anti-parallel spin alignments (the exchange interaction).

2. Consider a system of fermions with the Hamiltonian $H = H_0 + V$ where H_0 is a single-particle operator and V is a two-particle interaction. Let $|\psi_n\rangle$ be the multi-particle eigenstates of H so that $H|\psi_n\rangle = E_n|\psi_n\rangle$. The Hartree–Fock ground state is $|\Phi\rangle = \prod_{\mu \leq F} a_\mu^\dagger |0\rangle$, where F denotes the Fermi level.

   (a) Explain why the binding energy of a particle in a state $\lambda \leq F$ is given by $\epsilon_\lambda = \sum_n |\langle\psi_n|a_\lambda|\Phi\rangle|^2(E_0 - E_n)$ with $E_0 = \langle\Phi|H|\Phi\rangle$ the energy of the Hartree–Fock ground state.

   (b) Show that $\epsilon_\lambda = \langle\Phi|a_\lambda^\dagger[a_\lambda, H]|\Phi\rangle$.

   (c) Prove the relation $E_0 = \frac{1}{2}\langle\Phi|H_0|\Phi\rangle + \frac{1}{2}\sum_\lambda \epsilon_\lambda$.

3. (a) Calculate to first order in the inter-particle interaction $v(\mathbf{r} - \mathbf{r}')$ the energy of an $(N+1)$-particle system of spin $\frac{1}{2}$ fermions with one particle of momentum $\mathbf{p}$ outside an N-particle Fermi sea (a quasi-particle state). Repeat the computation for the state of $N-1$ particles with a particle of momentum $\mathbf{p}$ removed from an N-particle Fermi sea (a hole state). Measure the energies from the N-particle ground state energy.

   (b) Evaluate the quasi-particle and hole energies for a Coulomb interaction in the jellium model (uniform positive background).