1. Warm up on second quantization

Suppose we have a many-electron system with Coulomb interaction.

In the first quantization, the Hamiltonian can be written as

\[ H_1 = \sum_{i=1}^{N} -\frac{\hbar^2}{2m} \nabla_i^2 + U(r_i) \]

\[ H_2 = \frac{1}{2} \sum_{i \neq j} \frac{e^2}{|r_i - r_j|} \]

The easiest way to go from the first to the second quantization is through the field operator \( \psi^\dagger(r) \), which means the annihilation a particle at \( r \) with spin \( \sigma \). In terms of the field operator, \( H_1 \) and \( H_2 \) can be represented as

\[ H_1 = \int dr \ \psi_{\sigma}^\dagger(r) \left( -\frac{\hbar^2}{2m} \nabla^2 + U(r) \right) \psi_{\sigma}(r), \]

\[ H_2 = \frac{1}{2} \int dr_1 \ dr_2 \ \psi_{\sigma}^\dagger(r_1) \psi_{\sigma}^\dagger(r_2) \ \nu(r_1, r_2) \ \psi_{\sigma}(r_1) \psi_{\sigma}(r_2), \]

where \( \nu(r_1, r_2) = \frac{e^2}{|r_1 - r_2|} \).

a) Show that in a general single particle complete and orthogonal basis, by using the mode expansion

\[ \tilde{\psi}_\sigma(r) = \sum_{\omega} \phi_i(r) \ a_{\sigma \omega}, \]

where \( a_{\sigma \omega} \) is the annihilation operator for the state \( \phi_i(r) \).
we arrive at
\[ H_1 = \sum_{i,j} \langle i | H_1 | j \rangle a_i^{\dagger} a_j \]
\[ H_1 = \sum_{i,j} \left\{ \frac{\phi_i^*(w)\phi_j^*(w) + (\frac{\hbar^2}{2m} \nabla^2 + U(w)) \phi_i(w)\phi_j(w)}{1} \right\} a_i^{\dagger} a_j + a_i a_j^{\dagger} + a_i^{\dagger} a_j^* e^{i\kappa_0} \]

b) in the jellium model, \( U(w) \) is taken as constant. We can use the plane wave basis, i.e. \( \phi_{k\sigma} = \frac{1}{\sqrt{V}} e^{ikr} \) and \( a_{k\sigma}^* \). Show that
\[ H_1 = \sum_k \frac{-\hbar^2 k^2}{2m} a_{k\sigma} a_{k\sigma}^* \]
\[ H_2 = \frac{1}{2V} \sum_{k_1, k_2, q} V(q) \left( a_{k_1+q, \sigma} a_{k_1, \sigma} + a_{k_2, \sigma} a_{k_2, \sigma}^* \right) \]
(We assume the system is three dimensional).

2. Derive the Hartree-Fock equation from the variational principle.

a) Suppose we have a set of single particle basis \( \phi_{i_1}(w), \ldots, \phi_{i_n}(w) \) with associated annihilation operators \( a_{i_1, \sigma}, a_{i_2, \sigma}, \ldots, a_{i_n, \sigma} \).

Show that the expectation value of \( \langle \Psi | H | \Psi \rangle \), where
\[ |\Psi\rangle = a_{i_1, \sigma_1}^{\dagger} a_{i_2, \sigma_2}^{\dagger} \ldots a_{i_n, \sigma_n}^{\dagger} |0\rangle \] and \( H = H_1 + H_2 \) defined in problem 1, equals
\[ \langle \Psi | H | \Psi \rangle = \sum_{i, \omega_i} n_{\omega_i} \int dr \{ \phi_i^*(r) \left( -\frac{\hbar^2}{2m} \nabla^2 + U(r) \right) \phi_i(r) \}
\]

\[ + \frac{\alpha^2}{2} \sum_{j \neq o} n_{\omega_j} n_{\omega_o} \int dr dr' \left\{ \frac{1}{|r-r'|} \phi_i(r) \phi_i(r') \phi_j(r) \phi_j(r') \phi_o(r) \phi_o(r') \right\} \]

b) With the constraint \( \int dr |\phi_i(r)|^2 = 1 \) for \( i = 1, \ldots, n \),
show that, by variational principle, the Hartree-Fock equations read:

\[ \left\{ -\frac{\hbar^2}{2m} \nabla^2 + U(r) + \sum_{j \neq o} n_{\omega_j} \int dr' \frac{|\phi_j(r')|^2}{|r-r'|} \right\} \phi_i(r) |\sigma\rangle = \lambda_{i, \sigma} \phi_i(r) |\sigma\rangle, \]

where \( |\sigma\rangle \) is the spin eigenstate.

c) Show that, in the approximation of the jellium model,
the plane wave states where each electron fills in the Fermi sphere
satisfy the above equation.
Consider the state with every electron filling in the plane wave state in the Fermi sphere with Fermi wavevector $k_F$. The density correlation function is defined as

$$G(r, r') = \frac{\langle \varphi | \rho_\sigma (r) \rho_{\sigma'} (r') | \varphi \rangle - \langle \varphi | \rho_\sigma (r) | \varphi \rangle \langle \varphi | \rho_{\sigma'} (r') | \varphi \rangle}{\langle \varphi | \rho_\sigma | \varphi \rangle \langle \varphi | \rho_{\sigma'} | \varphi \rangle}.$$ 

a) Show that for $\sigma \neq \sigma'$, we have $G_{\sigma\sigma'} (r, r') = 0$.

b) Show that for $\sigma = \sigma'$, we have

$$G_{\sigma\sigma} (r, r') = - \left( \frac{1}{(2\pi)^3} \int d^3k \ e^{i \mathbf{k} \cdot (\mathbf{r} - \mathbf{r}')} \Theta (\mathbf{k}_F - \mathbf{k}_F) \right)^2$$

c) Do the above integral, and show

$$\frac{G_{\sigma\sigma} (r, r')}{\langle \varphi | \rho_\sigma | \varphi \rangle^2} = - 9 \left( \frac{x \cos x - \sin x}{x^3} \right)^2, \quad (x = \frac{k_F}{r-r'})$$

and plot this function.