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 $\psi^+_\sigma(r)$, 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

$$H_1 = \int d^3r \sum_\sigma \psi^+_\sigma(r) \left( -\frac{\hbar^2}{2m} \nabla^2 + U(r) \right) \psi^\sigma(r),$$

$$H_2 = \frac{1}{2} \int d^3r_1 d^3r_2 \psi^+_\sigma(r_1) \psi^+_\sigma(r_2) V(r_1 - r_2) \psi^\sigma(r_2) \psi^\sigma(r_1),$$

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

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

$$\psi^\sigma(r) = \sum_i \phi^\sigma_i(r) a_i \omega,$$

where $a_i \omega$ is the annihilation operator for the state $\phi^\sigma_i(r)$.
we arrive at
\[ H_1 = \sum_{i,j} \sum_{\sigma} \langle i | H_1 | j \rangle a^\dagger_{i \sigma} a_{j \sigma} = \sum_{ij} \left\{ \int \phi^*_i(r) \left( -\frac{\hbar^2}{2m} \nabla^2 + V(r) \right) \phi_j(r) \, dr \right\} a^\dagger_{i \sigma} a_{j \sigma} \]
\[ H_2 = \frac{\hbar^2}{2m} \sum_{ij \neq k} \int \, dr \, dr' \frac{\phi^*_i(r) \phi^*_j(r') \phi_i(r') \phi_j(r)}{r-r'} a^\dagger_{i \sigma} a^\dagger_{j \sigma} a_{i \sigma} a_{j \sigma} \]

b) In the jellium model, \( V(r) \) 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

\[ H_1 = \sum_k \frac{\hbar^2 k^2}{2m} a^\dagger_{k \sigma} a_{k \sigma}, \quad \text{and} \]
\[ H_2 = \frac{1}{2V} \sum_{k_1 k_2 q} V(q) \ a^\dagger_{k_1 - q, \sigma} a^\dagger_{k_2 + q, \sigma} a_{k_1 \sigma} a_{k_2 \sigma}, \quad \text{where} \ V(q) = \frac{4\pi e^2}{q^2}. \]

(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 \( \phi_{i_1}(r) \ldots \phi_{i_n}(r) \) with associated annihilation operators \( a_{i_1 \sigma}, a_{i_2 \sigma}, \ldots, a_{i_n \sigma} \). Show that the expectation value of \( \langle \Phi^- | H | \Phi^- \rangle \), where

\[ |\Phi^-\rangle = a^\dagger_{i_1 \sigma_1} a^\dagger_{i_2 \sigma_2} \ldots a^\dagger_{i_n \sigma_n} |10\rangle \quad \text{and} \quad H = H_1 + H_2 \quad \text{defined in problem 1}, \]

equals
\[
\langle \Psi | H | \Psi \rangle = \sum_{i,\omega_i} n_{i\omega_i} \int dr \left\{ \phi_i^*(r) \left( -\frac{\hbar^2}{2m} \nabla^2 + U(r) \right) \phi_i(r) \right\} \\
+ \frac{e^2}{2} \sum_{j,\omega} n_{j\omega} n_{j\omega'} \int dr dr' \left\{ \frac{1}{1r-r'1} \phi_i^*(r) \phi_j(r) \phi_j^*(r') \phi_i(r') \right\}
\]

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

\[
\left\{ -\frac{\hbar^2}{2m} \nabla^2 + U(r) + \sum_{j,\omega} n_{j\omega} \int dr' \frac{|\phi_j(r')|^2}{1r-r'1} \right\} \phi_i(r) |0\rangle
\]

\[
- \left\{ \sum_{j,\omega} n_{j\omega} \int dr' \frac{\phi_i^*(r') \phi_j(r')}{1r-r'1} \phi_i(r') |0\rangle \right\} = \lambda_{i,\sigma} \phi_i(r) |0\rangle,
\]

where \( |0\rangle \) 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.
(3) Exchange hole: \( \sqrt{\Psi} \)

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

\[
G_{\sigma\sigma'}(r, r') = \frac{\langle \Psi | \rho_{\sigma}(r) \rho_{\sigma'}(r') | \Psi \rangle - \langle \Psi | \rho_{\sigma}(r) | \Psi \rangle \langle \Psi | \rho_{\sigma'}(r') | \Psi \rangle}{\langle \Psi | \rho_{\sigma} | \Psi \rangle}.
\]

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

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

\[
G_{\sigma\sigma}(r, r') = -\left[ \frac{L}{(2\pi)^3} \int d^3k \ e^{ik \cdot (r-r')} \Theta (k - k_F) \right]^2.
\]

c) Do the above integral, and show

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

and plot this function.