Phys 211 B, HW problems (1)

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 σ. In terms of the field operator, H_1 and H_2 can be represented as

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

$$H_2 = \frac{1}{2}\int dr_1\, dr_2\, \psi_\sigma^\dagger(r_1)\,\psi_{\sigma'}^\dagger(r_2)\, V(r_1 - r_2)\, \psi_{\sigma'}(r_2)\, \psi_\sigma(r_1).$$

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

a) Show that in a general single particle complete and orthogonal $\underbrace{\text{basis}}_{\varphi_i(r)}$, by using the mode expansion

$$\psi_\sigma(r) = \sum_{i\sigma} \phi_i(r)\, a_{i\sigma},$$

where $a_{i\sigma}$ is the annihilation operator for the state $\varphi_i(r)$, we arrive at

$$H_1 = \sum_{i,j} \langle i | H_1 | j \rangle a_{i\sigma}^{\dagger} a_{j\sigma} = \sum_{ij} \left\{ \int \phi_i^*(r) \left(-\frac{\hbar^2}{2m} \nabla^2 + U(r) \right) \phi_j(r) dr \right\} a_{i\sigma}^{\dagger} a_{j\sigma}$$

$$H_2 = \frac{e^2}{2} \sum_{\substack{ijlk \\ \sigma\sigma'}} \int dr dr' \frac{\phi_i^*(r) \phi_j^*(r') \phi_l(r') \phi_k(r)}{|r-r'|} a_{i\sigma}^{\dagger} a_{j\sigma'}^{\dagger} a_{l\sigma'} a_{k\sigma}$$

b) in the jellium model, $U(r)$ is taken as constant. We can using the plane wave basis, i.e. $\varphi_{k\sigma}(r) = \frac{1}{\sqrt{V}} e^{i\vec{k}\vec{r}}$ and $a_{k\sigma}$. Show that

$$H_1 = \sum_k \frac{\hbar^2 k^2}{2m} a_{k\sigma}^{\dagger} a_{k\sigma}, \text{ and}$$

$$H_2 = \frac{1}{2V} \sum_{k_1 k_2 q} V(q) a_{k_1-q,\sigma}^{\dagger} a_{k_2+q,\sigma'}^{\dagger} a_{k_2\sigma'} a_{k_1\sigma}, \text{ where } V(q) = \frac{4\pi e^2}{q^2}.$$

(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 $\phi_{i1}(r) \cdots \phi_{in}(r)$ with associated annihilation operators $a_{i_1\sigma}$; $a_{i_2\sigma}, \cdots a_{in,\sigma}, \cdots$.

Show that the expectation value of $\langle \Psi | H | \Psi \rangle$, where $|\Psi\rangle = a_{i_1\sigma_1}^{\dagger} a_{i_2,\sigma_2}^{\dagger} \cdots a_{i_n\sigma_n}^{\dagger} |0\rangle$ and $H = H_1 + H_2$ defined in problem 1,

equals

$$\langle\Psi|H|\Psi\rangle = \sum_{i\sigma_i} n_{i\sigma_i} \int dr \left\{ \phi_i^*(r)\left(-\frac{\hbar^2}{2m}\nabla^2 + u(r)\right)\phi_i(r)\right\}$$

$$+ \frac{e^2}{2}\sum_{ij\sigma\sigma'} n_{i\sigma} n_{j\sigma'} \int dr dr' \left\{ \frac{|\phi_i(r)|^2 |\phi_j(r')|^2}{|r-r'|} - \delta_{\sigma\sigma'} \frac{\phi_i^*(r)\phi_j^*(r')\phi_j(r)\phi_i(r')}{|r-r'|} \right\}.$$

b) with the constraint $\int dr |\phi_i(r)|^2 = 1$ for $i=1,\cdots n$.

Show that, by the variational principle, the Hartree-Fock equations reads

$$\left\{-\frac{\hbar^2}{2m}\nabla^2 + u(r) + \sum_{j\sigma'} n_{j\sigma'} \int dr' \frac{|\varphi_j(r')|^2}{|r-r'|}\right\} \phi_i(r)|\sigma\rangle$$

$$-\left\{\sum_j n_{j\sigma'} \delta_{\sigma\sigma'} \int dr' \frac{\varphi_j^*(r')\varphi_j(r)}{|r-r'|} \phi_i(r')|\sigma\rangle\right\} = \lambda_{i,\sigma}\phi_i(r)|\sigma\rangle.$$

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.

③ exchang hole: $|\Psi\rangle$

Conside 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

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

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

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

$$G_{\sigma\sigma}(r r') = -\left[\frac{1}{(2\pi)^3}\int d^3\vec{k}\; e^{i\vec{k}\cdot(\vec{r}-\vec{r}')}\; \theta(k_F - k_F)\right]^2$$

c) Do the above integral, and show

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

and plot this function.