

PHYSICS 320: Problem Set No. 3
 Due: Fri. Sep. 11 2009

1. Consider the ground state of an electronic system of the sort discussed in class

$$|GS\rangle = \prod_m c_m^\dagger |0\rangle,$$

where $|0\rangle$ is the vacuum state and m labels the set of filled single particle states. $\{\psi_m(\mathbf{r})\}$ are the corresponding wavefunctions.

- (a) What is $\langle \rho(\mathbf{r}) \rangle$? $\rho(\mathbf{r})$ is the density operator and $\langle \dots \rangle$ denotes the expectation value in the state $|GS\rangle$.
- (b) Now, assume that the electron-electron interaction in a solid can be thought of as coming from each electron interacting with a “mean field” electron density $\langle \rho(\mathbf{r}) \rangle$ through the Coulomb interaction. Show that the resultant single electron Schrödinger equation you obtain contains the Hartree term but not the Fock term.

2. In deriving the Hartree-Fock (HF) equations, we obtained the following direct and exchange integrals

$$\begin{aligned} U_{\alpha\beta} &= \int \int d\mathbf{r}_1 d\mathbf{r}_2 |\psi_\alpha(\mathbf{r}_1)|^2 \frac{e^2}{|\mathbf{r}_1 - \mathbf{r}_2|} |\psi_\beta(\mathbf{r}_2)|^2, \\ J_{\alpha\beta} &= \int \int d\mathbf{r}_1 d\mathbf{r}_2 \psi_\alpha^*(\mathbf{r}_1) \psi_\beta^*(\mathbf{r}_2) \frac{e^2}{|\mathbf{r}_1 - \mathbf{r}_2|} \psi_\beta(\mathbf{r}_1) \psi_\alpha(\mathbf{r}_2). \end{aligned}$$

Let h_α be the expectation value of a one body term in the single particle state α . The occupied states from the set $\{\alpha\}$ are numbered from 1 to N in some way, where N is the total number of fermions in the system.

- (a) What is the total energy E of this many body state in HF theory?
- (b) What is the energy ϵ_α of the single particle state α ? Show that this energy can be interpreted as the energy required to add a particle to the state α .
- (c) From the above, you can see that $E \neq \sum_{\alpha=1}^N \epsilon_\alpha$. Why? Show that $E = \sum_{\alpha=1}^N e_\alpha$, where

$$e_\alpha = \epsilon_\alpha - \sum_{\beta=\alpha}^N (U_{\alpha\beta} - J_{\alpha\beta}).$$

Comment briefly on why this makes sense.

3. The expression for the single particle energy in the Jellium model

$$\epsilon(\mathbf{p}) = \frac{p^2}{2m} - \frac{e^2 p_F}{\pi \hbar} \left(1 + \frac{p_F^2 - p^2}{2p p_F} \log \left| \frac{p + p_F}{p - p_F} \right| \right),$$

where $p = |\mathbf{p}|$.

- (a) What is the density of states as a function of energy in the vicinity of the Fermi energy? Show that it is zero at the Fermi energy.
- (b) Now assume that the interaction between the electrons in the Jellium model is the screened Coulomb interaction of the form $e^{-\kappa r}/r$. Calculate the single particle energy $\epsilon(\mathbf{p})$ by putting this form of the interaction into the exchange term. Show that the density of states at the Fermi energy is no longer zero.

4. For small values of r_s , the electron system in the Jellium model can be treated perturbatively in the interaction.

- (a) Calculate the energy per electron as a function of r_s for the Jellium model in the HF approximation. Express your answer in Rydbergs. $1 \text{ ry} = me^4/2\hbar^2 = 13.6 \text{ eV}$. Remember that an electron has two possible spin states \uparrow and \downarrow .

(b) The energy calculated above is the first order correction to the energy of the free electron gas. It can be shown that the second order correction requires the calculation of terms which look like

$$\epsilon_{\alpha_1, \alpha_2}^{(2)} = -\frac{2m}{\hbar^2} \sum_{\alpha_3, \alpha_4} \frac{|\langle \alpha_1, \alpha_2 | V | \alpha_3, \alpha_4 \rangle|^2}{k_4^2 + k_3^2 - k_2^2 - k_1^2},$$

where α_1 and α_2 are short for the set of momentum and spin labels (\mathbf{k}_1, s_1) and (\mathbf{k}_2, s_2) . The form of this term comes from second order perturbation theory in V and corresponds to the scattering of two electrons in state α_1 and α_2 into virtual states α_3 and α_4 and back. Show that for $s_1 = s_2 = \uparrow$, $\epsilon_{\alpha_1, \alpha_2}^{(2)}$ is infinite in the following way:

i. First calculate

$$\langle \alpha_1, \alpha_2 | V | \alpha_3, \alpha_4 \rangle = \frac{1}{\Omega^2} \int \int d\mathbf{r} d\mathbf{r}' e^{i(\mathbf{k}_3 - \mathbf{k}_1) \cdot \mathbf{r}} \frac{e^2}{|\mathbf{r} - \mathbf{r}'|} e^{i(\mathbf{k}_4 - \mathbf{k}_2) \cdot \mathbf{r}'}.$$

Ω is the total volume of the system. (*Hint: It will help to use the Fourier transform of the Coulomb potential.*)

ii. Now, put the expression you obtain into the one for $\epsilon_{\alpha_1, \alpha_2}^{(2)}$ and show that the result is infinite. Convert the sums over momenta into integrals and use the identity

$$\int d\mathbf{k} f(\mathbf{k}) \delta(\mathbf{k} - \mathbf{k}_0) \delta(\mathbf{k} - \mathbf{k}_0) = f(\mathbf{k}_0) \Omega.$$

It might also help to define the variable $\mathbf{q} = \mathbf{k}_1 - \mathbf{k}_3$.

Remark: The Brueckner-Gellmann theory removes divergences like the one above by going to infinite order in perturbation theory. This involves summing a series of infinite terms with alternating signs to obtain a finite answer.

5. The HF approximation leads to ferromagnetism at sufficiently low densities as mentioned in class. To see this
 - (a) Calculate the energy per electron assuming they all have the same spin. This is the ferromagnetic state.
 - (b) Find the value of the electron density at which the above energy per electron becomes lower than that for an equal number of up and down spin electrons.
 - (c) Check the stability of the ferromagnetic state against the flipping of the spin of one electron.
6. Consider the simple model of a 3D Wigner crystal discussed in class, where each unit cell is taken to be an electrically neutral sphere. The sphere has a radius $r_s a_0$ with a single electron at its centre and uniform positive charge in its volume.
 - (a) The crystal can be treated classically to a first approximation and the total energy is just the sum of the electrostatic energies of each unit cell. Calculate this energy per unit cell as a function of r_s . Once again, express your answer in Rydbergs.
 - (b) The above calculation was classical. The first quantum correction comes from the zero point oscillation of the electron in each unit cell assuming the positive charges to be stationary. How does the zero point energy per unit cell scale with r_s ?