MATERIALS PHYSICS II FALL 2007 HOMEWORK PROBLEMS 3

Return to Robert (mailbox Physics 2nd floor) by Tuesday 2.10.2007 at noon.

Comment: working through the weekly problems as team work is completely acceptable and even recommended, as far as each person writes down and returns his/her own solutions!

1. The classical electrostatic energy of an electron density distribution $n(\mathbf{r})$ is

$$E_{es}[n] = \frac{e^2}{2}\int d\mathbf{r}\int d\mathbf{r}'\frac{n(\mathbf{r})n(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}.$$

Evaluate the functional derivative $\delta E_{es}/\delta n$.

2. Consider for simplicity a system of only two electrons. Approximate the total wave function $\Psi(\mathbf{r}_1 s_1, \mathbf{r}_2 s_2)$ with a Slater determinant. Derive the expectation value of the Hamiltonian, $E = <\Psi|H|\Psi>$, where $H = h_1(\mathbf{r}_1, s_1) + h_2(\mathbf{r}_2, s_2) + v(|\mathbf{r}_1 - \mathbf{r}_2|)$, apply the variational principle with Lagrange multipliers ϵ and recover Hartree-Fock equations.

3. Calculate Fourier transform $\tilde{\phi}_s(\mathbf{k})$ of the screened Coulomb potential (Yukawa potential) $\phi_s(\mathbf{r}) = -e\exp(-k_0 r)/r, \quad k_0 > 0$:

$$\tilde{\phi}_s(\mathbf{k}) = \int e^{-i\mathbf{k}\cdot\mathbf{r}}\phi_s(\mathbf{r})\,d\mathbf{r}.$$

What is the Fourier transform of the bare (unscreened) Coulomb potential $\phi(\mathbf{r})$?

4. Fill in the details of the derivation (lectures) of the single-electron eigenvalue, eq. (1) below, and the total energy of the system, eq. (2), for jellium. Use normalized plane waves as trial functions. F(x) is the Lindhard dielectric function and $x = k_i/k_F$. (Hint: Marder pp 212-214 or Ashcroft-Mermin pp. 334-336.)

$$\varepsilon_i = \frac{\hbar^2 k_i^2}{2m} - \frac{2e^2 k_F}{\pi}F(x) \qquad (1)$$

$$E = N\left(\frac{3}{5}\varepsilon_F - \frac{3}{4}\frac{e^2 k_F}{\pi}\right) \qquad (2)$$

5. Show that near the band minimum (**k=0**) the Hartree-Fock one-electron energy

$$\varepsilon(k) = \frac{\hbar^2 k^2}{2m} - \frac{2e^2 k_F}{\pi}F(x)$$

where $x = k/k_F$ and

$$F(x) = \frac{1}{4x}\left[(1-x^2)ln\left|\frac{1+x}{1-x}\right| + 2x\right]$$

is parabolic in k:

$$\varepsilon(k) \approx \frac{\hbar^2 k^2}{2m^*},$$

where m* is the effective mass:

$$\frac{m^*}{m} = \frac{1}{1 + 0.22(r_s/a_0)}.$$