MATERIALS PHYSICS II FALL 2004 HOMEWORK PROBLEMS 2

Return to Kimmo by Tuesday 21.9.2004 at 14:00

1. The classical electrostatic energy of an electron density distribution n(r) is

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

Evaluate the functional derivative $\delta E_{es}/\delta n$. **(1 point)**

2. Read through the material about Wigner crystals given in Thursdays (9.9.) lecture and answer briefly (max. a half page / question): **(3 points)**
(a) Describe the two melting mechanisms that are observed.
(b) Discuss the trends in the corresponding melting temperatures.
(c) What is a magic electron cluster?

3. (2 points) Derive the Koopman's theorem (See Marder problem 9.2). Start from the Hartree-Fock equations (9.33) and show that the single-particle eigenenergies are

$$\varepsilon_k = \int \psi_k^*(\mathbf{r}) h \psi_k(\mathbf{r}) d\mathbf{r} + \sum_j \iint v\{|\psi_k(\mathbf{r})|^2 |\psi_j(\mathbf{r}')|^2 - \psi_k^*(\mathbf{r})\psi_j^*(\mathbf{r}')\psi_j(\mathbf{r})\psi_k(\mathbf{r}')\} d\mathbf{r}\, d\mathbf{r}'. \quad (1)$$

Use equation (9.22) to show that the total energy

$$E = \sum_k \varepsilon_k - \sum_{k<j} \iint v\{|\psi_k(\mathbf{r})|^2 |\psi_j(\mathbf{r}')|^2 - \psi_k^*(\mathbf{r})\psi_j^*(\mathbf{r}')\psi_j(\mathbf{r})\psi_k(\mathbf{r}')\} d\mathbf{r}\, d\mathbf{r}' \quad (2)$$

Here $\psi_k(\mathbf{r})$ are the Hartree-Fock eigenfunctions, $h = -\hbar^2\nabla^2/2m + U(\mathbf{r})$ is the single-particle operator and $v(\mathbf{r} - \mathbf{r}') = e^2/|\mathbf{r} - \mathbf{r}'|$ is the interaction. One should notice that the total energy is not simply a sum over the eigenvalues.

Now assume that if the eigenfunctions and -values do not change appreciably when one electron is extracted from the highest level, the ionization energy is $E_N - E_{N-1} = \varepsilon_N$. This is known as Koopman's theorem.

Finally use the previous result (2) to show that the total energy in the jellium is given by the Marder's equation (9.48). Evaluate that sum to obtain the total energy of the jellium (result is given in eq. (9.49)).