MATERIALS PHYSICS II FALL 2007 HOMEWORK PROBLEMS 1

Return to Hannu (mailbox Nanobuilding 2nd floor) by Tuesday 18.9.2007 at noon

Comments: 1-3 should be easy, 4 requires thinking, help is available in books for 5 and 6 involves numerical work.

1. Derive the energy density of electron states, $D(\epsilon)$, for one-, two- and three-dimensional free-electron gas systems.

2. Derive the pressure of 3D free-electron gas at zero temperature.

3. Derive the bulk modulus of 3D free-electron gas.

4. *A simple model for a monovalent close-packed FCC metal.* Assume that the valence electron density of the metal (1 electron per atom) is uniformly distributed inside close-packed (touching) spheres, centered at fcc lattice sites. Let the radius of the spheres be R.
(a) Show that the electrostatic energy (electron-ion and electron-electron energy) of the electron in one sphere with a positive ion (charge $+e$) at the center, is given by

$$U_{es} = -\frac{9e^2}{40\pi\epsilon_0 R}.$$

(b) Show that the quantum mechanical kinetic energy of (free) electrons inside the sphere is

$$U_{kin} = \frac{3\hbar^2(9\pi/4)^{2/3}}{10mR^2}.$$

(c) The total energy per sphere (atom) in this model is then $U_T = U_{es} + U_{kin}$. Find the equilibrium distance between the nearest-neighbour atoms, R_{eq}, and the optimal total energy (= cohesive energy per atom), $U_T(R_{eq})$. Evaluate R_{eq} and $U_T(R_{eq})$ in Ångstroms and electron volts, respectively, and compare to experimental nearest-neighbour distances and cohesive energies of typical (monovalent) fcc-metals, like Cu, Ag and Au. (Cu: 3.61 Å and 3.49 eV; Ag: 4.09 Å and 2.95 eV ; Au: 4.08 Å and 3.81 eV)

5. *The Sommerfeld expansion.* The Sommerfeld expansion helps to evaluate integrals that are of the form

$$\int_{-\infty}^{\infty} H(\epsilon) f(\epsilon) d\epsilon \qquad (1)$$

and meet two conditions: (i) f is the Fermi function $f(\epsilon) = [exp((\epsilon - \mu)/k_B T) + 1]^{-1}$ and (ii) $H(\epsilon)$ vanishes at the lower limit of the integral and does not diverge faster than ϵ^k at the upper limit. Show that under these conditions, in the neighborhood of $\epsilon = \mu$, the integral (1) can be evaluated as

$$\int_{-\infty}^{\infty} H(\epsilon) f(\epsilon) d\epsilon = \int_{-\infty}^{\mu} H(\epsilon) d\epsilon + \sum_{n=1}^{\infty} (k_B T)^{2n} a_n \frac{d^{2n-1}}{d\epsilon^{2n-1}} H(\epsilon)|_{\epsilon=\mu}$$

where a_n:s are dimensionless constants

$$a_n = \int_{-\infty}^{\infty} \frac{x^{2n}}{(2n)!} (-\frac{d}{dx} \frac{1}{e^x + 1}) dx \quad ; \quad x = (\epsilon - \mu)/k_B T$$

Hint: See e.g., Marder p 146 , Ashcroft-Mermin Appendix C. (application to μ, C_v in Elliott p 209-301)

6. (a) Consider the electron density appropriate for aluminum. Assuming the conduction electrons (3 per atom, $s^2 p^1$) to be free noninteracting fermions, find the chemical potential numerically to two place accuracy at 0 K, 300 K, and 10000 K. (b) Estimate the chemical potential at these temperatures also from the Sommerfeld expansion (using the lowest nontrivial order) and compare with (a). Hint for (a): the key equations are

$$n = N/V = \int d\epsilon D(\epsilon) f(\epsilon), \qquad f(\epsilon) = 1/(exp(\beta(\epsilon - \mu)) + 1)$$