Solid State Physics

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Assignment II: Crystal Bonding, Free Electron & Band Theory

Submission due date: 30/05/2025

Q.1) The CsCl ionic crystal has a bcc structure. Ionic radii of Cs and Cl are 0.165nm and 0.181nm and their atomic weights are 133 and 35.5 respectively. Calculate the density of CsCl.

Q.2) Cohesive energy of a pair of atoms/molecules is given as a combination of attactive and repulsive potential $U(|\mathbf{r}|) = -\frac{a}{r^m} + \frac{b}{r^n}$, where the symbols have their usual meaning. Show that **(a)** the potential can be redefined into

$$U(|\mathbf{r}|) = -\frac{a}{r^m}\left[1 - \left(\frac{m}{n}\right)\frac{r_0^{n-m}}{r^{n-m}}\right],$$

and **(b)** the point of inflection (where slope and curvature both are zero) r_1 and point of minimum potential energy r_0 are related by

$$r_1 = r_0\left[\frac{n+1}{m+1}\right]^{(n-m)^{-1}}.$$

Q.3) Suppose that the energy of two particles in the field of each other is given by $U(|\mathbf{r}|) = -\frac{a}{r} + \frac{b}{r^8}$, where r is the distance between the centres of the particles. **(a)** Justify that the two particles form a stable compound for $r = r_0 = \left[\frac{8b}{a}\right]^{1/7}$ and **(b)** the potential energy of the two particles in stable configuration is $-\frac{7}{8}\frac{a}{r_0}$. **(c)** Hence demonstrate that if the particles are pulled apart, the molecules will break as soon as $r = \left[\frac{36b}{a}\right]^{1/7}$ and the minimum force required to break the molecule is $\left[\frac{7}{9}\right]\frac{a^{9/7}}{(36b)^{2/7}}$.

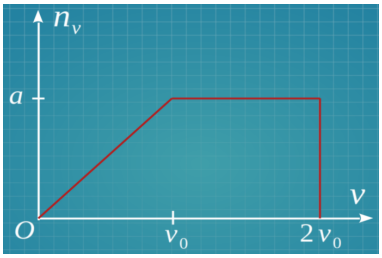
Q.4) **(a)** According to the Drude-Jellium model for a metal at temperature T, a conduction electron gets collided with an ion at time $t = 0$. Assuming that the temporal distribution of the electron to have another collision with an ion at time t is Poissonian,

$$p(t) = \frac{1}{\tau}e^{-t/\tau},$$

evaluate **(i)** the average, **(ii)** the (mean) square, and **(iii)** standard deviation (SD) of the time interval for the electron to have its next collission. Taking the obtained SD as the time uncertainty, estimate the quantum mechanical energy uncertainty and compare that with the energy uncertainty obtained classically (Maxwellian).

Q.5) **(a)** The quantity $(v - v_{rms})^2 = v^2 - 2vv_{rms} + v_{rms}^2$ is defined as the squared deviation of electron speed (Maxwellian) from root mean square (rms) speed. Calculate the rms deviation of this quantity for classical electron gas in metals. Given the average, root mean square and most probable speed are $\bar{v} = \sqrt{\frac{8k_BT}{m\pi}}, v_{rms} = \sqrt{\frac{3k_BT}{m}}$ and $v_m = \sqrt{\frac{2k_BT}{m}}$, where symbols have their usual meaning. **(b)** Show also that their exists 57% probability for the conduction electrons to have emerged with a speed greater than v_m.

Q.6)



Consider an imaginary speed distribution of an electron gas in a metal shown above, that consist of N conduction electrons with the number of electrons within velocity range v and $v + dv$ is given by $dn_v = n_v dv$. **(i)** Express the parameter 'a' that represents the maximum of n_v in terms of N and v_0. **(ii)** Mathematically obtain the distribution function $n_v(v)$ and **(iii)** using that, calculate $\bar{v}$ and v_{rms}. **(iv)** What fraction of the total electrons will have velocity between $3v_0/2$ and $2v_0$?

Q.7) **(a)** In Sodium, free electrons per cubic centimeter are 2.5×10^{28}. Calculate the Fermi energy and Fermi velocity. Given, $h = 6.625 \times 10^{-34} Js, m = 9.1 \times 10^{-31} kg$. **(b)** Consider Silver in the metallic state with one free electron per atom. Calculate the Fermi energy. Given, density of silver is $10.5 gm/cm^3$ and atomic weight is 108, $N = 6.02 \times 10^{23}/gmatom$. **(c)** Aluminium metal crystallites form fcc structure. If each atom contributes single electron as free electron and lattice constant $a = 4Å$, treating conduction electrons as free electron Fermi gas, calculate Fermi energy E_F, Fermi wave vector k_F and total kinetic energy per unit volume at $T = 0°K$.

Q.8) Show that **(a)** the number of possible wave functions in any energy band is equal to the number of unit cells, and **(b)** a band can accomodate $2N$ electrons, where N is the number of atoms in the crystal.

Q.9) **(a)** The potential of an electron in a one dimensional lattice is of the same type as that used in the Kronig-Penney model for the delta-function potential. In the limit $V_0 ab << \hbar^2/m$, find at $k = 0$ the energy of the lowest energy band. **(b)** For the same problem show that the band gap at $k = \frac{\pi}{a}$ is $2V_0 \frac{b}{a}$. **(c)** Also, show that the energy of the lowest energy band is $E = \frac{\hbar^2 P}{m a^2}$.

Q.10) **(a)** Show for a square lattice (in two dimensions) that the kinetic energy of a free electron at a corner of the first zone is higher than that of an electron at the midpoint of a side face of the zone by a factor of 2. **(b)** What is the corresponding factor for a simple cubic lattice (in three dimensions)? **(c)** What bearing might the earlier obtained result have on the conductivity of divalent metals?