

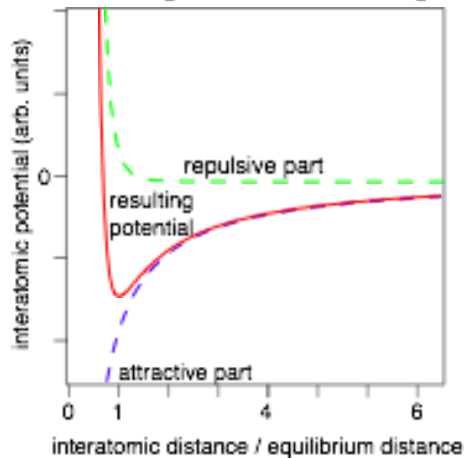
# Draft of solution Exam TFY4220, Solid State Physics, 28. May 2016.

## Problem 1 (20%) Introductory questions

(full answers can be found in the books and lecture notes, here just a few keywords.. )

1a) Lennard-Jones; Attractive from Coulomb and repulsive from Pauli principle..

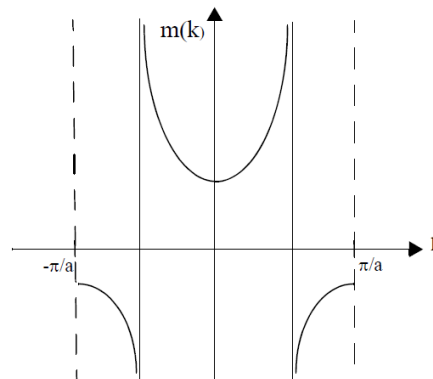
$$V_{LJ} = 4\epsilon \left[ \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^6 \right] = \epsilon \left[ \left( \frac{r_m}{r} \right)^{12} - 2 \left( \frac{r_m}{r} \right)^6 \right],$$



1b) Plot  $E(k)$  – some energies are forbidden, Electron Bragg scattering at zone boundaries, standing waves.. Fermi surface defined for metals. Surface in  $k$ -space with constant energy  $E_F$ . Chemical potential or Fermi level

1c) Fermi energy= the energy of the highest occupied single particle state at zero temperature (empty for higher energies and full for lower)

Fermi level (the chemical potential) = the thermodynamic work required to add one electron to the system, -the energy level of an electron, such that at thermodynamic equilibrium this energy level would have a 50% probability of being occupied at any given time (from Fermi-Dirac statistics), depends on temperature. At zero temperature, the energy  $E = \mu$  divides the occupied levels from the empty ones. Therefore,  $\mu(T = 0)$  is the Fermi energy. Fermi energy well defined for metals, Fermi level much more general, we use it in semiconductors.



1d) effective electron mass is inversely proportional to the curvature of the electron band. We include the effect of the periodic potential into the mass of the electron so that we still can use the free electron model.. mass is not changed, but the electron behave as if the mass is changed.. ) See book.

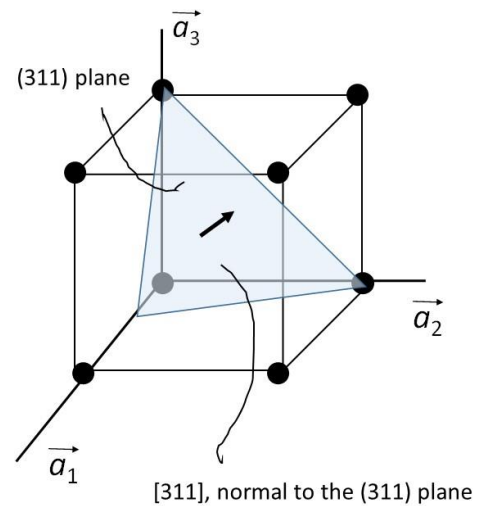
**Problem 2 (15%) Multiple Choices**

- 1 c)
- 2 b)
- 3 d)
- 4 a)
- 5 d)
- 6 c)
- 7 b)
- 8 a)
- 9 a)
- 10 b)

**Problem 3 (25%) Structure and Diffraction**

3a) For the (311) face, the intercept on the  $\mathbf{a}_1$  axis is  $1/3$  what it is on the  $\mathbf{a}_2$  and  $\mathbf{a}_3$  axes, because the Miller Index is the inverse of the intercepts. See figure. For a cubic material, the [311] direction will be normal to the (311) plane.

Calculation of distance between planes in a cubic crystal is done in exercise 4c) (can also be done in other ways, and also with  $(hkl) = (311)$ )



c) The unit plane normal is

$$\hat{\mathbf{n}} = \frac{\mathbf{n}}{|\mathbf{n}|} = \frac{h\mathbf{a}_1 + k\mathbf{a}_2 + l\mathbf{a}_3}{a\sqrt{h^2 + k^2 + l^2}}. \quad (14)$$

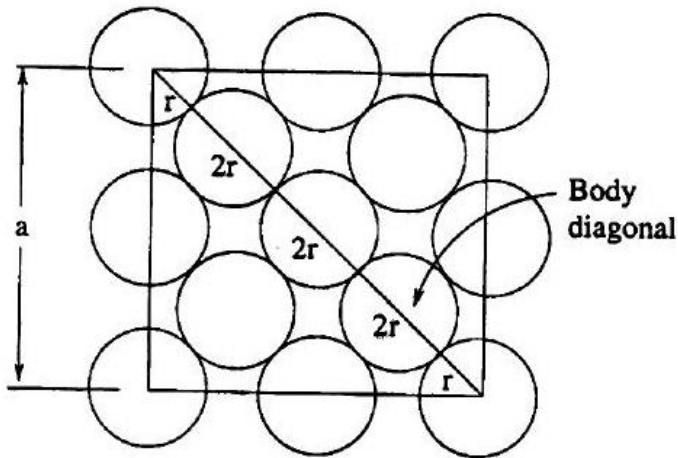
We may now find the distance between two neighbouring planes by translating along one of the lattice vectors and projecting this translation on the unit plane normal. Translating the full length of the lattice vector  $\mathbf{a}_1$  we pass  $h$  planes, such that the translation to get to the neighbouring plane is  $\mathbf{a}_1/h$ . The distance between two planes is therefore

$$d_{hkl} = \frac{1}{h} \mathbf{a}_1 \cdot \hat{\mathbf{n}} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}. \quad (15)$$

Translations along the other lattice vectors yield the same result.

In this case, with (hkl) equal (311) we have  $d_{311} = \frac{a}{\sqrt{3^2+1^2+1^2}} = \frac{a}{\sqrt{11}}$

3b) We should find the packing fraction of Si (diamond structure). We have two atoms in basis in a fcc structure, which give 8 atoms in the unit cell. Along the body diagonal there are 4 spheres with radius  $r$ , making  $8r = \sqrt{3} a$  which make the packing fraction equal  $\frac{V_{atoms}}{V_{unit\ cell}} = \frac{8 \cdot (4\pi/3)r^3}{a^3} = \frac{\sqrt{3}}{16} \approx 0.34$



First and second nearest neighbors; The atoms in the diamond structure have 4 nearest neighbors and 12 second nearest neighbors.

3c) NaCl Bravais lattice is fcc with two atoms (ions) in the basis; they are  $\text{Cl}^-$  in (000) and  $\text{Na}^+$  in  $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$

3d) Two atoms in basis – in this case  $\text{Cl}$  in (000) and  $\text{Na}$  in  $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ . This group repeats in all four Bravais lattice points  $(0,0,0)$ ,  $(\frac{1}{2}, \frac{1}{2}, 0)$ ,  $(0, \frac{1}{2}, \frac{1}{2})$  and  $(\frac{1}{2}, 0, \frac{1}{2})$

$S_G = F_{hkl} = \sum_j f_j \exp(-i\vec{G}_{hkl} \cdot \vec{r}_j)$  We have 8 atoms –  $\text{Cl}$  in  $(0,0,0)$ ,  $(\frac{1}{2}, \frac{1}{2}, 0)$ ,  $(0, \frac{1}{2}, \frac{1}{2})$  and  $(\frac{1}{2}, 0, \frac{1}{2})$  and

$\text{Na}$  in  $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ ,  $(0, 0, \frac{1}{2})$ ,  $(\frac{1}{2}, 0, 0)$  and  $(0, \frac{1}{2}, 0)$  This gives

$$F_{hkl} = f_{\text{Cl}}(1 + e^{\pi i(h+k)} + e^{\pi i(k+l)} + e^{\pi i(h+l)}) + f_{\text{Na}}(e^{\pi i(h+k+l)} + e^{\pi i(k)} + e^{\pi i(h)} + e^{\pi i(l)}) \text{ Can be simplified to}$$

$$F_{hkl} = (f_{\text{Cl}} + f_{\text{Na}} e^{\pi i(h+k+l)})(1 + e^{\pi i(h+k)} + e^{\pi i(k+l)} + e^{\pi i(h+l)})$$

This gives

$$F_{hkl} = 4(f_{\text{Cl}} + f_{\text{Na}}), \text{ hkl are all even (strong)}$$

$$F_{hkl} = 4(f_{\text{Cl}} - f_{\text{Na}}), \text{ for hkl all odd (weak)}$$

$$F_{hkl} = 0 \text{ hkl mixed (no reflection)}$$

3e) We see more reflections in KBr than in KCl. We see that the weak reflections from d) are extinct in KCl. The reason for this is that the atomic form factor for  $K^+$  and  $Cl^-$  are very similar. They are atom number 17 and 19, and as ions they have the same number of electrons. Between  $K^+$  and  $Br^-$  there is a difference of 8 electrons, and the atomic form factors will be different, contributing to some intensity in the weak reflections (which are the difference between the form factors)

3f) We can read out the scattering angle to be about 46,3 degrees. Using Bragg's law for the (311) reflection, and the formula for distance between planes found in a), we can find the wavelength to be:

$$2d \sin \theta = n\lambda$$

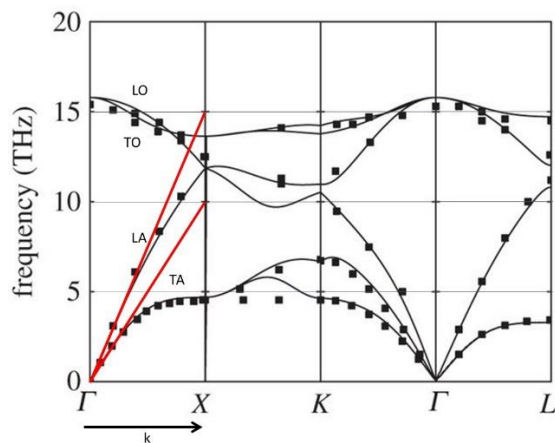
$$\lambda = 2 \cdot 6,598\text{\AA} / \sqrt{11} \cdot \sin(23,1) = 1.55\text{\AA}$$

Looks very reasonable..

#### Problem 4 (20%) Phonons

4a) wave vector  $k$  is the horizontal axis. Dispersion relation shows frequency as function of  $k$  vector -) The figure shows the dispersion relation for phonons in 3D, different directions in the reciprocal space. Two type of branches, optical and acoustical, LA and TA modes – In 3D and a with  $s$  atoms per primitive unit cell (in basis) we have  $3s$  dispersion curves,  $3$  acoustical and  $3s-3$  optical – here the two transversal modes are degenerated in some directions. We have 2 atoms in the primitive unit cell (basis). . (In fact, the material is Silicon – not asked for 😊 )

The acoustic waves are the ones going to zero when  $k$  goes to zero. Typically, longitudinal (compressive) waves travel faster in materials than transversal (shear) waves do, we therefore know that the lowest branch is the TA and the very highest is the LO branch. TA, LA, TO and LO are marked in the figure under. The wave vector  $k$  varies from zero at the  $\Gamma$  point, and increases along the different directions according to the figure to the right (in the exercise). The X point corresponds to the  $[100]$  direction.



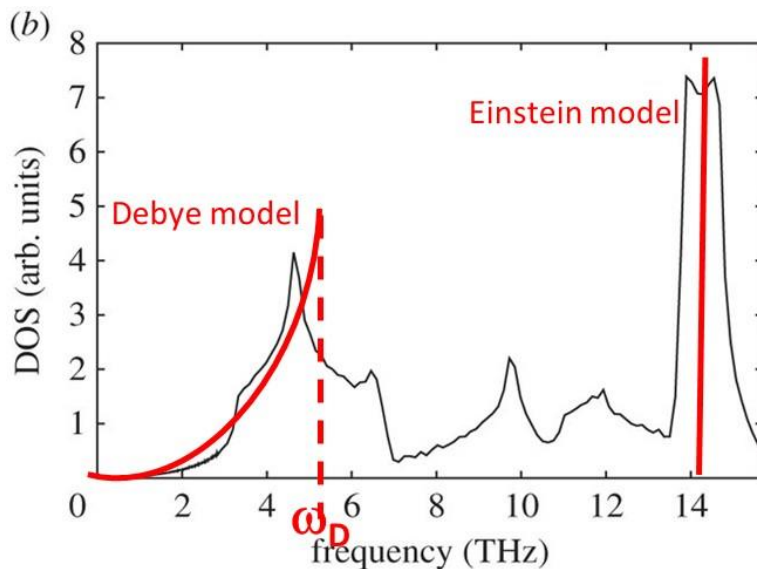
b) The density of states is the projection of states down to the c) We make a straight line from  $k=0$ , see red line in figure above, the slope will correspond to the speed of sound. The symmetry point X corresponds to  $(0, 0, 2\pi/a)$ , which gives a length of k-vector from  $\Gamma$  to X equal  $(2\pi/5.43) \text{ \AA}^{-1}$ . Speed of sound (Debye model) then given by

$$\text{TA: } v_T = \frac{d\omega(k)}{dk} = 10 \cdot 10^{12} \text{ Hz} \cdot 2\pi / (2\pi \cdot (5.43 \cdot 10^{-10} \text{ m})^{-1}) = 5400 \text{ m/s}$$

$$\text{LA: } v_L = \frac{d\omega(k)}{dk} = 15 \cdot 10^{12} \text{ Hz} \cdot 2\pi / (2\pi \cdot (5.43 \cdot 10^{-10} \text{ m})^{-1}) = 8150 \text{ m/s}$$

The tabulated values are 5840 m/s and 8430 m/s.

4c) To find the density of states for phonons, we project the dispersion relation down on the frequency axis, thinking of a quasi-continued dispersion relation. It will be like the one under, where the DOS for the two models are drawn in. The Debye model assumes a linear dispersion relation, which will give a parabola as a function of frequency (works best for low frequencies and low temperatures). The Einstein model assumes that all phonons have the same frequency, and will give a  $\sim$ delta function (works best for optical modes).



d) Umklapp processes – See Kittel and lecture notes (phonon-phonon scattering where total momentum is not conserved.. k-vector into another Brillouin zone, adds lattice vector  $G$ ) – Umklapp processes – anharmonic effects, limit thermal conductivity – increase thermal resistivity..

**Problem 5 (20%) Electrons – and semiconductors**

5a) We assume the conduction electrons are a free electron gas. No interaction with ions or lattice, or interaction between conduction electrons. Charged particles; follow the Pauli principle  $E(k) = \frac{\hbar^2}{2m} k^2$ . The Fermi energy is the highest occupied energy, corresponding to the Fermi energy wave vector  $k_F$ , corresponding to a sphere in 3D. The number of states inside the sphere with radius  $k_F$  is N. The volume in k-space which is occupied by one state is given so that the size of the material is  $V = L^3$  in real space; and is  $\left(\frac{2\pi}{L}\right)^3$ . There is one allowed wave vector for each  $\left(\frac{2\pi}{L}\right)^3$ . This will then give:

$$N = 2 \frac{\frac{4}{3} \pi k_F^3}{\left(\frac{2\pi}{L}\right)^3} = \frac{k_F^3 V}{3\pi^2} \text{ which gives } k_F = \left(\frac{3\pi^2 N}{V}\right)^{1/3} \text{ as should be shown. This gives the Fermi energy}$$

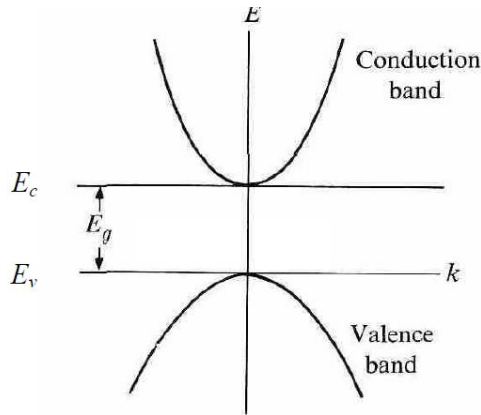
$$E_F = \frac{\hbar^2}{2m} \left(\frac{3N\pi^2}{V}\right)^{2/3} . \text{ From this expression we can now find the number of states less than E, given}$$

$$\text{by } N(E): E_F = \frac{\hbar^2}{2m} \left(\frac{3N(E)\pi^2}{V}\right)^{2/3}$$

$$\text{gives } N(E) = \frac{V}{3\pi^2} \left(\frac{E2m}{\hbar^2}\right)^{3/2} \text{ Then we can find}$$

$$D(E) = \frac{dN}{dE} = \frac{V}{3\pi^2} \left(\frac{2m}{\hbar^2}\right)^{3/2} \cdot \frac{3}{2} E^{1/2} = \frac{V}{2\pi^2} \left(\frac{2m}{\hbar^2}\right)^{3/2} E^{1/2} . \text{ We see that } C = \frac{V}{2\pi^2} \left(\frac{2m}{\hbar^2}\right)^{3/2}$$

5b)



We assume an empty conduction band and a filled valence band.

Assuming the free electron model we have for the valence band  $E = E_v - \frac{\hbar^2}{2m_h} k^2$  and for the conduction band  $E = E_c + \frac{\hbar^2}{2m_e} k^2$ . The masses are the effective masses..

Expression for the density of states  $D_c(E)$  in the conduction band is then (using results from a));

$$D_c(E) = \frac{V}{2\pi^2} \left( \frac{2m_e}{\hbar^2} \right)^{3/2} (E - E_c)^{1/2}.$$

We can do this  $f_e(E) = \frac{1}{e^{(E-\mu)/k_B T} + 1} \approx e^{-(E-\mu)/k_B T}$  because the band gap in semiconductors ( $\sim 1$  eV) is usually much larger than  $k_B T$  and therefore  $(E - \mu) \gg k_B T$ .

Concentration  $n$  of electrons in the conduction band:

$$n = \frac{N}{V} \int_{E_c}^{\infty} f_e(E) \cdot D(E) dE = \frac{1}{V} \int_{E_c}^{\infty} e^{-(E-\mu)/k_B T} \cdot \frac{V}{2\pi^2} \left( \frac{2m_e}{\hbar^2} \right)^{3/2} (E - E_c)^{1/2} dE$$

$$n = \frac{1}{2\pi^2} \left( \frac{2m_e}{\hbar^2} \right)^{3/2} e^{\mu/k_B T} \int_{E_c}^{\infty} e^{-E/k_B T} \cdot (E - E_c)^{1/2} dE$$

This was done in the lectures and in Kittel on page 206. We have to use the integral  $\int_0^{\infty} u^{1/2} e^{-u} du = \frac{\sqrt{\pi}}{2}$

The answer becomes:

$$n = 2 \left( \frac{m_e k_B T}{2\pi \hbar^2} \right)^{3/2} e^{\frac{(\mu - E_C)}{k_B T}}$$

In the same way we can find  $p$  to be equal to  $p = 2 \left( \frac{m_p k_B T}{2\pi \hbar^2} \right)^{3/2} e^{\frac{(E_V - \mu)}{k_B T}}$ .

When we calculate the product  $pn$ ,  $\mu$  will disappear, and with  $E_g = E_C - E_V$  we get the given formula -

$$np = 4 \left( \frac{k_B T}{2\pi \hbar^2} \right)^3 (m_e m_h)^{3/2} \cdot e^{(-E_g/k_B T)},$$

this shows the T dependence of the charge density concentration.

We can then calculate the chemical potential for the intrinsic semiconductor, by using the fact that  $n=p$ , and get :

$$\mu = \frac{E_g}{2} + \frac{3}{4} k_B T \ln \left( \frac{m_h}{m_e} \right)$$

5d) We introduce atoms with more electrons. That means, we will get a donor level inside the band gap, where electrons will very easily (at room temperature) be thermally excited to the conduction band. We will therefore have many more electrons in the conduction band. We will have an extrinsic, n-type semiconductor.  $n$  (concentration of charge carriers in the conduction band) will increase, the energy bands will move relative to the Fermi level (or chemical potential). The band gap of the original material will not change much, as the donor level is so close to the conduction band (P in Silicon is about 0.04 eV compared to the bandgap of 1.1 eV).

To change the band gap in a semiconductor we can alloy the system (add some Aluminium to GaAs for example). You can also add nanoparticles, or make quantum dots/2D/3D structures..