

## Solution to written exam in SOLID STATE PHYSICS F0053T AND F7045T

Examination date: 2017-06-02

The solutions are just suggestions. They may contain several alternative routes.

This is a combined solution for the courses F0053T and F7045T.

**For F0053T use solutions 1, 2, 3, 6 and 7.****For F7045T use solutions 1, 2, 3, 4, and 5.**

1. (a) The primitive vectors ( $\hat{a}_1$  and  $\hat{a}_2$ ) are: For structure A  $\hat{a}_1 = a$  and  $\hat{a}_2 = b$ . For structure B (the same as A)  $\hat{a}_1 = a$  and  $\hat{a}_2 = b$ . For structure C  $\hat{a}_1 = \frac{1}{2}(a + b)$  and  $\hat{a}_2 = \frac{1}{2}(a - b)$ .
- (b) For a direct lattice the relation  $\hat{a}_i \cdot \hat{a}_j^* = 2\pi\delta_{ij}$  defines the reciprocal lattice. As  $\hat{a}_1$  and  $\hat{a}_2$  are at right angles the reciprocal lattice vectors for structure A are  $\hat{a}_1^* = 2\pi \frac{\hat{a}_1}{|\hat{a}_1|^2}$  and  $\hat{a}_2^* = 2\pi \frac{\hat{a}_2}{|\hat{a}_2|^2}$ . The vectors  $\frac{\hat{a}_1}{|\hat{a}_1|}$  and  $\frac{\hat{a}_2}{|\hat{a}_2|}$  are unit vectors.
- (c) The general reciprocal lattice vector is  $\hat{G} = n\hat{a}_1^* + m\hat{a}_2^*$ . The scattering relation is  $k - k' = \Delta k = \hat{G}$ . The reciprocal vector can be written as  $\hat{G} = n2\pi \frac{\hat{a}_1}{\hat{a}_1 \cdot \hat{a}_2} + m2\pi \frac{\hat{a}_2}{\hat{a}_1 \cdot \hat{a}_2} = n2\pi \hat{i}/a_2 + m2\pi \hat{j}/a_1$ , where  $\hat{i}$  is a unit vector in the direction of  $\hat{a}_1$  and  $\hat{j}$  is a unit vector in the direction of  $\hat{a}_2$ . The desired form is  $\hat{G} = n2\pi \hat{i}/a_2 + m2\pi \hat{j}/a_1$ .

2. (a) From the graph it is evident that this experiment has been done at very low temperatures. One may assume that the temperature is well below the Debye temperature. The specific heat  $C_v$  will have a phonon contribution and a contribution from the free electrons:

$C_v = C_v^{el} + C_v^{ph}$ . The phonon contribution is (at low temperatures):

$$C_v^{ph} = \frac{12\pi^4}{5} Nk_B \left(\frac{T}{\Theta_D}\right)^3 = AT^3. \text{ The free electron contribution is: } C_v^{el} = \frac{\pi^2}{2} Nk_B \frac{T}{T_F} = \gamma T, \quad T_F = E_F/k_B$$

We draw a graph of  $C_v/T$  against  $T^2$  accordingly  $\frac{C_v}{T} = \frac{12\pi^4}{5\Theta_D^3} Nk_B T^2 + \frac{\pi^2 Nk_B^2}{2E_F} = \gamma + AT^2$ .

This will be a straight line in a graph of  $C_v/T$  against  $T^2$ .

- (b) The Debye temperature  $\Theta_D$  can be determined from the slope  $A = 2.57\text{mJ/mole K}^4$ .

$$\frac{12\pi^4}{5\Theta_D^3} Nk_B = A, \text{ solving for } \Theta_D \text{ gives } \Theta_D = 91.1\text{K}$$

- (c) From the intersection with the C/T axis we get  $\gamma = 2.08\text{mJ/mole K}^2$ . From this we get  $E_F$  accordingly to  $\gamma = \frac{\pi^2}{2} Nk_B \frac{k_B}{E_F}$  where  $E_F = 2.7209 \cdot 10^{-19}\text{J} = 1.698\text{eV}$ .

From crystal structure data we can calculate  $E_F$  Potassium has a BCC lattice with

$$a = 5.225\text{\AA}. \quad \epsilon_F = \frac{\hbar^2}{2m} \left(\frac{3\pi^2 N}{V}\right)^{\frac{2}{3}}$$

Now can calculate for the electron mass

$$m = \frac{\hbar^2}{2\epsilon_F} \left(\frac{3\pi^2 N}{V}\right)^{\frac{2}{3}} = \frac{(1.055 \cdot 10^{-34})^2}{2 \cdot 1.698 \cdot 1.601 \cdot 10^{-19}} \left(\frac{3\pi^2 \cdot 2}{(5.225 \cdot 10^{-10})^3}\right)^{\frac{2}{3}} = 1.138508 \cdot 10^{-30}\text{kg} = 1.25m_0$$

3. All have mono atomic cubic structure. Structure factor

$S_G(v_1 v_2 v_3) = \sum_j f_j e^{-i2\pi(v_1 x_j + v_2 y_j + v_3 z_j)}$ , BCC has atoms at  $x_1 = y_1 = z_1 = 0$  and  $x_2 = y_2 = z_2 = \frac{1}{2}$ , diffraction condition  $S = 0$  if  $v_1 + v_2 + v_3 = \text{odd integer}$ , and  $S = 2f$  if  $v_1 + v_2 + v_3 = \text{even integer}$ .

FCC has atoms at  $000, 0\frac{1}{2}\frac{1}{2}, \frac{1}{2}0\frac{1}{2}, \frac{1}{2}\frac{1}{2}0$ , diffraction condition

$S = 4f$  if  $v_1, v_2, v_3$  are all even integers or are all odd integers, and

$S = 0$  if one or two of  $v_1, v_2, v_3$  are even integers. The possible hkl are 111, 200, 220, 311, 222, 400 ...

And finally diamond (not primitive) is an FCC structure with basis consisting of two sites  $000, \frac{1}{4}\frac{1}{4}\frac{1}{4}$  ie a total of 8 sites (conventional cube) at  $000, 0\frac{1}{2}\frac{1}{2}, \frac{1}{2}0\frac{1}{2}, \frac{1}{2}\frac{1}{2}0, \frac{1}{4}\frac{1}{4}\frac{1}{4}, \frac{1}{4}\frac{3}{4}\frac{3}{4}, \frac{3}{4}\frac{1}{4}\frac{3}{4}, \frac{3}{4}\frac{3}{4}\frac{1}{4}$ . For Diamond an extra term is multiplied onto the FCC structure factor this consists of  $(1 + e^{-i\frac{\pi}{2}(h+k+l)})$  this will make some of the FCC lines to disappear when it is zero. The condition is  $\frac{\pi}{2}(h+k+l) = \pi(\text{odd integer})$ . The possible hkl are 111, 220, 311, 400, ... (Note the missing 200:  $2+0+0 = 2$  where  $2/2 = 1$  is an odd integer and 222:  $2+2+2=6$  where  $6/2=3$  is an odd integer.)

Braggs diffraction condition is  $2d(hkl) \sin(\theta) = \lambda$  where  $d(hkl) = a/\sqrt{h^2 + k^2 + l^2}$ .

(a) Start sorting out the bcc lattice (fcc and diamond are similar) and calculate ratios for,

$$\frac{\sin(\theta_1)}{\sin(\theta_2)} = \frac{\sqrt{h_1^2+k_1^2+l_1^2}}{\sqrt{h_2^2+k_2^2+l_2^2}}, \text{ smallest angles, (110) and (200) give ratio } \frac{\sqrt{2}}{\sqrt{4}} = 0.707. \frac{\sin(42.2/2)}{\sin(49.2/2)} = 0.865$$

$$\text{and } \frac{\sin(28.8/2)}{\sin(41.0/2)} = 0.710 \text{ and } \frac{\sin(42.8/2)}{\sin(73.2/2)} = 0.612. \text{ Sample B is BCC check also } \frac{\sin(28.8/2)}{\sin(50.8/2)} = 0.580$$

and  $\frac{\sqrt{2}}{\sqrt{6}} = 0.577$  seems fine. Now we have two samples left try them out for FCC smallest angle  $n = 1$ , (111) and (200) give ratio  $\frac{\sqrt{3}}{\sqrt{4}} = 0.866$ . we see directly that sample A is FCC this means that sample C has to be diamond.

A=fcc, B=bcc, C=diamond.

(b) Calculate  $a$  from Braggs diffraction condition we get  $a = \lambda\sqrt{h^2 + k^2 + l^2}/2 \sin(\theta)$ . This gives with  $\lambda = 1.5\text{\AA}$ . For bcc we get  $a = 1.5\sqrt{2}/2 \sin(28.8/2) = 4.26\text{\AA}$ . Similarly we arrive at  $a_{fcc} = 3.61\text{\AA}$  and for diamond structure (111) gives the smallest angle  $a_{diamond} = 3.56\text{\AA}$  (formfactor  $S_G = 4f(1 + i)$ ).

4. Varje molekyl ger 6 elektroner detta ger t theten  $n = 6 \cdot 6.02310^{23} \cdot 880/0.078 = 4.077 \cdot 10^{28} \text{m}^{-3}$ . hexagonen approximeras med en cirkel, omkrets =  $6 \times 1.4 \text{\AA} = 2\pi r$  och  $r^2 = (3 \cdot 1.4/\pi)^2$ . Detta ger (CK sid 419)
- $$\chi = -4.077 \cdot 10^{28} \cdot (1.60 \cdot 10^{-19})^2 4\pi \cdot 10^{-7} (3 \cdot 1.410^{-10}/\pi)^2 / (6 \cdot 9.1 \cdot 10^{-31}) = 4.310^{-6}$$

5. (a) At the maximum of absorption the photons have sufficient energy to excite electrons from the valence band to empty states just above the edge of the valence band. The energy of the Acceptor states is given by the photon energy  $E_a = \frac{hc}{\lambda}$  with  $\lambda = 59.1\mu\text{m}$  we get  $E_a = 0.021\text{eV}$
- (b) At room temperature  $T_{room} = 300\text{K}$  we have  $k_B T_{room} = 0.021\text{eV}$  and hence all acceptor states are ionised ie NO ABSORPTION (all acceptor states have already an electron so they are already occupied and the photons cannot excite an electron to already filled levels). The experiment is performed at very low temperatures (liquid He).
- (c) Photons with  $\lambda = 1700\text{\AA}$  have the energy  $E_a = \frac{hc}{\lambda} = 7.3\text{eV}$ . This tells us the following about the bandgaps:  
 $E_g^{\text{window glass}} < 7.3\text{eV} < E_g^{\text{quarts glass}}$

6. (a)  $i\hbar \frac{\partial^2}{\partial t^2} \cos \omega t = -i\hbar \omega \frac{\partial}{\partial t} \sin \omega t = -i\hbar \omega^2 \cos \omega t$  **YES**
- (b)  $\frac{\partial}{\partial x} e^{ikx} = ik e^{ikx}$  **YES**
- (c)  $\frac{\partial}{\partial x} e^{-ax^2} = -2ax e^{-ax^2}$  **NO**
- (d)  $\frac{\partial}{\partial x} \cos kx = -k \sin kx$  **NO**
- (e)  $\frac{\partial}{\partial x} kx = k$  **NO**
- (f)  $\hat{P} \sin(kx) = \sin(-kx) = -\sin(kx)$  **YES**
- (g)  $-i\hbar \frac{\partial}{\partial z} C(1+z^2) = -i\hbar C(0+2z)$  **NO**
- (h)  $-\frac{\hbar}{2} \frac{\partial}{\partial z} C e^{-3z} = -\frac{\hbar}{2} C(-3) e^{-3z} \propto \psi(z)$  **YES**
- (i)  $\frac{C}{2} (z^2 - \frac{\partial^2}{\partial z^2}) z e^{-\frac{1}{2}z^2} = ?$  This has to be done in some steps. Start by doing this derivative first:  $-\frac{\partial^2}{\partial z^2} z e^{-\frac{1}{2}z^2} = -\frac{\partial}{\partial z} (e^{-\frac{1}{2}z^2} - z^2 e^{-\frac{1}{2}z^2}) = -(-z e^{-\frac{1}{2}z^2} - 2z e^{-\frac{1}{2}z^2} + z^3 e^{-\frac{1}{2}z^2}) = 3z e^{-\frac{1}{2}z^2} - z^3 e^{-\frac{1}{2}z^2}$ .
- Now you go back to the start:  $\frac{C}{2} (z^2 - \frac{\partial^2}{\partial z^2}) z e^{-\frac{1}{2}z^2} = \frac{C}{2} (z^3 e^{-\frac{1}{2}z^2} + 3z e^{-\frac{1}{2}z^2} - z^3 e^{-\frac{1}{2}z^2}) = \frac{C}{2} (3z e^{-\frac{1}{2}z^2}) = \propto \psi(z)$  **YES**
7. (a) The total wave function has to be normalised which implies that the sum of the squared coefficients equals one.  $A^2(2^2 + 3^2 + 1^2 + 1^2) = 1$  resulting in  $A^2 = \frac{1}{15}$  and hence  $A = \frac{1}{\sqrt{15}}$ .
- (b) The probability is given by the absolute square of the coefficients.  
 $(\Psi(\mathbf{r}, t=0) = \frac{1}{\sqrt{15}} (2\psi_{100}(\mathbf{r}) - 3\psi_{210}(\mathbf{r}) + \psi_{320}(\mathbf{r}) - \psi_{322}(\mathbf{r})))$   
 The probabilities are (in order)  $\frac{4}{15}, \frac{9}{15}, \frac{1}{15}, \frac{1}{15}$ . as a check they sum up to 1 as they should do.
- (c) The energy of a single eigenstate is given by:  $E_n = -\frac{13.56}{n^2}$  eV. The expectation value is given by  $\langle E \rangle = \frac{4}{15} (-\frac{13.56}{1^2}) + \frac{9}{15} (-\frac{13.56}{2^2}) + \frac{1}{15} (-\frac{13.56}{3^2}) + \frac{1}{15} (-\frac{13.56}{3^2}) = -13.56 (\frac{4}{15} + \frac{9}{60} + \frac{1}{135} + \frac{1}{135}) = -13.56 \frac{233}{540} = -5.807868 \approx -5.81$  eV
- The operator  $\mathbf{L}^2$  has eigenvalues  $\hbar^2 l(l+1)$ . The expectation value is given by  $\langle \mathbf{L}^2 \rangle = \frac{4}{15} \cdot 0 + \frac{9}{15} \cdot (\hbar^2 1(1+1)) + \frac{1}{15} (\hbar^2 2(2+1)) + \frac{1}{15} (\hbar^2 2(2+1)) = \frac{30}{15} \hbar^2 = 2\hbar^2$
- The operator  $L_z$  has eigenvalues  $\hbar m_l$ . The expectation value is given by  $\langle L_z \rangle = \frac{4}{15} \cdot 0 + \frac{9}{15} \cdot 1\hbar + \frac{1}{15} \cdot 0 + \frac{1}{15} (2\hbar) = \frac{11}{15} \hbar$