

Solution to written exam in SOLID STATE PHYSICS F0053T AND F7045T

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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 unit cell: Cu fcc: 1, K bcc: 1, Po sc: 1.
 (b) The cubic unit cell: Cu fcc: 4, K bcc: 2, Po: 1.
 (c) Copper has fcc structure with a side length of the unit cube cell of $a = 3.61\text{\AA}$. Nearest neighbours like $(0,0,0)$ and $(\frac{1}{2}, \frac{1}{2}, 0)$ have a distance of $\sqrt{2}\frac{a}{2} = \frac{a}{\sqrt{2}} = 2.55\text{\AA}$. Next nearest neighbours like $(0,0,0)$ and $(0,0,1)$ have a distance $a = 3.61\text{\AA}$.
2. $C_v = C_v^{el} + C_v^{ph}$. As the temperature in question (300K) is well above the Debye temperature (160K) we can use Dulong-Petits law for the phonons $C_v^{ph} = 3Nk_B$. For the electron contribution $C_v^{el} = \frac{\pi^2}{2}Nk_B\frac{T}{T_F}$, $T_F = E_F/k_B$ and $E_F = \frac{\hbar^2}{2m} \left(\frac{3\pi^2 N}{V} \right)^{2/3}$. For Na we have $\rho = 971\text{kg/m}^3$, atomic weight = 22.9898u some calculations gives $T_F = 36599.353\text{K}$. Fraction contributed by the electrons: $F = \frac{C_v^{el}}{C_v^{el} + C_v^{ph}} = \frac{1}{1 + \frac{6T_F}{\pi^2 T}} \approx 0.0133$.
3. **Stephane:** Svaret på c från annan uppgift. I c startar man från c_v data.

- (a) We start to determine v_{sph} first. Data for: Ar has fcc structure and $a = 5.31\text{\AA}$. One mole contains $6.0221 \cdot 10^{23}$ atoms. In the Debye approximation we have for the specific heat C_v

$$C_v = \frac{12\pi^4}{5} Nk_B \left(\frac{T}{\Theta} \right)^3 \quad (1)$$

where $k_B = 1.3807 \cdot 10^{-23}$ J/K is Boltzmanns constant and Θ is the Debye temperature. Start to determine Θ from the slope of the line, $slope = 2.57269$ mJ/mol K⁴.

$$\Theta = \sqrt[3]{\frac{12\pi^4 Nk_B}{5 \cdot slope}} = 91.0801\text{K} \quad (2)$$

From the Debye temperature Θ we can determine the velocity of sound.

$$\Theta = \frac{\hbar v_{sph}}{k_B} \sqrt[3]{\frac{N6\pi^2}{V}} \quad (3)$$

and we solve for v_{sph}

$$v_{sph} = \frac{\Theta k_B}{\hbar} \sqrt[3]{\frac{V}{N6\pi^2}} = 1023 \text{ m/s} \approx 1.0 \text{ km/s} \quad (4)$$

- (b) Now we continue with the phonon dispersion figure, and we restrict it to the part of the figure marked by [1 0 0]. As the frequency ω is related to the wavevector k by

$$\omega = kv_{disp} \quad (5)$$

for small k we have to determine the slope of the dispersion graph for small k and we have v_{disp} .

The meaning of [1 0 0] is the direction we go from $k = 0$ out to the Brillouin zone boundary. The direction is given in conventional cube directions. Referring to Fig 15 page 43 Kittel this means going from the centre along the x (or y or z) direction to the small square on the side of the conventional cube. The separation between [1 0 0] planes in an fcc structure is $a/2$ and hence the zone boundary is at $2\pi/a$ and therefore $k_{max} = 2\pi/a$ at the zone boundary.

- i. line with large slope. At $\epsilon = 10.0\text{MeV}$ the reduced $k/k_{max} = k_{red}$ is 0.80 and we get

$$v_1 = \frac{\epsilon a}{\hbar 2 \pi k_{red}} = \frac{10.0 \cdot 10^{-31} \cdot 1.60218 \cdot 10^{-19} \cdot 5.31 \cdot 10^{-10}}{1.05457 \cdot 10^{-34} \cdot 0.80 \pi 2} \text{ m/s} = 1604.9465 \text{ m/s} \approx 1.60 \text{ km/s} \quad (6)$$

- ii. line with small slope. At $\epsilon = 10.0\text{MeV}$ reduced k_{red} is 1.13 and we get

$$v_2 = \frac{\epsilon a}{\hbar 2 \pi k_{red}} = \frac{10.0 \cdot 10^{-31} \cdot 1.60218 \cdot 10^{-19} \cdot 5.31 \cdot 10^{-10}}{1.05457 \cdot 10^{-34} \cdot 1.13 \pi 2} \text{ m/s} = 1136.2453 \text{ m/s} \approx 1.14 \text{ km/s} \quad (7)$$

- (c) We see that v_{sph} and the v_{disp} agree fairly well. One expects v_{sph} to be somewhere in the range of v_{disp} . However from web-elements (<http://www.shef.ac.uk/chemistry/web-elements/>) we find (bulk properties) $v_{sound} = 319$ m/s in agreement with the calculation for v_{disp} . For other inert gases we find He 970 m/s, Ne 936 m/s, Kr 1120 m/s and Xe 1090 m/s. So Argon seems to be an outsider, but one has to be careful how the experiments are done in detail (here we have single crystal properties).

4. The number of Bohr magnetons is given by $p = g\sqrt{J(J+1)}$ where $g = 1 + \frac{J(J+1)+S((S+1)-L(L+1))}{2J(J+1)}$.

		m_l							S	L	J	g	p
		-3	-2	-1	0	1	2	3					
Cr ³⁺	d ³				↑	↑	↑		3/2	3	3/2	2/5	0,775
Cu ³⁺	d ⁹		↑	↑↓	↑↓	↑↓	↑↓		1/2	2	5/2	1,2	3,55
Tb ³⁺	f ⁸	↑	↑	↑	↑	↑	↑	↑↓	3	3	6	3/2	9,72

5. (a) Germanium is a semiconductor with a band gap of $E_g = 0.67\text{eV}$. Doping it with Phosphorus (P) that is an element VI element, that makes it a donor impurity. The ionization energy is 12.0 meV. As room temperature is about 25 meV this will ionize all the donor atoms. The molar weight of Germanium is $M_{Ge} = 72,64\text{g/mole}$ and for Phosphorus it is $M_P = 30,97\text{g/mole}$. Density of Germanium $\rho_{Ge} = 5323\text{kg/m}^3$.

Calculate the number of donor atoms

$$N_d = 3.191mg = \frac{6,022 \cdot 10^{23} \cdot 3.191 \cdot 10^{-3}}{30,97} = 6.20478 \cdot 10^{19} \quad (8)$$

The volume of one kg of Germanium is $V_{Ge} = \frac{1}{5323} = 1.87864 \cdot 10^{-4} \text{m}^3$.

At room temperature all donors are ionized. The density of ionized donors will be

$$N_d^+ = \frac{6.20478 \cdot 10^{19}}{1.87864 \cdot 10^{-4}} = 3.3028 \cdot 10^{23} \text{m}^{-3}. \quad (9)$$

The condition for neutrallity is

$$n = N_d^+ + p. \quad (10)$$

The law of mass action gives:

$$n * p = n_i^2 = 4 \left(\frac{k_B T}{2\pi\hbar^2} \right)^3 (m_e m_h)^{3/2} e^{-E_g/k_B T} \quad (11)$$

$$n_i = 2 \left(\frac{1.3806 \cdot 10^{-23} \cdot 293}{2\pi \cdot 1.054^2 \cdot 10^{-68}} \right)^{3/2} (1.2 \cdot 0.2)^{3/4} (9.1094 \cdot 10^{-31})^{3/2} e^{-(0.67 \cdot 1.6022 \cdot 10^{-19}/2 \cdot 1.3806 \cdot 10^{-23} \cdot 293)} \quad (12)$$

$$n_i = 1.4373 \cdot 10^{19} \text{m}^{-3}. \quad (13)$$

We see that $n_i \ll N_d^+$ and using equation 10 we conclude that all electrons in the conduction band originate from ionized donors. Ie $n \approx N_d^+$ and $p \approx 0$.

(b) donor and n type

(c) For the graph.

I In the high temperatures behaviour will be intrinsic $n = p = n_i \propto e^{-E_g/2k_B T}$ and $n > N_d^+$.

II For a intermediate temperature range (including room temperature) the n and p will be fairly constant, $n \approx N_d^+$ and $p \approx 0$.

III As temperature is lowered further the concentrations will change as electrons are caught by the ionized donors. As temperature is lowered $n \approx N_d^+$ will go to zero exponentially.

6. (a) $i\hbar \frac{\partial^2}{\partial t^2} \sin \omega t \cos \omega t = i\hbar \omega \frac{\partial}{\partial t} (\cos^2 \omega t - \sin^2 \omega t) = -i\hbar \omega^2 2(\sin \omega t \cos \omega t) \propto \psi(t)$ **YES**
- (b) $i\hbar \frac{\partial^2}{\partial t^2} (\cos^2 \omega t - \sin^2 \omega t) = -i\hbar \omega^2 4 \frac{\partial}{\partial t} (\sin \omega t \cos \omega t) = -i\hbar \omega^2 4(\cos^2 \omega t - \sin^2 \omega t) \propto \psi(t)$ **YES**
- (c) $\frac{\partial}{\partial x} \sin kx = k \cos kx \propto \psi(x)$ **NO**
- (d) $\frac{\partial}{\partial x} kx^2 = k2x \propto \psi(x)$ **NO**
- (e) $\frac{C}{2} (z^2 - \frac{\partial^2}{\partial z^2}) z e^{-\frac{1}{2}z^2} = ?$ 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**
- (f) $\frac{\partial}{\partial x} (e^{ikx} + e^{-ikx}) = ik(e^{ikx} - e^{-ikx}) \propto \psi(x)$ **NO**
- (g) $\hat{P} \cos(kx) = \cos(-kx) = \cos(kx) = \psi(x)$ **YES**
- (h) $-\frac{\hbar}{2} \frac{\partial}{\partial z} C e^{-\omega z} = -\frac{\hbar}{2} C (-\omega) e^{-\omega z} \propto \psi(z)$ **YES**

(i) $-i\hbar\frac{\partial}{\partial z}C(1+z^3) = -i\hbar C(0+3z^2) \approx \psi(z)$ **NO**

7. This is a 2 dimensional problem with a Schrödinger equation (where $V(x, y) = 0$) like

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\Psi(x, y) - \frac{\hbar^2}{2m}\frac{d^2}{dy^2}\Psi(x, y) = E\Psi(x, y)$$

This equation is separable and the ansatz $\Psi(x, y) = \psi(x) * \psi(y)$ gives the following result

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi_x(x) - \frac{\hbar^2}{2m}\frac{d^2}{dy^2}\psi_y(y) = E_x\psi_x(x) + E_y\psi_y(y)$$

ie two independent one dimensional Schrödinger equations one for the variable x and one for y . We therefore solve the one dimensional problem first and after that we construct the two dimensional solution. To find the eigenfunctions we need to solve the Schrödinger equation which is (in the region where $V(x)$ is zero)

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\Psi = E\Psi \rightarrow \frac{d^2}{dx^2}\Psi + k^2\Psi = 0 \text{ where } k^2 = \frac{2mE}{\hbar^2}$$

Solutions are of the kind:

$$\Psi(x) = A \cos kx + B \sin kx$$

Now we need to take the boundary conditions for the wave function Ψ ($\Psi(-\frac{a}{2}) = \Psi(\frac{a}{2}) = 0$) into account.

$$A \cos(-\frac{ka}{2}) + B \sin(-\frac{ka}{2}) = 0 \text{ and } A \cos(\frac{ka}{2}) + B \sin(\frac{ka}{2}) = 0$$

Adding the two conditions gives: $\cos(\frac{ka}{2}) = 0$ and subtracting them gives $\sin(\frac{ka}{2}) = 0$. These two conditions cannot be fulfilled at the same time, so either A or B has to be zero. We start with $A = 0$ and we get the following solution: The normalising constant $B = \sqrt{\frac{2}{a}}$ you get from the condition $\int_{-a/2}^{a/2} |\Psi|^2 dx = 1$. The condition $\sin(\frac{ka}{2}) = 0$ gives $\frac{ka}{2} = \frac{\pi}{2} * (\text{even} - \text{integer})$. The solution is:

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right) \text{ with eigenenergies } E_n = \frac{n^2\pi^2\hbar^2}{2Ma^2} \text{ where } n = 2, 4, 6, \dots \quad (14)$$

In a similar way the other function is analysed ($A = 0$) which gives: The condition $\cos(\frac{ka}{2}) = 0$ gives $\frac{ka}{2} = \frac{\pi}{2} * (\text{odd} - \text{integer})$. The solution is:

$$\psi_n(x) = \sqrt{\frac{2}{a}} \cos\left(\frac{n\pi x}{a}\right) \text{ with eigenenergies } E_n = \frac{n^2\pi^2\hbar^2}{2Ma^2} \text{ where } n = 1, 3, 5, \dots \quad (15)$$

The eigenfunctions in the y direction are the same as for the x direction as the potential is similar for this direction. Now we have the eigenfunctions of the one dimensional problem and the solution to the 2 dimensional problem is readily produced. The eigenfunctions are:

$$\Psi_{n,m}(x, y) = \psi_n(x) \cdot \psi_m(y) \text{ eigenenergies } E_{n,m} = E_n + E_m \text{ where } n = 1, 2, \dots \text{ and } m = 1, 2, \dots \quad (16)$$

In the area where the potential is infinite the wave function is equal to zero.

An **alternative route** taken by many students has been to present a calculation with the following boundary conditions: Ψ ($\Psi(0) = \Psi(a) = 0$) into account. In this case the solution is for these boundary conditions:

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right) \text{ with eigenenergys } E_n = \frac{n^2\pi^2\hbar^2}{2Ma^2} \text{ where } n = 1, 2, 3, \dots \quad (17)$$

This solution has to be adapted to the boundary conditions related to this exam problem:

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}\left(x + \frac{a}{2}\right)\right) \text{ with eigenenergys } E_n = \frac{n^2\pi^2\hbar^2}{2Ma^2} \text{ where } n = 1, 2, 3, \dots \quad (18)$$

$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a} + \frac{n\pi}{2}\right) = \sqrt{\frac{2}{a}} \left(\sin\left(\frac{n\pi x}{a}\right) \cdot \cos\left(\frac{n\pi}{2}\right) + \cos\left(\frac{n\pi x}{a}\right) \cdot \sin\left(\frac{n\pi}{2}\right)\right)$. We see that we recover the solution in eq (14), (15) and (16) as we let n run from 1 to ∞ .

b) Now we turn to the question of **parity**, ie whether the wave function is *odd* or *even* under a change of coordinates from (x, y) to $(-x, -y)$. The one dimensional eigenfunctions in eq (14) and (15) have a definite parity. The functions in (14) are odd whereas the functions in (15) are even. As the eigenstates for the 2 dimensional system are formed from eq (16) ie products of functions that are even or odd the total function itself will be either even or odd as well.

The four lowest eigenenergies are given by

$$E_{n,m} = \frac{\pi^2\hbar^2}{2Ma^2}(n^2 + m^2), \text{ where the 4 lowest are } (n^2 + m^2) = 2, 5, 8, 10.$$

When we form the eigenstates we need to keep track of the parity of the $\psi_n(x)$ and $\psi_m(y)$. It is therefore necessary to have the functions in the form like in eq (14) and (15) to identify the parity as odd or even. This is difficult if you try with functions like eq (18) even though it is a correct eigenstate it is hard to identify their parity.

$$\begin{aligned} E_{1,1} &= \text{one state } (n^2 + m^2 = 2) & \mathbf{even * even} &= \text{even} \\ E_{1,2} = E_{2,1} &= \text{two states } (n^2 + m^2 = 5) & \mathbf{odd * even} &= \text{odd} \\ E_{2,2} &= \text{one state } (n^2 + m^2 = 8) & \mathbf{odd * odd} &= \text{even} \\ E_{1,3} = E_{3,1} &= \text{two states } (n^2 + m^2 = 10) & \mathbf{even * even} &= \text{even} \end{aligned}$$

So of the four energies (states) only one is **odd** and three are **even**.