

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) 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):

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

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 Θ_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

$$a = 5.225 \text{ \AA} \text{ (PH)} \text{ or } a = 5.23 \text{ \AA} \text{ (Fysika)}. \text{ The Fermi energy is given by } \epsilon_F = \frac{\hbar^2}{2m} \left(\frac{3\pi^2 N}{V} \right)^{\frac{2}{3}}.$$

Now we can calculate for the electron mass

$$m = \frac{\hbar^2}{2\epsilon_F} \left(\frac{3\pi^2 N}{V} \right)^{\frac{2}{3}} = \frac{(1.05457 \cdot 10^{-34})^2}{2 \cdot 1.698 \cdot 1.6022 \cdot 10^{-19}} \left(\frac{3\pi^2 \cdot 2}{(5.225 \cdot 10^{-10})^3} \right)^{\frac{2}{3}} = 1.138508 \cdot 10^{-30} \text{ kg} = 1.25 m_0$$

We may also calculate $\frac{N}{V}$ as follows. In Fysika we find the density $\rho = 862 \text{ kg/m}^{-3}$ and the molar weight $M = 39,0938 \text{ g/mole}$. $\frac{N}{V} = \frac{\rho N_A}{M} \frac{862 \cdot 6.02214 \cdot 10^{23}}{39,0938 \cdot 10^{-3}} = 1.327854 \cdot 10^{28} \text{ m}^{-3}$.

Now we can calculate for the electron mass

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2. Använd Braggs lag för att bestämma miller indexen (hkl) för topparna. $d = \lambda/(2 \sin(\beta/2))$ där d är plan avståndet och $\beta/2 = \theta$. Vidare har vi för planavståndet $\left(\frac{d_{hkl}}{a} \right)^2 = \frac{1}{h^2 + k^2 + l^2}$ där a är enhetskubens kantlängd (ej känd). Följande tabell görs upp för att bestämma $h^2 + k^2 + l^2$ för topparna. Våglängden för $K_\alpha = 1,542 \text{ \AA}$. Det kan vara svårt att avgöra vilken topp som är först i spektrat. Vi satsar till att börja med att den första är den kraftiga toppen vid 31 grader. De två första försöken (f1 och f2 i tabellen) visar att det blir ingen ordning på siffrorna. Tredje försöket (f3) där fungerar det.

(β)	27.50	31.04	45.60	56.58	66.34	75.36	84.06
$(\theta = \beta/2)$	13.75	15.52	22.80	28.29	33.17	37.68	42.03
d	3.2438	2.8814	1.9896	1.6268	1.4092	1.2613	1.1516
$1/d^2$	0.095038	0.12045	0.25262	0.37786	0.50356	0.62858	0.75404
f1 $x = 2/0.12045$		2.0000	4.1946	6.2741			
f2 $x = 3/0.12045$		3.0000	6.2919	9.4112			
f3 $x = 3/0.095038$	3.0000	3.8021	7.9741	11.9276	15.8955		
<i>integers</i>	3	4	8	12	16		

Sista raden i tabellen ger de sökta heltalen $h^2 + k^2 + l^2$.

En analys av strukturfaktorn för de 4 kubiska gittren ger (räkningar erfordras se tex Kittel) ger 4 serier av tillåtna (hkl) index. För fcc är denna serie:

(hkl)	111	220	311	222	400	331	422	511	333
$h^2 + k^2 + l^2$	3	8	11	12	16	19	24	27	27

Vi ser att det saknas ett plan, det som ger 11 dvs 311 reflexionen. En inspektion av spektrat ser man att det finns en svag topp vid $\beta = 54.00$. En analys ger $d = 1.69827$ och $1/d^2 = 0.34672$ för att ge 10.945 vilket motsvarar den saknade linjen i tabellen. Så pulvret består av ett material med fcc struktur. Att två linjer syns så svagt beror på att det finns flera atomer i den primitiva cellen.

Även a låter sig bestämmas till $\sqrt{3} \cdot 3.2438 = 5.616 \text{ \AA}$ (tabell 5.6402 \AA), det frågas dock ej efter denna uppgift, provet bestod av NaCl ett material med fcc struktur och 2 atomer i den primitiva cellen.

3. (a) Potassium has a bcc structure with a lattice constant $a = 5.225 \text{ \AA}$ (conventional cell). The reciprocal lattice is hence an fcc with a with a size of $a_{reciprocal} = \frac{4\pi}{a}$, see figure in collection of formulas. Γ is located at the origin and H is on the surface of the unit cube. The distance between Γ and N is the shortest distance from the origin (centre of Fermi sphere) to the surface of the BZ. This distance is $\frac{\pi}{a}\sqrt{2} = \frac{\pi}{5.225} \cdot 10^{-10} \sqrt{2} = 0.8503 \cdot 10^{10} \text{ m}^{-1}$
Some sources state $a=5.328 \text{ \AA}$. This distance is $\frac{\pi}{a}\sqrt{2} = \frac{\pi}{5.328} \cdot 10^{-10} \sqrt{2} = 0.8339 \cdot 10^{10} \text{ m}^{-1}$
 - (b) The radius of the Fermi sphere is given by (2 electrons, bcc) for the $a = 5.225 \text{ \AA}$.
 $k_F = \left(\frac{3\pi^2 N}{V}\right)^{1/3} = \left(\frac{3\pi^2 2}{a^3}\right)^{1/3} = \left(\frac{3\pi^2 2}{5.225^3} 10^{30}\right)^{1/3} = 0.74599 \cdot 10^{10} \text{ m}^{-1}$. We conclude that $0.74599 < 0.8503$ ie. the Fermi sphere is inside the 1 BZ, $0.74599/0.8503 = 87.7 \%$.
The radius of the Fermi sphere is given by (2 electrons, bcc) for the $a = 5.328 \text{ \AA}$.
 $k_F = \left(\frac{3\pi^2 N}{V}\right)^{1/3} = \left(\frac{3\pi^2 2}{a^3}\right)^{1/3} = \left(\frac{3\pi^2 2}{5.328^3} 10^{30}\right)^{1/3} = 0.7316 \cdot 10^{10} \text{ m}^{-1}$. We conclude that $0.7316 < 0.834$ ie. the Fermi sphere is inside the 1 BZ, $0.7316/0.834 = 87.7 \%$. The same as expected.
4. As this is not a problem concerned with to much accuracy you may set $\hbar = 1 \cdot 10^{-34} \text{ Js}$.
 - a) For the valence band we have $\epsilon = -\frac{\hbar^2 k^2}{2m_h}$ and hence we have $m_h = +5 \cdot 10^{-32} \text{ kg}$,
 - b) For the valence band we have $\epsilon_h = \frac{\hbar^2 k^2}{2m_h}$ and hence we have
 $\epsilon_h = +10^{-19} \text{ J}$,

c) For the hole momentum we have $\mathbf{p}_h = -\hbar\mathbf{k}$ and hence we have

$$\mathbf{p}_h = -10^{-25}\hat{\mathbf{k}}_x \text{kg m/s},$$

d) For the hole velocity we have $\mathbf{v}_h = \frac{1}{\hbar} \frac{d\epsilon}{d\mathbf{k}}$ and hence we have

$$\mathbf{v}_h = -2 \cdot 10^6 \hat{\mathbf{k}}_x \text{m/s}$$

5. The conductivity is given by $\sigma = ne\mu_e + pe\mu_h$. Assuming we are in the intrinsic regime we have for the density of electrons $n = p = n_i$ and hence the resistance is given by

$$R \propto 1/\sigma \propto n_i \propto e^{E_g/2k_B T}.$$

We only keep track of the exponentials and assume the algebraic expression in T in n_i does not change a lot compared to the exponential. If the sample is intrinsic will show in a graph of $\ln(R)$ vs $1/T$.

To analyse the data we note that

$$\ln(R) \propto \frac{E_g}{2k_B} \frac{1}{T}.$$

In the table below data is processed accordingly:

$T(^{\circ}\text{C})$	R	T (K)	$1/T$	$\ln(R)$
22.0	182	295	$3.390 \cdot 10^{-3}$	5.204
48.0	92.0	321	$3.115 \cdot 10^{-3}$	4.522
72.0	53.0	345	$2.899 \cdot 10^{-3}$	3.970
97.0	32.0	370	$2.703 \cdot 10^{-3}$	3.466
127	17.2	400	$2.500 \cdot 10^{-3}$	2.845

If we draw $\ln(R)$ as a function of $1/T$ and if the data follows a straight line we calculate its slope.

$$\frac{E_g}{2k_B} = \frac{5.204 - 2.845}{(3.390 - 2.500) \cdot 10^{-3}} = 2650.6$$

and hence we can calculate E_g accordingly:

$$E_g = \frac{2650.6 \cdot 2 \cdot 1.38 \cdot 10^{-23}}{1.602 \cdot 10^{-19}} = 0.457 \text{eV}.$$

$$E_g = 0.46 \text{eV}$$

6. (a) There are several ways to determine A . One is to integrate and use the normalization condition to solve for A . A different path (done here) is to write the given wave function in terms of eigenfunctions (here particle in a box). The eigenfunctions are (PH)

$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right)$. We can directly conclude that the given wave function consists of $n = 1$, $n = 5$ and $n = 7$ functions, we can write:

$$\psi(x, 0) = \frac{\sqrt{13}}{\sqrt{8a}} \sin\left(\frac{\pi x}{a}\right) + \frac{1}{2\sqrt{a}} \sin\left(\frac{5\pi x}{a}\right) + \frac{A}{\sqrt{a}} \sin\left(\frac{7\pi x}{a}\right)$$

$$\psi(x, 0) = \frac{\sqrt{13}\sqrt{2}}{4\sqrt{a}} \sin\left(\frac{\pi x}{a}\right) + \frac{\sqrt{2}}{2\sqrt{2} \cdot a} \sin\left(\frac{5\pi x}{a}\right) + \frac{A\sqrt{2}}{\sqrt{2} \cdot a} \sin\left(\frac{7\pi x}{a}\right) =$$

$$\frac{\sqrt{13}}{4}\psi_1(x, 0) + \frac{1}{\sqrt{8}}\psi_5(x, 0) + \frac{A}{\sqrt{2}}\psi_7(x, 0)$$

As all three eigenfunctions are orthonormal the normalisation integral reduces to $\frac{13}{16} + \frac{1}{8} + \frac{A^2}{2} = 1$ and hence $A = \frac{1}{\sqrt{8}}$ (≈ 0.354).

- (b) The wave function contains only $n = 1$, $n = 5$ and $n = 7$ eigenfunctions and therefore the only possible outcome of an energy measurement are $E_1 = \frac{\hbar^2\pi^2}{2ma^2}$ with probability $\frac{13}{16}$ and $E_5 = \frac{\hbar^2\pi^2}{2ma^2}25$ with probability $\frac{1}{8}$ and $E_7 = \frac{\hbar^2\pi^2}{2ma^2}49$ with probability $\frac{1}{16}$.

The average energy is given by

$$\langle E \rangle = \frac{13}{16}E_1 + \frac{1}{8}E_5 + \frac{1}{16}E_7 = \frac{\hbar^2\pi^2}{2ma^2}\left(\frac{13}{16} + \frac{1}{8} \cdot 25 + \frac{1}{16} \cdot 49\right) = \frac{112}{16} \cdot \frac{\hbar^2\pi^2}{2ma^2} = 7 \cdot \frac{\hbar^2\pi^2}{2ma^2}$$

- (c) The time dependent solution is given by $\Psi(x, t) = \sum_{n=1}^{\infty} c_n \psi_n(x) e^{-iE_n t/\hbar}$ and hence

$$\Psi(x, t) = \sqrt{\frac{13}{16}}\psi_1(x, 0)e^{-i\frac{\hbar\pi^2 t}{2ma^2}} + \frac{1}{\sqrt{8}}\psi_5(x, 0)e^{-i\frac{25\hbar\pi^2 t}{2ma^2}} + \frac{1}{4}\psi_7(x, 0)e^{-i\frac{49\hbar\pi^2 t}{2ma^2}}$$

7. The Carbon ion has $Z = 6$ and hence the energy levels are $E_n = -\frac{488.16}{n^2}$ eV for a carbon ion with just one electron (Hydrogen like). Try to find a start of the series. In order to do that we calculate the energies of the spectral lines. The energy of a spectral line has to be matched to a energy difference between two levels of the Carbon ion. The energy of $\lambda = 207.80$ nm is $E = h\nu = \frac{hc}{\lambda} = \frac{6.626 \cdot 10^{-34} \cdot 2.9979 \cdot 10^8}{207.80 \cdot 10^{-9} \cdot 1.6022 \cdot 10^{-19}} = 5.9663$ eV . A similar calculation gives the energy for the other lines in the series: 9.56395, 11.8989 and 13.4997 eV.

As the Balmer series in Hydrogen is for transitions down to level $n=2$ we (see from E_n) have to go higher up in n for the Carbon ion as the energies for a transition to the level $n = 2$ in Carbon would be far to large.

We can solve the problem in two ways either in a sophisticated way or by brute force.

The sophisticated way. Using the fact that can assume levels are adjacent we let n be the quantum number for the lower level and m for a level above, we have no knowledge of how n and m relate. We know however that for the next level (higher in energy) we have down to n from level $m + 1$. One can form the following two equations

$$5.9663eV = 488.16\left(\frac{1}{n^2} - \frac{1}{m^2}\right)eV \text{ and}$$

$$9.56395eV = 488.16\left(\frac{1}{n^2} - \frac{1}{(m+1)^2}\right)eV$$

we only need two of the lines to form an appropriate set of equations. (You can use the other pairs of lines as well to form two equations.) Subtracting one equation from the other to eliminate n you get $3.59765 = 488.16\left(\frac{1}{m^2} - \frac{1}{(m+1)^2}\right)$ and finally

$\frac{1}{m^2} - \frac{1}{(m+1)^2} = 0.007369817273025237627$. Solving for m you arrive at $m = 6$. If you do not want to solve the equation above you just try some different values of m until you find $m = 6$ that solves the equation. Now we use the result for m in $5.9663eV = 488.16\left(\frac{1}{n^2} - \frac{1}{6^2}\right)eV$ to solve for n and we arrive at $n = 5$.

Then there is also the tour of brute force ie just trial and error: If we try $n=5$ we have transitions from $m=6, 7, 8, 9$, etc. The corresponding energies will be: $488.16(\frac{1}{5^2} - \frac{1}{6^2})=5.97$ eV, the next one will be: $488.16(\frac{1}{5^2} - \frac{1}{7^2})=9.56$ eV, $488.16(\frac{1}{5^2} - \frac{1}{8^2})=11.899$ eV and so on. So these are down to $n=5$ from level $m=6, 7, 8$ and 9 .