

Solution to written exam in SOLID STATE PHYSICS F0053T AND F7045T

Examination date: 2018-09-01

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. **rectangular unit cell, the q are lattice points**, *basis of letters associated with each lattice point, PRIMITIVE UNIT CELL.*

q	p	d	b	q	p	d	b	q	p	d	b	Q	p	d	b	...
d	b	q	p	d	b	<i>q</i>	<i>p</i>	d	b	Q	p	d	b	Q	p	...
q	p	d	b	q	p	<i>d</i>	<i>b</i>	q	p	d	b	Q	p	d	b	...
d	b	q	p	d	b	q	p	d	b	q	p	d	b	q	p	
.
.
.

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

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

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 $(\frac{d_{hkl}}{a})^2 = \frac{1}{h^2+k^2+l^2}$ där a är enhetskubens kantlängd (ej känd). Följande tabell görs upp för att bestämma $h^2 + k^2 + l^2$ för topparna.

(θ)	28.44/2	47.32/2	56.14/2	69.12/2	76.34/2	76.56/2	88.02/2
d	3.13867	1.9212	1.6385	1.35914	1.2476	1.2445	1.109698
$1/d^2$	0.10151	0.27093	0.37248	0.54134	0.64246	0.64567	0.81206
$x = 2/0.10151$	2.00000	5.338					
$x = 3/0.10151$	3.00000	8.007	11.008	15.999	18.987	19.082	23.999

Sista raden i tabellen ger de sökta heltalen $h^2 + k^2 + l^2$. även a låter sig bestämmas till $\sqrt{3} \cdot 3.13867 = 5.436\text{\AA}$, det frågas dock ej efter denna uppgift.

3. (a) Avståndet mellan (111)-plan i en kubisk kristall ges av $d = a/\sqrt{h^2 + k^2 + l^2} = a/\sqrt{3}$, vilket är storleken på den endimensionella kristallens primitiva enhetscell. Eftersom kristallen innehåller två typer av atomer har dispersionsrelationen en akustisk och en optisk gren.

(b) Serieutveckling av dispersionsrelationen för akustiska vågor ger

$$\omega^2 = C \frac{M_1 + M_2}{M_1 M_2} - C \sqrt{\left(\frac{M_1 + M_2}{M_1 M_2}\right)^2 - \frac{4 \sin^2(Ka/2)}{M_1 M_2}} \approx C \frac{M_1 + M_2}{M_1 M_2} \left(1 - \sqrt{1 - \frac{K^2 d^2}{M_1 M_2} \left(\frac{M_1 M_2}{M_1 + M_2}\right)^2}\right) \approx C \frac{K^2 d^2}{2(M_1 + M_2)}.$$

Detta ger

$$v = \frac{\partial \omega}{\partial K} = d \sqrt{\frac{C}{2(M_1 + M_2)}} \Rightarrow C = 6(M_1 + M_2) \left(\frac{v}{a}\right)^2 = 13.8 \text{ N/m},$$

där massorna är 22.99u och 35.45u för natrium respektive klor.

(c) Konserveringslagarna är $\hbar\omega = \hbar\Omega$ för energi och $\hbar k = \hbar K$ för rörelsemängd. Eftersom ljusets hastighet är mycket större än fononernas hastighet inses att fotonens dispersionskurva måste vara mycket brantare än fononens. I praktiken blir den vertikal och skär endast de optiska fononernas där $K = 0$. Detta ger

$$\omega^2 = 2C \frac{M_1 + M_2}{M_1 M_2} \Rightarrow \lambda = \frac{2\pi c}{\omega} = \frac{2\pi c}{\sqrt{2C(M_1 + M_2)/M_1 M_2}} = 54.6 \text{ } \mu\text{m}.$$

4. The magnetic response of the salt is paramagnetic (see labb excercises) The Iron ion is Fe^{3+} and the electronic configuration is $3d^5$ ie the d-shell has 5 electrons outoff 10 possible. Applying Hund's rules we find $S=2.5$, $L=0$ and $J=2.5$ and hence $g = 2$. This gives $p = 5.916$

($p_{quenched} = 5.916$) The Paramagnetic susceptibility (Curie law) is given by $\chi = \frac{\mu_0 n p_{eff}^2 \mu_B^2}{3k_B T} = \frac{C}{T}$. The density is $\rho = 3.1 \cdot 10^3 \text{ kg/m}^3$ and the molar weight is ($\text{Fe}_2(\text{SO}_4)_3$) is $M=0.39988 \text{ kg/m}^3$. Hence the density ρ corresponds to 7752.31 mole/m^3 . The number of Fe ions is 2 per unit, and the density will be $9.33843 \cdot 10^{27} / \text{m}^3$. Taken at a temperature of $T=300\text{K}$ we arrive at $\chi = 0.0028411 \approx 0.0028$. This is a saturated value and $p = 5.916$.

5. Combining $\sigma = e(n\mu_e + p\mu_h) = 1/\rho$ and $n_i = p_i = 2 \left(\frac{k_B T}{2\pi\hbar^2}\right)^{3/2} (m_e m_h)^{3/4} e^{-E_g/2k_B T}$ As the mobility μ only depends algebraically on T the reistance will be dominated by the exponential. Hence we have $R \propto e^{E_g/2k_B T} \rightarrow \ln(R) = \text{constant} + E_g/2k_B T$. Plotting $\ln(R)$ versus $1/T$ will produce a straight line and from the slope ($E_g/2k_B = 3917.82157$) we calculate $E_g \approx 0.68\text{eV}$.

6. (a) Let the commutator act on a wave function $\Psi(y)$ and $p_y = -i\hbar \frac{d}{dy}$

$$[y^2, p_y^2]\Psi(y) = -\hbar^2\left(y^2\frac{d^2\Psi(y)}{dy^2} - \frac{d^2(y^2\Psi(y))}{dy^2}\right) = -\hbar^2\left(y^2\frac{d^2\Psi(y)}{dy^2} - y^2\frac{d^2\Psi(y)}{dy^2} - 4y\frac{d\Psi(y)}{dy} - 2\Psi(y)\right) = +\hbar^2 2\Psi(y) + 4y\hbar^2\frac{d\Psi(y)}{dy} = (+\hbar^2 2 + i4\hbar y p_y)\Psi(y) \text{ concluding for the commutator:}$$

$$[y^2, p_y^2] = +2\hbar^2 + 4i\hbar y p_y = +2\hbar^2 + 4\hbar^2 y \frac{d}{dy} .$$

- (b) The energy levels for a hydrogen like system are given by: $E_n = -13.6\frac{Z^2}{n^2}$ [eV], here we have $Z = 4$: $\Delta E = E(2s) - E(1s) = E_2 - E_1 = -13.54 \cdot \left(\frac{16}{2^2} - \frac{16}{1^2}\right) = 13.54 \cdot \frac{16 \cdot 3}{4} = 162.48$ eV
- (c) The angular part of the wave function can be written as a spherical harmonic:

$$3 \cos^2 \theta - 1 \propto Y_{20}$$

Which gives $l = 2$ och $m = 0$. The part depending on r (r^2/a_μ^2) $e^{-r/3a_\mu}$ corresponding to the principal quantum number $n = 3$ och $l = 2$ consistent with Y_{20} .

7. (a) The parity of a hydrogen eigenfunction $\psi_{nlm_l}(\mathbf{r})$ is given by $(-1)^l$. The given wave function $\Psi(\mathbf{r})$ consists of eigenfunctions with different parity. Hence $\Psi(\mathbf{r})$ has no definite parity.

- (b) The probability is given by the absolute square of the coefficients.

$$(\Psi(\mathbf{r}, t = 0) = \frac{1}{\sqrt{15}} (3\psi_{100}(\mathbf{r}) - 2\psi_{210}(\mathbf{r}) + \psi_{310}(\mathbf{r}) - \psi_{322}(\mathbf{r})))$$

The probabilities are (in order) $\frac{9}{15}, \frac{4}{15}, \frac{1}{15}, \frac{1}{15}$. 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 $\langle E \rangle = \frac{9}{15}\left(-\frac{13.56}{1^2}\right) + \frac{4}{15}\left(-\frac{13.56}{2^2}\right) + \frac{1}{15}\left(-\frac{13.56}{3^2}\right) + \frac{1}{15}\left(-\frac{13.56}{3^2}\right) = -13.56\left(\frac{9}{15} + \frac{4}{60} + \frac{1}{135} + \frac{1}{135}\right) = -9.240889 \approx -9.24$ eV

The operator \mathbf{L}^2 has eigenvalues $\hbar^2 l(l+1)$. The expectation value is given by

$$\langle \mathbf{L}^2 \rangle = \frac{9}{15} \cdot 0 + \frac{4}{15}(\hbar^2 1(1+1)) + \frac{1}{15}(\hbar^2 1(1+1)) + \frac{1}{15}(\hbar^2 2(2+1)) = \frac{4 \cdot 2 + 2 + 6}{15} \hbar^2 = \frac{16}{15} \hbar^2$$

The operator L_z has eigenvalues $\hbar m_l$. The expectation value is given by

$$\langle L_z \rangle = \frac{9}{15} \cdot 0 + \frac{4}{15} \cdot 0 + \frac{1}{15} \cdot 0 + \frac{1}{15}(\hbar 2) = \frac{2}{15} \hbar$$