

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 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. För GaAs (fcc) är strukturfaktorn:

$$S = [f_{\text{Ga}} + f_{\text{As}} e^{-i\frac{\pi}{2}(h+k+l)}] * [1 + e^{-i\pi(h+k)} + e^{-i\pi(h+l)} + e^{-i\pi(k+l)}]$$

denna ger de vanliga fcc villkoren

$$S = 0, \text{ if } (hkl) \text{ är en blandning av jämna och udda tal.}$$

$$\neq 0 \text{ för övriga kombinationer}$$

Ger Miller indexen för GaAs: **(111)**, **(200)**, **(220)**, **(311)**, (222), (400), (331).

För kisel (diamant) är strukturfaktorn:

$$S = f_{\text{Si}} [1 + e^{-i\frac{\pi}{2}(h+k+l)}] * [1 + e^{-i\pi(h+k)} + e^{-i\pi(h+l)} + e^{-i\pi(k+l)}]$$

ett sätt att se det

$$S = 0, \text{ om } h+k+l = 2 + 4n$$

$$= 0, \text{ om } (hkl) \text{ blandning av jämna/udda tal}$$

$$\neq 0 \text{ för övriga kombinationer}$$

alternativt sätt att se det

$$S \neq 0, \text{ om om } (hkl) \text{ alla är udda}$$

$$\neq 0, \text{ om } (hkl) \text{ alla är jämna och } h+k+l = 4n$$

$$= 0 \text{ för övriga kombinationer}$$

Ger Miller indexen för kisel: **(111)**, **(220)**, **(311)**, **(400)**, (331). Notera att (200) och (222) inte finns med.

3. For a metal the specific heat consists of two parts. One is the contribution from the electrons

$$C_v^f = \frac{\pi^2}{2} N k_B \frac{T}{T_F} = \gamma T,$$

and the other is the contribution from the lattice (phonons)

$$C_v^{ph} = \frac{12\pi^4}{5} Nk_B \frac{T^3}{\Theta_D^3} = \alpha T^3.$$

The total specific heat is the sum of both contributions

$$C_v = C_v^{ph} + C_v^f = \gamma T + \alpha T^3.$$

Hence, a graph of $\frac{C_v}{T}$ versus T^2 will produce a straight line. The intersection of the line at $T = 0$ will give γ and the slope will give α . From the slope α we find the Debye temperature Θ_D . The slope of the line in a graph of C_v/T vs T^2 is 0.609 .

$$\Theta_D = \left(\frac{12\pi^4 Nk_B}{5\alpha} \right)^{\frac{1}{3}} = 148\text{K}$$

4. (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:
 $E_g^{\text{window glass}} < 7.3\text{eV} < E_g^{\text{quarts glass}}$

5. We have $n_i = p_i = 2\sqrt{\frac{k_B T}{2\pi\hbar^2}} (m_e m_h)^{3/4} e^{-E_g/2k_B T} = 1.44 \cdot 10^{15} \text{ m}^{-3}$. This gives $\sigma_0 = ne\mu_e + pe\mu_h = 4.86 \cdot 10^{-5} \Omega^{-1} \text{ m}^{-2}$ for pure silicon. Sb is a donor and the concentration of donor atoms is $N_d = 10^{-6} \cdot \frac{8}{a^3} = 4.99 \cdot 10^{22} \text{ m}^{-3}$. We also have the relations $np = n_i^2 = p_i^2$ and $p + N_d^+ = n + N_a^-$. With $N_a^- = 0$ and $N_d^+ = N_d$, this gives $n^2 - N_d n - n_i^2 = 0$. Since $N_d \gg n_i$, we get $n \approx N_d$ and $p \approx 0$. Finally, we calculate $\sigma = ne\mu_e + pe\mu_h = 1.28 \cdot 10^3 \Omega^{-1} \text{ m}^{-2} = 26 \cdot 10^6 \sigma_0$.

6. (a) Let the commutator act on a wave function $\Psi(x)$ and $p_x = -i\hbar \frac{d}{dx}$
 $[x^2, p_x^2]\Psi(x) = -\hbar^2 \left(x^2 \frac{d^2\Psi(x)}{dx^2} - \frac{d^2(x^2\Psi(x))}{dx^2} \right) = -\hbar^2 \left(x^2 \frac{d^2\Psi(x)}{dx^2} - x^2 \frac{d^2\Psi(x)}{dx^2} - 4x \frac{d\Psi(x)}{dx} - 2\Psi(x) \right) =$
 $+ \hbar^2 2\Psi(x) + 4x\hbar^2 \frac{d\Psi(x)}{dx} = (+\hbar^2 2 + i4\hbar x p_x) \Psi(x)$ concluding for the commutator:
 $[x^2, p_x^2] = +2\hbar^2 + 4i\hbar x p_x$.

- (b) The energy levels for a hydrogen like system are given by: $E_n = -13.6 \frac{Z^2}{n^2} [\text{eV}]$, here we have $Z = +3$: $\Delta E = E(2s) - E(1s) = E_2 - E_1 = -13.54 \cdot \left(\frac{9}{2^2} - \frac{9}{1^2} \right) = 13.54 \cdot \frac{27}{4} = 91, 53 \text{ eV}$

(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. 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 $\Psi(x, y) = \psi(x) \cdot \psi(y)$ 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 therefor 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:

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right) \text{ with eigenenergys } E_n = \frac{n^2 \pi^2 \hbar^2}{2Ma^2} \text{ where } n = 2, 4, 6, \dots \quad (1)$$

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:

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

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:

$$\Psi_{n,m}(x, y) = \psi_n(x) \cdot \psi_m(y) \text{ eigenenergys } E_{n,m} = E_n + E_m \text{ where } n = 1, 2, \dots \text{ and } m = 1, 2, \dots \quad (3)$$

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:

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right) \quad \text{with eigenenergys } E_n = \frac{n^2\pi^2\hbar^2}{2Ma^2} \quad \text{where } n = 1, 2, 3, \dots \quad (4)$$

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

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

$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a} + \frac{n\pi}{2}\right) = \sqrt{\frac{2}{a}} \left(\sin\left(\frac{n\pi x}{a}\right) \cdot \cos\left(\frac{n\pi}{2}\right) + \cos\left(\frac{n\pi x}{a}\right) \cdot \sin\left(\frac{n\pi}{2}\right)\right)$. We see that we recover the solution in eq (1), (2) and (3) as we let n run from 1 to ∞ .

b) The ground state eigenfunction is given by (using eq. (2))

$$\Psi_{n=1,m=1}(x, y) = \psi_1(x) \cdot \psi_1(y) = \sqrt{\frac{2}{a}} \cos\left(\frac{\pi x}{a}\right) \cdot \sqrt{\frac{2}{a}} \cos\left(\frac{\pi y}{a}\right) \quad (6)$$

The next lowest state eigenfunction is given by (using eq. (2) and (1)). Note there are two eigenfunctions with the same energy ($\Psi_{n=1,m=2}(x, y)$) you may use either one of them.

$$\Psi_{n=2,m=1}(x, y) = \psi_2(x) \cdot \psi_1(y) = \sqrt{\frac{2}{a}} \sin\left(2\frac{\pi x}{a}\right) \cdot \sqrt{\frac{2}{a}} \cos\left(\frac{\pi y}{a}\right) \quad (7)$$

Orthogonality is defined as

$$\int_x \int_y \Psi_{n_1,m_1}(x, y) \Psi_{n_2,m_2}(x, y) = \delta_{n_1,n_2} \delta_{m_1,m_2} \quad (8)$$

by explicit calculation

$$\int_{x=-a/2}^{a/2} \int_{y=-a/2}^{a/2} \left(\frac{2}{a} \cos\left(\frac{\pi x}{a}\right) \cdot \cos\left(\frac{\pi y}{a}\right)\right) \cdot \left(\frac{2}{a} \sin\left(2\frac{\pi x}{a}\right) \cdot \cos\left(\frac{\pi y}{a}\right)\right) = \text{calculations} = 0 \quad (9)$$

this is a separable integral (in x and y), suggestion do the integral in x first as this will be zero as they belong to different eigenvalues. Thus the calculation ends with a zero as it should.