

Solution to written exam in SOLID STATE PHYSICS F0053T AND F7045T

Examination date: 2016-08-27

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) $C_v = C_v^{el} + C_v^f$. Plotta C_v/T mot T^2 detta blir en rät linje enligt: Fononbidraget
 $C_v = \frac{12\pi^4}{5} Nk_B \left(\frac{T}{\Theta}\right)^3 = AT^3$. Elektronbidraget är linjärt (γT) i temperaturen
 $C_v^{el} = \frac{\pi^2}{2} Nk_B \frac{T}{T_F}$, $T_F = E_F/k_B$ Plotta $\frac{C_v}{T} = \frac{12\pi^4}{5\Theta^3} Nk_B T^2 + \frac{\pi^2 Nk_B^2}{2E_F}$ ur lutningen (0.0030075)
 fås $\Theta_D = 87\text{K}$ och ur skärningspunkten (0.001989) med y-axeln fås $E_F = 1.9 \text{ eV} = 3.0 \cdot 10^{-19} \text{ J}$.
- (b) $\epsilon_F = \frac{\hbar^2}{2m} \left(\frac{3\pi^2 N}{V}\right)^{\frac{2}{3}}$ kalium är bcc med $a = 5.225 \text{ \AA}$. ($k_F = 7.45 \cdot 10^9$). Effektiva massan ges av
 $m = \frac{\hbar^2}{2\epsilon_F} \left(\frac{3\pi^2 N}{V}\right)^{\frac{2}{3}} = \frac{(1.055 \cdot 10^{-34})^2}{2 \cdot 1.9 \cdot 1.601 \cdot 10^{-19}} \left(\frac{3\pi^2 \cdot 2}{(5.225 \cdot 10^{-10})^3}\right)^{\frac{2}{3}} = 1.0174667 \cdot 10^{-30} \text{ kg} = 1.117 m_0$
2. (a) Natrium har bcc struktur med $a = 4.2906 \text{ \AA}$. reciproka gittret är då fcc med kantlängden $\frac{4\pi}{a}$ (se figur formelsamling). Punkten Γ ligger i origo punkten H ligger på ytan av enhetskuben. Avståndet mellan Γ och punkten N är den kortaste sträckan. Dess längd är $\frac{\pi}{a} \sqrt{2} = 1.035 \cdot 10^{10} \text{ m}^{-1}$
- (b) Fermisfären har en radie som ges av
 $k_F = \left(\frac{3\pi^2 N}{V}\right)^{1/3} = \left(\frac{3\pi^2 \cdot 2}{4.2906^3} 10^{30}\right)^{1/3} = 0.9084 \cdot 10^{10} \text{ m}^{-1}$ Vi ser att $0.9084 < 1.035$ dvs Fermisfären skär ej 1 BZ, $0.9084/1.035 = 87.8 \%$.
3. 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
 $S = 0$, if (hkl) är en blandning av jämna och udda tal.
 $\neq 0$ 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
 $S = 0$, om $h+k+l = 2 + 4n$
 $= 0$, om (hkl) blandning av jämna/udda tal
 $\neq 0$ för övriga kombinationer
 alternativt sätt att se det
 $S \neq 0$, om om (hkl) alla är udda
 $\neq 0$, om (hkl) alla är jämna och $h+k+l = 4n$
 $= 0$ för övriga kombinationer

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

4. 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 $\sigma = ne\mu_e + pe\mu_h = 1.28 \cdot 10^3 \Omega^{-1} \text{ m}^{-2} = 26 \cdot 10^6 \sigma_0$.

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

		m_l						S	L	J	p	
		-3	-2	-1	0	1	2					3
Eu ²⁺	f ⁷	↑	↑	↑	↑	↑	↑	↑	7/2	0	7/2	7,94
Yb ³⁺	f ¹³	↑	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	1/2	3	7/2	4,54
Tb ³⁺	f ⁸	↑	↑	↑	↑	↑	↑	↑↓	3	3	6	9,72

6. Note: As the task is 'solve the Schrödinger equation' failing to do so will result in nought points.

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 on 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 ($\Psi(0) = \Psi(a) = 0$) into account.

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

From the first relation we get $A = 0$. From the second we get $B \sin(ka) = 0$ where $ka = n\pi$ with $n = 1, 2, 3, \dots$ and hence $k = \frac{n\pi}{a}$. The normalising constant $B = \sqrt{\frac{2}{a}}$ you get from the condition $\int_{-a/2}^{a/2} |\Psi|^2 dx = 1$.

The solution is:

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

By analogy the y directions is treated in a similar fasion but with a different size of box.

The solution is:

$$\psi_m(y) = \frac{2}{\sqrt{a}} \sin\left(\frac{2m\pi y}{a}\right) \text{ with eigenenergys } E_m = \frac{2m^2\pi^2\hbar^2}{Ma^2} \text{ where } m = 1, 2, 3, \dots \quad (2)$$

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.

b) The ground state eigenfunction is given by (using eq. (3))

$$\Psi_{n=1,m=1}(x, y) = \psi_1(x) \cdot \psi_1(y) = \sqrt{\frac{2}{a}} \sin\left(\frac{\pi x}{a}\right) \cdot \frac{2}{\sqrt{a}} \sin\left(\frac{2\pi y}{a}\right) \quad (4)$$

The next lowest state (in energy) eigenfunction is given by (using eq. (1) and (2)). Note there is only one eigenfunction as $(\Psi_{n=1,m=2}(x, y))$ has an higher energy.

$$\Psi_{n=2,m=1}(x, y) = \psi_2(x) \cdot \psi_1(y) = \sqrt{\frac{2}{a}} \sin\left(2\frac{\pi x}{a}\right) \cdot \frac{2}{\sqrt{a}} \sin\left(\frac{2\pi y}{a}\right) \quad (5)$$

Orthogonality is defined as

$$\int_x \int_y \Psi_{n_1,m_1}(x, y) \Psi_{n_2,m_2}(x, y) = \delta_{n_1,n_2} \delta_{m_1,m_2} \quad (6)$$

by explicit calculation

$$\int_{x=0}^a \int_{y=0}^{a/2} \left(\frac{2\sqrt{2}}{a} \sin\left(\frac{\pi x}{a}\right) \cdot \sin\left(\frac{2\pi y}{a}\right) \right) \cdot \left(\frac{2\sqrt{2}}{a} \sin\left(2\frac{\pi x}{a}\right) \cdot \sin\left(\frac{2\pi y}{a}\right) \right) = \text{calculations} = 0 \quad (7)$$

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.

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 the same parity. Hence $\Psi(\mathbf{r})$ has a definite parity.

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

$$(\Psi(\mathbf{r}, t = 0) = \frac{1}{\sqrt{15}} (3\psi_{100}(\mathbf{r}) - 2\psi_{200}(\mathbf{r}) + \psi_{320}(\mathbf{r}) - \psi_{322}(\mathbf{r})))$$

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 $\langle E \rangle = \frac{9}{15}(-\frac{13.56}{1^2}) + \frac{4}{15}(-\frac{13.56}{2^2}) + \frac{1}{15}(-\frac{13.56}{3^2}) + \frac{1}{15}(-\frac{13.56}{3^2}) = -13.56(\frac{9}{15} + \frac{4}{60} + \frac{1}{135} + \frac{1}{135}) = -9.240889 \approx -9.24$ eV

The operator \mathbf{L}^2 has eigenvalues $\hbar^2 l(l+1)$. The expectation value is given by $\langle \mathbf{L}^2 \rangle = \frac{9}{15} \cdot 0 + \frac{4}{15} \cdot 0 + \frac{1}{15}(\hbar^2 2(2+1)) + \frac{1}{15}(\hbar^2 2(2+1)) = \frac{12}{15}\hbar^2 = \frac{4}{5}\hbar^2$

The operator L_z has eigenvalues $\hbar m_l$. The expectation value is given by $\langle L_z \rangle = \frac{9}{15} \cdot 0 + \frac{4}{15} \cdot 0 + \frac{1}{15} \cdot 0 + \frac{1}{15}(\hbar 2) = \frac{2}{15}\hbar$