LULEÅ UNIVERSITY OF TECHNOLOGY
Division of Physics

Solution to written exam in Solid State Physics F0019T and F7006T

Examination date: 2015-06-05
The solutions are just suggestions. They may contain several alternative routes.
This is a combined solution for the courses F0019T and F7006T.
For F0019T use solution 1, 2, 3, 4 and 5.
For F7006T use solution 2, 3, 4, 5 and 6 with an offset of -1.

1. The eigenfunctions and eigenvalues of the free-particle Hamiltonian are found by solving the time-independent Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2u(x)}{dx^2}+V(x)u(x)=Eu(x),$$

with $V(x)$ zero everywhere. Thus, the eigenvalue equation reads

$$\frac{d^2u(x)}{dx^2}+k^2u(x)=0,$$

where $k^2=2mE/\hbar^2$. The eigenfunctions are given by the plane waves e^{ikx} and e^{-ikx}, or linear combinations of these, as *e.g.* $\sin kx$ and $\cos kx$.

(a) The wave function of the particle at $t=0$ is given by

$$\psi(x,0)=\cos^3(kx)+\sin^3(kx).$$

This is not an eigenfunction in itself but it can be written as sum of eigenfunctions using the Euler relations

$$\psi(x,0)=\left(\frac{e^{ikx}+e^{-ikx}}{2}\right)^3+\left(\frac{e^{ikx}-e^{-ikx}}{2i}\right)^3= \quad (1)$$

$$\frac{1}{8}\left(e^{i3kx}+3e^{ikx}+3e^{-ikx}+e^{-i3kx}\right)-\frac{1}{8i}\left(e^{i3kx}-3e^{ikx}+3e^{-ikx}-e^{-i3kx}\right)= \quad (2)$$

$$\frac{3}{4}\cos(kx)+\frac{1}{4}\cos(3kx)+\frac{3}{4}\sin(kx)-\frac{1}{4}\sin(3kx) \quad (3)$$

Thus, $\psi(x,0)$ can be written as a superposition of plane waves with two different values of $k_1=k$ and $k_2=3k$.

(b) The energy of a plane wave e^{ikx} is given by $E=\hbar^2k^2/2m$. Thus, the energy of e^{ik_1x} (or e^{-ik_1x}) is $E_1=\hbar^2k^2/2m$ and the energy of e^{ik_2x} (or e^{-ik_2x}) is $E_2=\hbar^2k_2^2/2m=9\hbar^2k^2/2m$.

(c) The function $u(x)=e^{ikx}$ is a solution to the the time-independent Schrödinger equation. The corresponding solutions to the time-dependent Schrödinger equation are given by $u(x)T(t)$,with $T(t)=e^{-iEt/\hbar}$. Therefore, $u(x)T(t)=e^{i(kx-Et/\hbar)}$. A sum of solutions of this form is also a solution, since the Schrödinger equation is linear. This means that if $\psi(x,0)$ is given by equation (3), then the time dependent solution is given by

$$\psi(x,t)=\frac{1}{8}\left(e^{i3kx}+e^{-i3kx}\right)e^{-iE_2t/\hbar}+\frac{3}{8}\left(e^{ikx}+e^{-ikx}\right)e^{-iE_1t/\hbar}+ \quad (4)$$

$$-\frac{1}{8i}\left(e^{i3kx}-e^{-i3kx}\right)e^{-iE_2t/\hbar}+\frac{3}{8i}\left(e^{ikx}-e^{-ikx}\right)e^{-iE_1t/\hbar} \quad (5)$$

where

$$E_1=\frac{\hbar^2k^2}{2m} \quad \text{and} \quad E_2=\frac{9\hbar^2k^2}{2m} \quad (6)$$

2. (a) Rubidium has a bcc structure with a lattice constant a = 5.590 Å(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 $\frac{\pi}{a}\sqrt{2} = 0.795\ 10^{10}\mathrm{m}^{-1}$

   (b) The radius of the Fermi sphere is given by (2 electrons, bcc)
   $k_F = (\frac{3\pi^2 N}{V})^{1/3} = (\frac{3\pi^2 2}{a^3})^{1/3} = (\frac{3\pi^2 2}{5.590^3}10^{30})^{1/3} = 0.6972\ 10^{10}\mathrm{m}^{-1}$ We conclude that $0.697 < 0.795$ ie. the Fermi sphere is inside the 1 BZ, 0.697/0.795 = 87.7 % .

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

4. X-rays scatter against the electron distribution around the ions. In KCl the number the number of electrons around the K^+ and Cl^- ion are equal. The X-rays do not see an FCC lattice with a basis of K^+ and Cl^- ions but they see an SC lattice with similar electron distribution on each lattice site. Support motivations with Bragg scattering conditions and form factors.

5. $\sigma_i = n_i e\mu_e + p_i e\mu_h = n_i(\mu_e + \mu_h)$ och $n_i = 2(\frac{k_BT}{2\pi\hbar^2})^{\frac{3}{2}}(m_e m_h)^{\frac{3}{4}}e^{-E_g/2k_BT}$ insättning ger $n_i = 7.343\ 10^{-20}\ \mathrm{m}^{-3} \Rightarrow \sigma_i = 3.529\ 10^{-39}\ (\Omega\mathrm{m})^{-1}$. mycket mindre än det uppmätta. Om vi dopar blir konduktiviteten högre. Beteckna dopningskoncentrationen med N_d. $n = p + N_d$ och $np = n_i^2$ ger ekv system för p. $(p + N_d)p = n_i^2$ och $p = -\frac{N_d}{2} \pm \sqrt{(\frac{N_d}{2})^2 + n_i^2} \approx 0 \Rightarrow n = N_d$ och därmed blir $\sigma = N_d e\mu_e$ och $N_d = \frac{\sigma}{e\mu_e} \approx 1.1\ 10^6\mathrm{m}^3$.

6. (a) There are no free electrons at the Fermi surface. There is a band gap between valance and conduction band. Hence no electrons that can be in states where they can move so that the sum of k-vectors for all electrons becomes non-zero.

   (b) DOS in the Debye approximation $D(\omega) = V\omega^2/2\pi^2 v^3$, see page 122 CK.

   (c) $U = \int d\omega D(\omega)\langle n(\omega)\rangle\hbar\omega = ...= \frac{3Vk_B^4T^4}{2\pi^2v^3\hbar^3}\int_0^{x_D} dx\frac{x^3}{e^x-1}$. see page 122 CK. Gives T^4 dependence.

   (d) For phonons $C_v = 234Nk_B\left(\frac{T}{\Theta}\right)^3$. For electrons $C_v = \frac{1}{2}\pi^2 Nk_BT/T_F$. On C/T graph versus T^2 we get Θ from slope and ϵ_F from C/T at $T = 0$. Start with Θ, slope is (21.5-8)/100

millijoule/mole K^4 gives $\Theta^3 = 234 \cdot 6.022\ 10^{23}\ 1.381\ 10^{-23} \frac{100}{(21.5-8)10^{-3}} K^3$
$\to \Theta = 243.37K \approx 240K$ (from experiment $\Theta = 275K$.
$\frac{1}{2}\pi^2 N k_B T/T_F = 8 \frac{\text{mJ}}{\text{mol K}^4}$. Gives $T_F = 5.12996\ 10^3K$ and $e_F = k_B T_F = 0.442eV$. A value given in books is $\epsilon_F = 5.32eV$ a large difference from the fact that electrons are not at all free, see CK 155–157.