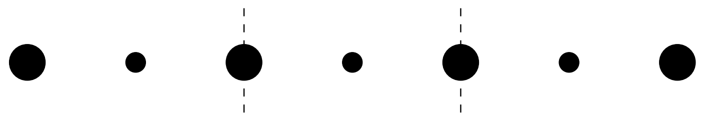

LULEÅ UNIVERSITY OF TECHNOLOGY
Division of Physics

Solution to written exam in Solid State Physics F0053T

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The solutions are just suggestions. They may contain several alternative routes.

1. (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 $\frac{\pi}{a}\sqrt{2} = 0.795\ 10^{10}\text{m}^{-1}$

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

2. 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)

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

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 Debey temperature Θ_D. The slope of the line in a graph of C_v/T vs T^2 is 0.609 .

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

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 endimesionella 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

$$\omega^2 = 2C\frac{M_1+M_2}{M_1M_2} \Rightarrow \lambda = \frac{2\pi c}{\omega} = \frac{2\pi c}{\sqrt{2C(M_1+M_2)/M_1M_2}} = 54.6\ \mu\text{m}.$$

4. Same/similar as problem 4.4 in Bransden & Joachain. In the region where the potential is zero ($x < 0$) the solutions are of the traveling wave form e^{ikx} and e^{-ikx}, where $k^2 = 2mE/\hbar^2$. A plane wave $\psi(x) = Ae^{i(kx-\omega t)}$ describes a particle moving from $x = -\infty$ towards $x = \infty$. The probability current associated with this plane wave is
$j = \frac{\hbar}{2mi} \mid A \mid^2 (e^{-ikx}\frac{\partial}{\partial x}e^{+ikx} - e^{+ikx}\frac{\partial}{\partial x}e^{-ikx}) =\mid A \mid^2 \frac{\hbar}{m}k =\mid A \mid^2 v$
A plane wave $\psi(x) = Be^{i(-kx-\omega t)}$ describes a particle moving the opposite direction from $x = \infty$ towards $x = -\infty$. The probability current associated with this plane wave is
$j = \frac{\hbar}{2mi} \mid B \mid^2 (e^{+ikx}\frac{\partial}{\partial x}e^{-ikx} - e^{-ikx}\frac{\partial}{\partial x}e^{+ikx}) = -\mid B \mid^2 \frac{\hbar}{m}k = -\mid B \mid^2 v$

a Solution for the region $x > 0$ where the potential is $V_0 = 4.5$eV. The potential step is larger than the kinetic energy 2.0 eV of the incident beam. The particle may therefore **not** enter this region classically. It will be totally reflected. In quantum mechanics we perform the following calculation: The two solutions for the two regions are:

$$\Psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & \text{for} \quad x < 0 \quad \text{where} \quad k^2 = 2mE/\hbar^2 \\ Ce^{\kappa x} + De^{-\kappa x} & \text{for} \quad x > 0 \quad \text{where} \quad \kappa^2 = 2m(V_0 - E)/\hbar^2 \end{cases}$$

we can put $C = 0$ as this part of the solution would diverge, and is hence not physical, as x approaches ∞. At $x = 0$ both the wavefunction and its derivative have to be continous functions, as the potential is everywhere finite. The derivative is:

$$\frac{\partial \Psi(x)}{\partial x} = \begin{cases} Aike^{ikx} - Bike^{-ikx} \\ -D\kappa e^{-\kappa x} \end{cases}$$

At $x = 0$ we arrive at the following two equations:

$$\begin{cases} A + B = D \\ iAk - iBk = -D\kappa \end{cases} \text{solving for} \begin{cases} \frac{D}{A} = \frac{2k}{k+\kappa} \\ \frac{B}{A} = \frac{k-i\kappa}{k+i\kappa} \end{cases} \text{solving for} \begin{cases} \frac{D}{A} = \frac{2}{1+i\sqrt{V_0/E-1}} \\ \frac{B}{A} = \frac{1-i\sqrt{V_0/E-1}}{1+i\sqrt{V_0/E-1}} \end{cases}$$

We can now calculate the coeficient of reflection, R The coeficients represent the following amplitudes: A is the incident beam, B is the reflected beam and C is the transmitted beam. The associated probability currents are denoted j_A, j_B and j_C. Conservation yields

$j_A = j_B + j_C$. Hence we can define the coeficient of reflection as the fraction of reflected flux $R = \frac{|j_B|}{|j_A|}$ and the coeficient of transmission as $T = \frac{|j_C|}{|j_A|}$

$$\left\{ R = \frac{|j_B|}{|j_A|} = \frac{B^2 k}{A^2 k} = 1 \right.$$

This is easily seen from the ratio B/A being the ratio of two complex number where one is the complex conjugate of the other and therefore having the same absolute value. Imidiately follows that $T = 0$ as the currents have to be conserved.

(b+c) Solution for the region $x > 0$ where the potential is $V_0 = 4.5\text{eV}$. The potential step is smaller than the kinetic energy 7.0eV or 5.0eV of the incident beam. The particle may therefore enter this region classically. It will however lose some of its kinetic energy. In quantum mechanics there is a probabillity for the wave to be reflected as well. The two solutions for the two regions are:

$$\Psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & \text{for} \quad x < 0 \quad \text{where} \quad k^2 = 2mE/\hbar^2 \\ Ce^{ik'x} + De^{-ik'x} & \text{for} \quad x > 0 \quad \text{where} \quad k'^2 = 2m(E - V_0)/\hbar^2 \end{cases}$$

whe can put $D = 0$ as there cannot be an incident beam from $x = \infty$. At $x = 0$ both the wavefunction and its derivative have to be continous functions. The derivative is:

$$\frac{\partial \Psi(x)}{\partial x} = \begin{cases} Aike^{ikx} - Bike^{-ikx} \\ Cik'e^{ik'x} \end{cases}$$

At $x = 0$ we arrive at the following two equations:

$$\begin{cases} A + B = C \\ Ak - Bk = Ck' \end{cases} \text{solving for} \begin{cases} \frac{C}{A} = \frac{2k}{k+k'} \\ \frac{B}{A} = \frac{k-k'}{k+k'} \end{cases} \text{solving for} \begin{cases} \frac{C}{A} = \frac{2\sqrt{E}}{\sqrt{E}+\sqrt{E-V_0}} \\ \frac{B}{A} = \frac{\sqrt{E}-\sqrt{E-V_0}}{\sqrt{E}+\sqrt{E-V_0}} \end{cases}$$

The coeficients represent the following amplitudes: A is the incident beam, B is the reflected beam and C is the transmitted beam. The associated probability currents are denoted j_A, j_B and j_C. Conservation yields $j_A = j_B + j_C$. Hence we can define the coeficient of reflection as the fraction of reflected flux $R = \frac{|j_B|}{|j_A|}$ and the coeficient of transmission as $T = \frac{|j_C|}{|j_A|}$ For the two cases in part b and c the coeficients are:

$$\begin{cases} R = \frac{|j_B|}{|j_A|} = \frac{B^2 k}{A^2 k} = \left(\frac{B}{A}\right)^2 = \left(\frac{\sqrt{E}-\sqrt{E-V_0}}{\sqrt{E}+\sqrt{E-V_0}}\right)^2 = \left(\frac{\sqrt{5.0}-\sqrt{0.5}}{\sqrt{5.0}+\sqrt{0.5}}\right)^2 = 0.26987 \\ T = \frac{|j_C|}{|j_A|} = \frac{C^2 k'}{A^2 k} = \left(\frac{C}{A}\right)^2 \frac{\sqrt{E-V_0}}{\sqrt{E}} = \left(\frac{2\sqrt{E}}{\sqrt{E}+\sqrt{E-V_0}}\right)^2 \frac{\sqrt{E-V_0}}{\sqrt{E}} = \left(\frac{2\sqrt{5.0}}{\sqrt{5.0}+\sqrt{0.5}}\right)^2 \frac{\sqrt{0.5}}{\sqrt{5.0}} = 0.73013 \end{cases}$$

$$\begin{cases} R = \frac{|j_B|}{|j_A|} = \frac{B^2 k}{A^2 k} = \left(\frac{B}{A}\right)^2 = \left(\frac{\sqrt{E}-\sqrt{E-V_0}}{\sqrt{E}+\sqrt{E-V_0}}\right)^2 = \left(\frac{\sqrt{7.0}-\sqrt{2.5}}{\sqrt{7.0}+\sqrt{2.5}}\right)^2 = 0.063437 \\ T = \frac{|j_C|}{|j_A|} = \frac{C^2 k'}{A^2 k} = \left(\frac{C}{A}\right)^2 \frac{\sqrt{E-V_0}}{\sqrt{E}} = \left(\frac{2\sqrt{E}}{\sqrt{E}+\sqrt{E-V_0}}\right)^2 \frac{\sqrt{E-V_0}}{\sqrt{E}} = \left(\frac{2\sqrt{7.0}}{\sqrt{7.0}+\sqrt{2.5}}\right)^2 \frac{\sqrt{2.5}}{\sqrt{7.0}} = 0.936563 \end{cases}$$

The last result could also be reached by $T + R = 1$.

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

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

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

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

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

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

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

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

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

where

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