Mando II

Task I

a) $\mathcal{K}$ - thermal conductivity.

σ - electrical — II —.

$$\mathcal{K} = \frac{1}{3} C_V v^2 \tau \quad , \quad v\text{-velocity} \ , \ \tau \text{- relaxation time}$$

$$\langle v \rangle^2 = \frac{3k_B T}{m_e} \quad , \quad C_V = C_{el} = \frac{3}{2} n_e k_B \text{ - heat capacity}$$

$$\Rightarrow \mathcal{K} = \frac{1}{3} \cdot \frac{3}{2} n_e k_B \cdot \frac{3k_B T}{m_e} \cdot \tau$$

$$\sigma = \frac{q^2 n_e}{m_e} \tau$$

$$\Rightarrow L = \frac{\mathcal{K}}{\sigma T} = \underline{\underline{\frac{3}{2} \frac{k_B^2}{q^2}}} \quad , \quad q = e$$

Good agreement with experiment because conductivity, both electrical and thermal, depend on movability of the electrons, which again is related to temperature.

b) $$C_{el} = \frac{\pi^2 N k_B T}{2 T_f}$$

$E_f = k_B T_f$

$$\Rightarrow \mathcal{K} = \frac{1}{3} \cdot \frac{\pi^2 N k_B T}{2 T_f} \cdot v_f^2 \cdot \tau_f$$

$$E_f = k_B T_f \Rightarrow T_f = \frac{E_f}{k_B} \Rightarrow \frac{1}{T_f} = \frac{k_B}{E_f}$$

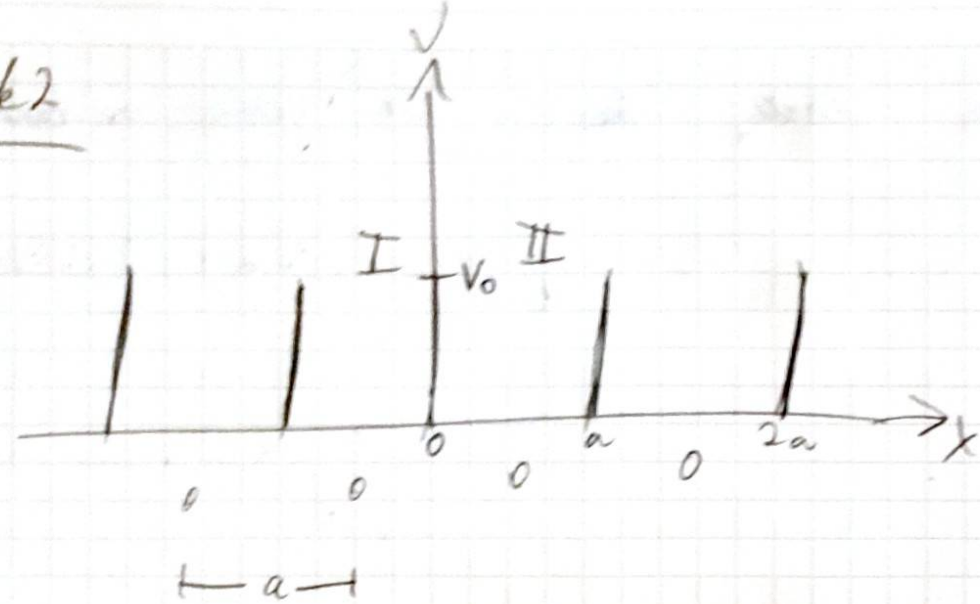
$$E_f = \frac{1}{2} m_e v_f^2 \Rightarrow v_f^2 = \frac{2 E_f}{m_e}$$

$$\Rightarrow \mathcal{K} = \frac{1}{3} \cdot \frac{\pi^2 N \cdot T \cdot k_B^2}{2 E_f} \cdot \frac{2 E_f}{m_e} \cdot \tau_f = \frac{\pi^2}{3 m_e} N T k_B^2 \tau_f$$

$$\sigma = \frac{e^2 N}{m_e} \tau_f$$

$$\Rightarrow \frac{\mathcal{K}}{\sigma T} = \frac{\pi^2}{3} \left(\frac{k_B}{e} \right)^2$$

Task 2



S.E: $\left(\frac{p^2}{2m_e} + V(x)\right)\psi = E\psi$ $\qquad \hat{p} = -i\hbar\hat{\nabla}$

$$= -\frac{\hbar^2}{2m_e}\frac{\partial^2}{\partial x^2}\psi + V(x)\psi = E\psi$$

$$V(x) = V_0 \sum_{j=0}^{N-1} \delta(x - ja)$$

In cell II, for $0<x<a$:

$$-\frac{\hbar^2}{2m_e}\frac{\partial^2}{\partial x^2}\psi = E\psi$$

$$\Rightarrow \frac{\partial^2}{\partial x^2}\psi = -k^2\psi \quad , \quad k = \frac{\sqrt{2m_e E}}{\hbar}$$

$$\Rightarrow \psi_2 = A\cos(kx) + B\sin(kx) \qquad (1)$$

By Blochs Theorem we have in cell I:

$$\psi_1(x) = e^{-iqa}\left\{A\cos[k(x+a)] + B\sin[k(x+a)]\right\}$$

At $x=0$, ψ must be continous, so

$$\psi_1(x) = \psi_2(x)$$

$$\Rightarrow A = e^{-iqa}\left[A\cos(ka) + B\sin(ka)\right] \quad (2)$$

Evaluating the S.E at the border via:

$$\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi + V\psi = E\psi\right)$$

$$\Rightarrow \lim_{\varepsilon\to 0} -\frac{\hbar^2}{2m}\underbrace{\int_{-\varepsilon}^{+\varepsilon}\frac{\partial^2}{\partial x^2}\psi}_{=\frac{\partial}{\partial x}\psi\Big|_{-\varepsilon}^{+\varepsilon}} + \int_{-\varepsilon}^{+\varepsilon} V\psi\,dx = \lim_{\varepsilon\to 0}\int_{-\varepsilon}^{+\varepsilon}\underbrace{E\psi}_{\text{finite}}\,dx = 0$$

From this we have

$$\Delta\left(\frac{\partial\psi}{\partial x}\right) = \frac{2m}{\hbar^2}V_0\psi(0)$$

Using this we get ...

$$\left.\frac{\partial \psi_2}{\partial x}\right|_{x=0} - \left.\frac{\partial \psi_1}{\partial x}\right|_{x=0} = \frac{2mV_0}{\hbar^2} A$$

$$\Rightarrow kB - e^{-iqa}\left[B\cos(ka) - A\sin(ka)\right] k = \frac{2mV_0}{\hbar^2} A \quad (3)$$

Solving (2) for A :

$$A = \frac{B\sin(ka)}{e^{iqa} - \cos(ka)}$$

Inserting this in (3) gives

$$kB - e^{-iqa}\left[kB\cos(ka) - \frac{kB\sin^2(ka)}{e^{iqa} - \cos(ka)}\right] = \frac{2mV_0}{\hbar^2} \frac{B\sin(ka)}{e^{iqa} - \cos(ka)}$$

$$\Rightarrow 1 - e^{-iqa}\left[\cos(ka) - \frac{\sin^2(ka)}{e^{iqa} - \cos(ka)}\right] = \frac{2mV_0}{\hbar^2 k} \frac{\sin(ka)}{e^{iqa} - \cos(ka)}$$

$$\Rightarrow e^{iqa} - \cos(ka) - e^{-iqa}\left(e^{iqa} - \cos(ka)\right)\left[\cos(ka) - \frac{\sin^2(ka)}{e^{iqa} - \cos(ka)}\right] = \frac{2mV_0}{\hbar^2 k}\sin(ka)$$

$$\Rightarrow e^{iqa} - \cos(ka) - e^{-iqa}\left(e^{iqa}\cos(ka) - \cos^2(ka) - \sin^2(ka)\right)$$

$$= \frac{2mV_0}{\hbar^2 k}\sin(ka)$$

$$\Rightarrow e^{iqa} - \cos(ka) - \cos(ka) + e^{-iqa}\cos^2(ka) + e^{-iqa}\sin^2(ka)$$

$$= \frac{2mV_0}{\hbar^2 k}\sin(ka)$$

$$\Rightarrow e^{iqa} - 2\cos(ka) + e^{-iqa} = \frac{2mV_0}{\hbar^2 k}\sin(ka)$$

$$\Rightarrow 2\cos(qa) = 2\cos(ka) + \frac{2mV_0}{\hbar^2 k}\sin(ka)$$

$$\Rightarrow \cos(qa) = \cos(ka) + \frac{mV_0}{\hbar^2 k}\sin(ka)$$

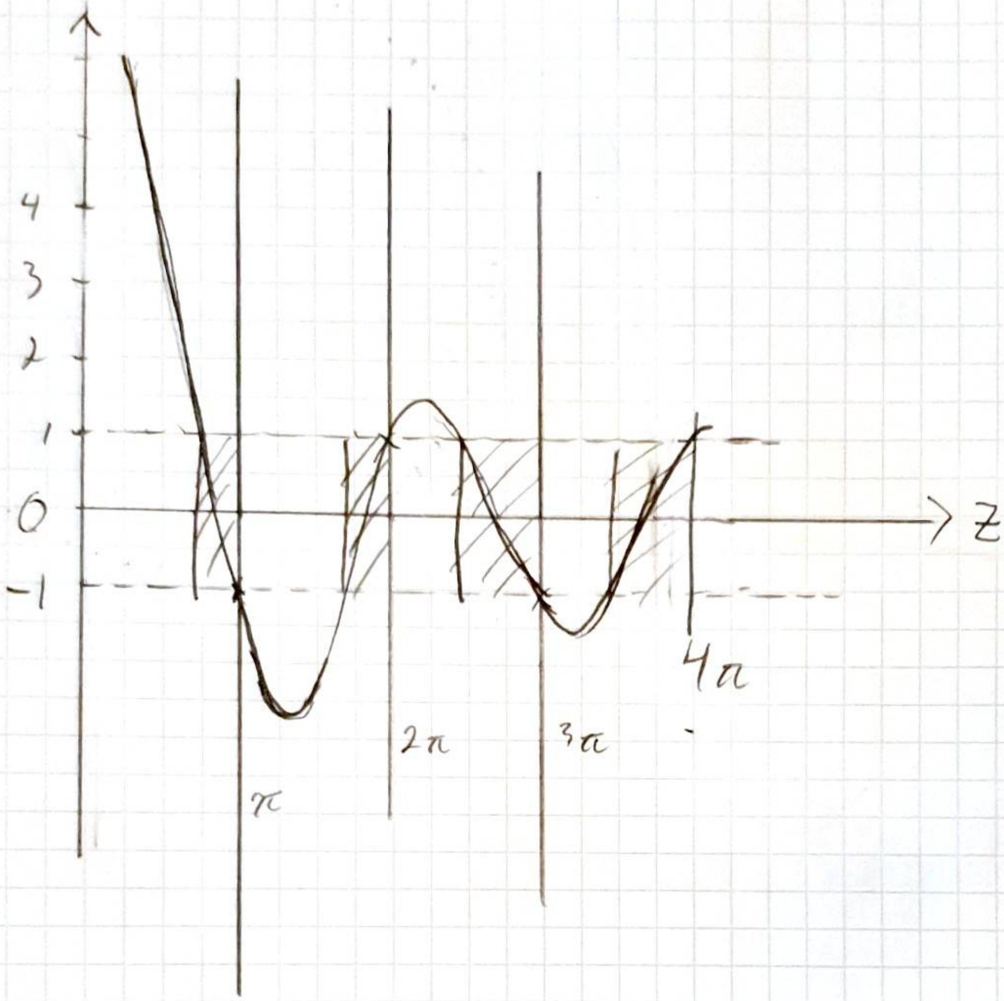
$$z = ka$$

$$\Rightarrow f(z) = \cos(z) + \frac{mV_0 a}{\hbar^2}\frac{\sin(z)}{z}$$

$$-1 \leq \cos(qa) \leq 1$$

$$\frac{mV_0 a}{\hbar^2} = \beta$$

For $\beta = 10$:



Since $\beta \sim V_0$, as $V_0 \to 0$ then $\cos(ka) \to \cos(qa)$ and there will be no forbidden energy zones. → No bandgaps. → Free electron.

As $V_0 \to \infty$ $\cos(qa) = V_0 \frac{\sin(z)}{z}$ and there will only be defined energylevels at $\lim_{z \to n2\pi} \frac{\sin(z)}{z}$. But at this limit the derivative will go to infinity, so only one z-value will be allowed and therefore only one energy level.

Task 3

S.C

# of atoms = 1

a) k_f?

$$k_{BZ} = \frac{\pi}{a} \quad , \ k_f = (3 \rho \pi^2)^{1/3}$$

ρ = Number of free electrons per unit volume

Monovalent crystal

volume in k-space?

$$\Rightarrow \rho = 1 \cdot \# \text{of atoms} / V = \frac{1}{V} = \frac{1}{a^3}$$

$$\Rightarrow k_f = \left(3 \frac{1}{a^3} \pi^2\right)^{1/3} = \frac{(3\pi^2)^{1/3}}{a}$$

$$\frac{k_f}{k_{BZ}} = 0{,}985$$

$\log_2(i) \Rightarrow \log_i(2)$, $i^x = 2$

b) If $k_f < k_{BZ}$ empty states available

$x \ln(i) = \ln 2$

$x = \frac{\ln 2}{i\pi/2}$

For each divalent atom added, an additional $\frac{1}{8}$ electron would accompany it.

$2^x = i$

$e^{x \ln 2} = i$

$$\Rightarrow \frac{1}{a^3}\left(\frac{n_1}{8} + \frac{2n_2}{8}\right) = \rho$$

n_1 - nr. of monovalent atoms, n_2 - nr. of divalent atoms

$n_1 + n_2 = 8 \rightarrow$ the total number of atoms whose $\frac{1}{8}$ is in the cell.

$$\Rightarrow k_f = \left(3 \cdot \left(\frac{n_1}{8} + \frac{2n_2}{8}\right) \cdot \frac{1}{a^3} \pi^2\right)^{1/3} = \frac{\pi}{a}$$

$$\Rightarrow \left(\frac{3}{8}\left(n_1 + 2n_2\right) \cdot \pi^2\right)^{1/3} = \pi$$

$$\Rightarrow \frac{3}{8}\left(n_1 + 2(8 - n_1)\right) \cdot \pi^2 = \pi^3$$

$$\Rightarrow \frac{3}{8}\left(n_1 + 16 - 2n_1\right) = \pi$$

$$\Rightarrow \frac{8\pi}{3} - 16 = -n_1, \quad n_1 = 7{,}6$$

$$\Rightarrow n_2 = 0{,}4$$

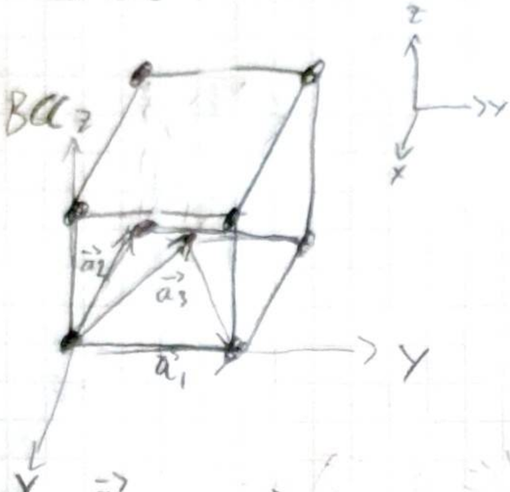
$\Rightarrow$ 0,4 atoms per 8 atoms are needed to satisfy $k_f = k_{BZ}$, or:

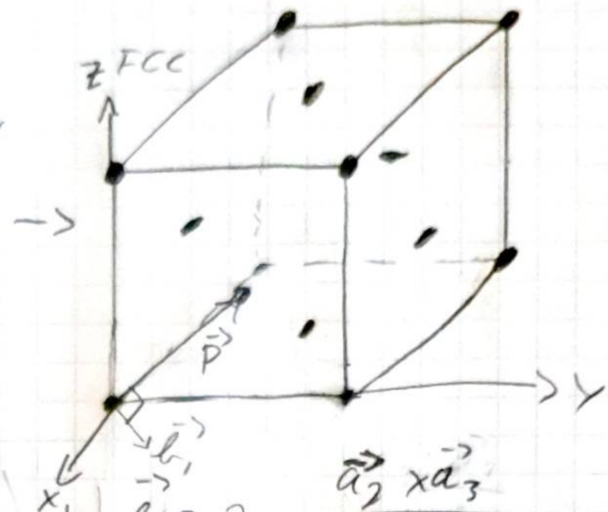
$$0{,}4 \cdot 5 = 2 \quad , \quad 8 \cdot 5 = 40$$

$\Rightarrow$ We need 5% divalent atoms

Adding electrons to the system will fill the band, allowing less movement of the electrons.

c) A BCC in reciprocal lattice is an FCC





$$\vec{a}_1 = a\vec{y}$$

$$\vec{a}_2 = a(-\vec{x})$$

$$\vec{a}_3 = \frac{1}{2}a(-\vec{x}+\vec{y}+\vec{z})$$

$$\vec{b}_1 = 2\pi\frac{\vec{a}_2\times\vec{a}_3}{\vec{a}_1\cdot(\vec{a}_2\times\vec{a}_3)}$$

$$\vec{b}_2 = 2\pi\frac{\vec{a}_3\times\vec{a}_1}{\vec{a}_2\cdot(\vec{a}_3\times\vec{a}_1)}$$

$$\vec{b}_3 = 2\pi\frac{\vec{a}_1\times\vec{a}_2}{\vec{a}_3\cdot(\vec{a}_1\times\vec{a}_2)}$$

$$\vec{a}_2\times\vec{a}_3 = a^2\begin{vmatrix}\vec{x} & \vec{y} & \vec{z}\\ -1 & 0 & 0\\ -\frac{1}{2} & \frac{1}{2} & \frac{1}{2}\end{vmatrix} = a^2\left(\frac{1}{2}\vec{y}\right) + a^2\vec{z}\left(-\frac{1}{2}\right)$$

$$\Rightarrow \vec{b}_1 = \frac{2\pi\cdot\frac{1}{2}a^2(\vec{y}-\vec{z})}{\frac{1}{2}a^3} = \frac{2\pi}{a}(\vec{y}-\vec{z})$$

$|\vec{p}| = |\vec{b}_1| = \frac{2\pi}{a}\sqrt{2}$ (Because we know the lattice is periodic).

$$\Rightarrow k_{BZ} = \frac{\sqrt{2}\,\pi}{a}$$

c) $k_f = \left(3 \cdot \frac{2}{a^3} \cdot \pi^2\right)^{1/3}$

$\Rightarrow \frac{k_f}{k_{BZ}} = \frac{(6\pi^2)^{1/3}}{\sqrt{2}\,\pi} = 0{,}8773$

d)

$k_f = k_{BZ}$:

$$\Rightarrow \left(3 \cdot \frac{x}{a^3} \pi^2\right)^{1/3} = \sqrt{2}\,\frac{\pi}{a}$$

$$3 \frac{X}{a^3} \pi^2 = \left(\sqrt{2}\,\frac{\pi}{a}\right)^3$$

$$X = \frac{(\sqrt{2}\pi)^3}{3\pi^2} = 2{,}96$$

$\Rightarrow$ We need 2,96 free electrons in order to satisfy $k_f = k_{BZ}$

$n_1 + 2n_2 = 2{,}96$ free electrons per cell

$n_1 + n_2 = 2$ atoms per conventional unit cell

$$n_1 + 4 - 2n_1 = 2{,}96$$

$$\Rightarrow 4 - 2{,}96 = n_1$$

$$\Rightarrow n_1 = 1{,}04$$

$$\Rightarrow n_2 = 0{,}96 \quad \Rightarrow \frac{n_2}{n_1+n_2} = 48\%\ Mg$$

e)

For a crystal to be an insulator, it must have an even number of electrons per primitive cell. This is because a full band is a lazy band (it restricts electron movement).

It will then be necessary to check if the bands overlap in energy.

Assuming we have an Alkali/Alkali earth alloy with a band overlap such as Na, then the conductivity will vary with the minimum conductivity appearing as each unit cell have $2n$ electrons. $n \in \mathbb{Z}$.