

1. (a) Bloch's theorem says that if the potential is periodic, ie. $U(\vec{x} + \vec{a}) = U(\vec{x})$, then the energy eigenfunctions satisfy $\psi(\vec{x} + \vec{a}) = e^{i\vec{k}\cdot\vec{a}}\psi(\vec{x})$ for some \vec{k} . This is important for a number of reasons. For instance, it shows that the eigenfunctions are extended in space and can be labeled with a momentum-like quantum number, thus justifying the free electron model for metals.
- (b) The Wiedemann-Franz law says that, for metals, the ratio $\kappa/(\sigma T)$ is independent of the material and amount of disorder. Since this result is derived from the free-electron model, it provides an experimental justification of that model.
- (c) For BiTe_2 , we have the bismuth contributing $2+3=5$ electrons, and each tellurium $2+4=6$ electrons. This gives a total of 17 electrons per unit cell. Since each band can take 2 electrons per unit cell, this means that we will have 8 filled bands and one half filled band, suggesting that this material is a metal.
For ZnGeP_2 , we have the zinc contributing 12 electrons, the germanium contributing 4 electrons, and each phosphorus 5 electrons. This gives a total of 26 electrons per unit cell. Since each band can take 2 electrons per unit cell, this means that we will have 13 filled bands, suggesting that this material is an insulator.
- (d) Van der Waals: induced dipole-dipole interaction; approximately 0.1 eV/atom.
Ionic: attraction between positive and negative ions; approximately 5 eV/atom.
Metallic: energy is lowered by delocalization of the electrons; approximately 1 eV/atom.
Covalent: localized electrons create an attraction between the ions; approximately 1 eV/atom.
2. (a) i. ISSP, page 138, equation (16):

$$k_F = (3\pi^2 n)^{1/3} = (3\pi^2 30)^{1/3} \times 10^6 = 9.6 \times 10^6 \text{ cm}^{-1}$$

ii.

$$v_F = \frac{\hbar k_F}{m^*} = \frac{\hbar k_F}{0.1m} = 1.1 \times 10^8 \text{ cm/s}$$

iii.

$$\begin{aligned} \frac{D(E_F)}{V} &= \frac{1}{2\pi^2} \left(\frac{2m^*}{\hbar^2} \right)^{3/2} E_F^{1/2} = \frac{1}{2\pi^2} \left(\frac{2m^*}{\hbar^2} \right)^{3/2} \left(\frac{\hbar^2 k_F^2}{2m^*} \right)^{1/2} = \frac{m^*}{\pi^2 \hbar^2} k_F = 8.03 \times 10^{44} \text{ J}^{-1} \text{ m}^{-3} \\ &= 8.03 \times 10^{31} \text{ erg}^{-1} \text{ cm}^{-3} \end{aligned}$$

- (b) At room temperature the dominant scattering mechanism will be phonons. The Debye temperature is typically smaller than room temperature, in which case the number of phonons in a mode $n \approx k_B T / (\hbar \omega)$. Therefore the resistivity, which is proportional to the number of phonons present, is proportional to T .
- (c) i. The hall coefficient is given by $R_H = 1/(nec)$ and so it tells us the density of carriers. The resistivity is $\rho = m/(ne^2\tau)$. Therefore,

$$\tau = \left(\frac{mc}{e} \right) \frac{R_H}{\rho}$$

Therefore, measuring the hall coefficient and the resistivity can be used to find the mean free time, assuming that m is the free electron mass.

ii. The density of states enters into the heat capacity (ISSP, page 144, equation 32):

$$C_V = \frac{\pi^2}{3} D(E_F) k_B^2 T = \gamma T$$

The slope γ can be measured from the slope of C_V versus T ; then

$$D(E_F) = \frac{\gamma}{k_B^2 \pi^2 / 3}$$

3. (a) Taylor expanding in Ka :

$$\frac{P}{Ka} (Ka - (Ka)^3/3 + \dots) + 1 - (Ka)^2/2 + \dots = 1 - (ka)^2/2 + \dots$$

which gives

$$P(1 - (Ka)^2/3) - (Ka)^2/2 \simeq -(ka)^2/2 + \dots$$

Rewriting:

$$(Ka)^2 \simeq \frac{P}{\frac{1}{2} + \frac{P}{3}} + \frac{(ka)^2}{2} \frac{1}{\frac{1}{2} + \frac{P}{3}} \simeq 2P + (ka)^2 \frac{1}{1 + \frac{2P}{3}}$$

and so

$$E(k) = \frac{\hbar^2}{ma^2} P + \frac{\hbar^2 k^2}{2m} \frac{1}{1 + \frac{2P}{3}}$$

Therefore the energy at $k = 0$ is raised, and the effective mass near $k = 0$ is increased slightly.

$$m^* = m \left(1 + \frac{2P}{3} \right)$$

(b) If the reciprocal lattice vectors are given by $\vec{G} = (2\pi/a)(n, m)$, then, writing $k = \alpha(\pi/a)(1, 0)$ where α goes from 0 to 1, gives

$$E_{nm}(\alpha) = \frac{\hbar^2}{2m} (\vec{k} + \vec{G})^2 = \frac{\hbar^2 \pi^2}{2ma^2} ((\alpha + 2n)^2 + 4m^2)$$

The band structure is shown in figure 1. One expects gaps to open up wherever two or more bands meet.

4. (a) For periodic boundary conditions, the single-valuedness of the wave-functions gives

$$e^{ikx} = e^{ik(x+L)} \Rightarrow e^{ikL} = 1 \Rightarrow k = \frac{2\pi n}{L} \quad n = \dots, -1, 0, 1, \dots$$

Therefore the distance between k points is $2\pi/L$.

(b) The $k = 0$ wavefunction is a non-zero constant everywhere in space, and in particular at the edges of the box. Outside, the wavefunction is zero. Therefore one cannot have a continuous wavefunction with $k = 0$.

(c) The longest allowed wavelength is $2L$, and so the smallest k is $k = 2\pi/(2L) = \pi/L$. Note then that $\cos(ka) = \cos(\pi/30) \simeq .978$. Then the gap is

$$E_g = (6 - 5(0.978)) - (-1)(6 - 5(0.978)) = 2(6 - 5(0.978)) = 2.22eV$$

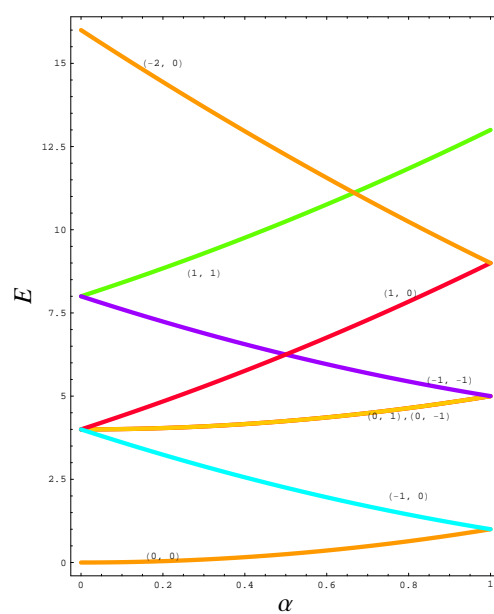


Figure 1: The energy band structure for Q3(b).