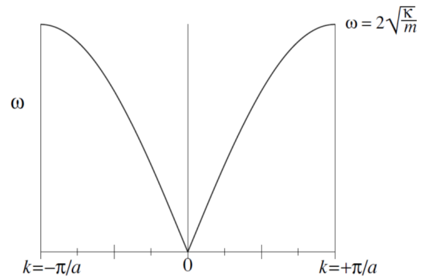
Condensed Matter Physics 2023
Quiz 5 (Week 12)

1. For the infinite one-dimensional chain (atoms of mass M connected by springs), sketch and describe the dispersion relation. Explain how it would vary for increasing M, and what is the value of the sound velocity and how to find it.

The dispersion relation is sketched below and is given by: $\omega(k) = 2\sqrt{\frac{\kappa}{M}}\left|\sin\left(\frac{ka}{2}\right)\right|$.



The dispersion can be plotted in the first Brillouin zone, between $k = -\pi/a$ and $k = \pi/a$, as it is periodic with periodicity $2\pi/a$. It is maximum at the Brillouin zone boundaries, where the group velocity $v_g = d\omega/dk$ is zero. Near the zone center ($k = 0$), i.e. at long wavelengths, it is linear and the group and phase velocities are the same.
With a larger value of M, the curve would flatten, with the value of the frequency becoming lower. The sound velocity is given by $v = \sqrt{\frac{\kappa a^2}{M}}$, as can be found by linearly expanding the dispersion relation near $k = 0$: $\omega(k) \simeq 2\sqrt{\frac{\kappa}{M}}\left|\frac{ka}{2}\right| = v|k|$.

2. The energy gap of ZnSe is 2.3 eV.
   (a) Is ZnSe transparent to visible light? Explain your answer.
   (b) How could you increase the electrical conductivity of this material? Give reasons.

(a) ZnSe will absorb photons with energy $E \geq E_g$, that is $E \geq 2.3$ eV. This means that violet-blue-green light is absorbed, and yellow-orange-red light is transmitted (see slide 6 of Lecture 14, including the table), and ZnSe is expected to have a yellowish-red color.

(b) There are two ways to increase the electrical conductivity of ZnSe in principle. Raising the temperature would increase the number of thermally activated charge carriers in the conduction band (electrons) and in the valence band (holes) and, thus, the conductivity. Alternatively, doping the material with either donor or acceptor elements would increase the number of electrons (holes) in the conduction (valence) band, respectively, again increasing the electrical conductivity. For example, we could achieve n-type conductivity by doping with Ga on the Zn site (Ga has one more electron in the valence shell than Zn); or we could achieve p-type conductivity by doping with As on the Se site (As has one less electron in the valence shell than Se).

3. If no electron-hole pairs were created in silicon (Si) until the temperature reached the value corresponding to the energy band gap, 1.12 eV, at which temperature would Si become conductive? [Hint: the thermal energy is given by $E_{\text{th}} = \frac{3}{2}k_B T$.] Could this physically happen given the temperature found?

The temperature corresponding to the energy band gap can be found by equating the thermal energy to the band gap: $\frac{3}{2}k_B T = E_g$. Hence,

$$T = \frac{2E_g}{3k_B} = \frac{2 \cdot 1.12 \cdot 1.602 \times 10^{-19}}{3 \cdot 1.38 \times 10^{-23}} = 8668 \text{ K}$$

This is well above the melting temperature of silicon (easy to search: 1414°C= 1687 K), so if this scenario was true, Si would melt before it could become conducting.

4. An intrinsic semiconductor has a simple cubic crystal structure with lattice parameter $a = 5.3$ Å. The valence (v) and conduction (c) bands are well approximated by:

$$\epsilon_v(\mathbf{k}) = A + B\left[\cos(k_x a) + \cos(k_y a) + \cos(k_z a)\right]$$

$$\epsilon_c(\mathbf{k}) = C - D\left[\cos(k_x a) + \cos(k_y a) + \cos(k_z a)\right]$$

with $A = -4.1$ eV, $B = 0.4$ eV and $D = 0.3$ eV,.

(a) Find C, knowing that the band gap is $E_g = 0.6$ eV. [Hint: at which $\mathbf{k}$ is ϵ_v maximum, and at which $\mathbf{k}$ is ϵ_c minumum?]

(b) Determine the values of the effective mass of electrons and holes at the bottom of the conduction band and top of the valence band, respectively.

(c) Determine the density of electrons in the conduction band and holes in the valence band at $T =$ 300 K.

From the expressions of $\epsilon_v(\mathbf{k})$ and $\epsilon_c(\mathbf{k})$ given, the top of the valence band and bottom of the conduction band are clearly at $\mathbf{k} = (0, 0, 0)$ (Γ point).

(a) The band gap is then given by $E_g = \epsilon_c(0) - \epsilon_v(0) = C - 3D - (A + 3B)$, so we obtain:

$$C = E_g + 3D + A + 3B = 0.6 + 3 \cdot 0.3 - 4.1 + 3 \cdot 0.4 = -1.4 \text{ eV}$$

(b) The bands are isotropic, so the effective masses at Γ are the same when we take k along k_x, k_y or k_z. The effective masses of the electrons (e) and holes (h) are:

$$m_e^* = \hbar^2 \left(\frac{\partial^2 \epsilon_c(0)}{\partial k_x^2}\right)^{-1} = \frac{\hbar^2}{a^2 D} = \frac{(1.05457 \times 10^{-34})^2}{(5.3 \times 10^{-10})^2 \cdot 0.3 \times 1.602 \times 10^{-19}} = 8.2{\times}10^{-31} \text{ kg} = 0.90\, m$$

$$m_h^* = -\hbar^2 \left(\frac{\partial^2 \epsilon_v(0)}{\partial k_x^2}\right)^{-1} = \frac{\hbar^2}{a^2 B} = \frac{(1.05457 \times 10^{-34})^2}{(5.3 \times 10^{-10})^2 \cdot 0.4 \times 1.602 \times 10^{-19}} = 6.2{\times}10^{-31} \text{ kg} = 0.68\, m$$

(c) In an intrinsic semiconductor, the density of electrons and holes is the same:

$$n_{\text{intrinsic}} = p_{\text{intrinsic}} = \sqrt{np} = \frac{1}{\sqrt{2}}\left(\frac{k_B T}{\pi \hbar^2}\right)^{3/2} (m_e^* m_h^*)^{3/4}\, e^{-E_g/(2k_B T)}$$

and using the effective masses we find:

$$n_i = p_i = \frac{1}{\sqrt{2}}\left(\frac{1.38 \times 10^{-23} \cdot 300}{\pi(1.05457 \times 10^{-34})^2}\right)^{3/2} (8.2{\cdot}6.2{\times}10^{-62})^{3/4} e^{-0.6/(2 \cdot 8.617 \times 10^{-5} \cdot 300)} = 1.6{\times}10^{20} \text{ m}^{-3}$$