Homework 8

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Problem 1 Consider a 1D chain of identical atoms with one atom per unit cell. Each atom donates Z electrons to the band structure. How many bands will be filled by electrons and briefly explain why?

Solution When the bands overlap with each other, we really can't say much about how many bands are filled, because we can distort the bands and make the number of filled bands as many as we want (Figure 1).

When there is no overlapping, if Z is even, then there are $Z/2$ bands filled, because a band can host N orbital modes and therefore it can host $2N$ electrons when spin is considered. There are ZN electrons in the band structure in total, so we need $ZN/2N = Z/2$ bands. If Z is odd, then we need to fill $(Z+1)/2$ bands, because $N(Z-1)$ electrons are hosted by $(Z-1)/2$ bands, and we need an additional band to host the rest N electrons.

Problem 2

Solution

(a) We have

$$k_1 = \frac{2\pi}{L} = \frac{2\pi}{Na}, \quad k_2 = \frac{\pi}{a}. \tag{1}$$

$$E' = \frac{\hbar^2}{2m}\left(\frac{\pi}{a}\right)^2. \tag{2}$$

$$E'' = \epsilon_{n=3,\boldsymbol{k}=\pi/a} = \frac{\hbar^2}{2m}\Big(\frac{\pi}{a} + \underbrace{\frac{2\pi}{a}}_{\boldsymbol{G}_{n=3}}\Big) = 9\frac{\hbar^2}{2m}\left(\frac{\pi}{a}\right)^2. \tag{3}$$

(b) From the band diagram,

$$\epsilon_{n=2,k} = \frac{\hbar^2}{2m}(k+G_2)^2 = \frac{\hbar^2}{2m}\left(k - \frac{2\pi}{a}\right)^2. \tag{4}$$

The group speed is

$$v = \frac{1}{\hbar}\frac{\partial \epsilon_{n=2,k}}{\partial k} = \frac{\hbar}{m}\left(k - \frac{2\pi}{a}\right) = -\frac{3\hbar\pi}{2ma}. \tag{5}$$

The effective mass is

$$\frac{1}{m^*} = \frac{1}{\hbar^2}\frac{\partial^2 \epsilon_{n=2,k}}{\partial k^2} = \frac{1}{m}, \quad m^* = m. \tag{6}$$

(c) Regardless of the shape, each band accommodates

$$\underbrace{2}_{\text{spin}} \cdot \frac{2k_2}{k_1} = 2N \tag{7}$$

electrons.

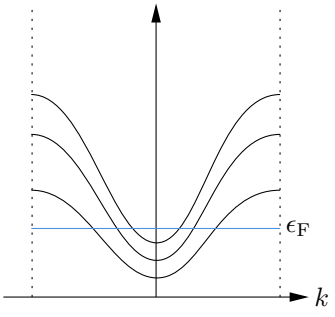

Figure 1: Overlapping bands and partial filling

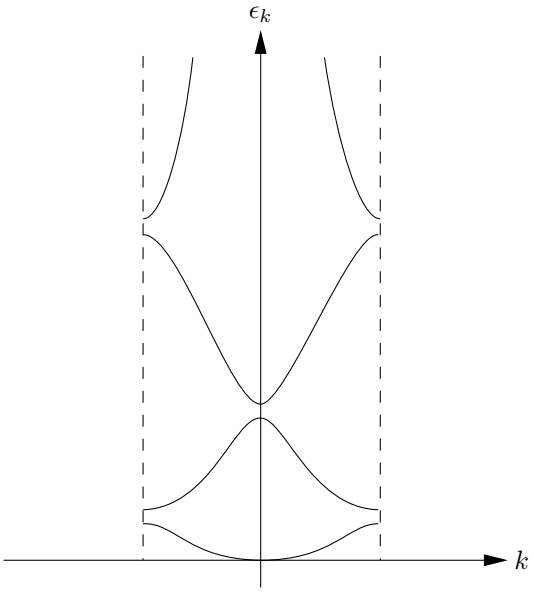

Figure 2: Empty lattice model after weak perturbation

(d) See Figure 2.

(e) TODO

Problem 4
Solution

(a) It has to be an insulator. Selective absorption of light of one particular color means there is a direct band gap corresponding to the energy of the photon of that color.

(b) The transmitted light is red, so the absorbed light is bluish, so the photon energy – and the direct band gap – is about 2.5 eV.

Problem 5
Solution

(a) We just need to find a material whose direct band gap falls in the visible light spectrum. This is the third material ($E_g = 1.42\,\text{eV}$), and it will be a red color LED.

(b) The smaller the direct band gap is, the easier it is to be a thermally activated conductor. So the conductivity of the second material ($E_g = 0.35\,\text{eV}$) turns on first.