$\boxed{\#7-1}$ Given One-dimensional crystal

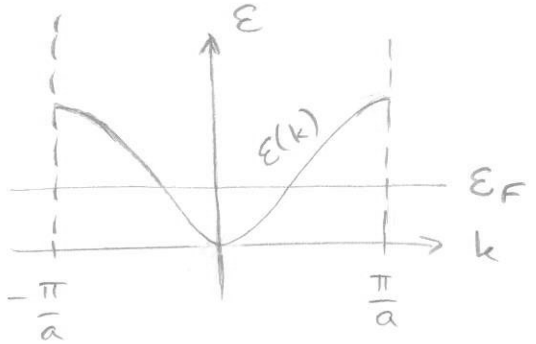
Lattice param. a, $\underbrace{\frac{1}{a} \text{ el / length unit}}_{}$ 1 el / unit cell

Lowest band $\varepsilon(k) = \varepsilon_0 \left(1 - \cos(ka)\right)$

Show: For electrons at ε_F : $m^* \to \infty$

What does it mean?

Solution



$$\frac{1}{m^*} = \frac{1}{\hbar^2} \frac{\partial^2 \varepsilon}{\partial k^2} =$$

$$= \frac{1}{\hbar^2} \varepsilon_0 \cos(ka) \cdot a^2$$

$$n = \frac{N \cdot 1}{L} = \int_0^{\varepsilon_F} g(\varepsilon)\, d\varepsilon \qquad \left(N = \int_0^{\varepsilon_F} D(\varepsilon)\, d\varepsilon \right)$$

$$D(\varepsilon)\, d\varepsilon = 2 \cdot \frac{L}{2\pi} \cdot 2 \cdot dk$$

spin — number of points per k-volume $\longleftrightarrow$ $\frac{2\pi}{L}$ k-volume per point — count positive k

$$g(\varepsilon)\, d\varepsilon = \frac{1}{L} \cdot D(\varepsilon)\, d\varepsilon = \frac{2}{\pi} dk$$

$$n = \frac{N}{L} = \int_0^{k_F} \frac{2}{\pi} dk = \frac{2}{\pi} k_F \implies k_F = \frac{\pi}{2} \cdot n = \frac{\pi N}{2L}$$

$$L = N \cdot a \implies k_F = \frac{\pi}{2a}$$

(if you think this is obvious!)
k-points are spaced uniformly along k-axis
2 el/cell fill band

set $k = k_F$ in $\frac{1}{m^*}$:

$$\left.\frac{1}{m^*}\right|_{\varepsilon_F} = \underbrace{\frac{1}{\hbar^2} \varepsilon_0 \cos\Big(\underbrace{\frac{\pi}{2a} \cdot a}_{\pi/2}\Big)}_{0} \cdot a^2 = 0$$

$\implies m^* \to \infty$ at ε_F

Interpretation: Electrons act as heavy particles if external force

#7:2

Given: Crystal with simple cubic (sc) structure

Unit cell, lattice param. a

Certain energy band

$$\mathcal{E}(\bar{k}) = -\mathcal{E}_0(\cos k_x a + \cos k_y a + \cos k_z a)$$

Electron with $\bar{k} = \bar{0}$ at $t = 0$

Electrical field E_x

Disregard resistance $\longrightarrow$ no scattering

a) **Wanted** $\bar{r}(t)$ if $\bar{r}(0)$ known (to within uncertainty)

Solution

$$\frac{d\bar{r}}{dt} = v_g(t) \qquad r(t) = \int_0^t v_g(t)\,dt$$

$$v_g(t) = \frac{1}{\hbar}\nabla_{\bar{k}}\mathcal{E}(\bar{k}(t))$$

$$\bar{F} = -e\bar{E} = \hbar\frac{d\bar{k}}{dt} \Longrightarrow \frac{d\bar{k}}{dt} = -\frac{eE_x}{\hbar}$$

$$\bar{k}(t) = \underbrace{\bar{k}(0)}_{\bar{0}} - \frac{eE_x}{\hbar}t \qquad \boxed{k_x = -\frac{eE_x}{\hbar}t}$$

$$\bar{v}_g(t) = \frac{1}{\hbar}\left(\frac{\partial\mathcal{E}(t)}{\partial k_x}, \frac{\partial\mathcal{E}(t)}{\partial k_y}, \frac{\partial\mathcal{E}(t)}{\partial k_z}\right) = +\frac{\mathcal{E}_0}{\hbar}\cdot a\left(\sin k_x a + \sin k_y a + \sin k_z a\right)$$

$$v_x(t) = \frac{\mathcal{E}_0 a}{\hbar}\sin\left(-\frac{eE_x}{\hbar}at\right)$$

$$x(t) = \int_0^t v_x(t)\,dt = \frac{\mathcal{E}_0 a}{\hbar}\cdot\frac{1}{\frac{eE_x}{\hbar}a}\cos\left(-\frac{eE_x}{\hbar}at\right) =$$

$$= \underline{\underline{\frac{\mathcal{E}_0}{eE_x}\cos\left(\frac{eE_x}{\hbar}at\right)}}$$

b) $\left.\begin{array}{l}\mathcal{E}_0 = 1\text{ eV}\\ E_x = 1\text{ V/cm}\end{array}\right\} \Longrightarrow \underline{x_{max} = ?} \qquad x_{max} = \frac{1\text{ eV}}{e\cdot 1\text{ V/cm}} = \underline{\underline{1\text{ cm}}}$

Not expected motion; very long distance without scattering

#7:3 Given: s.c. $\mathcal{E}(k) = A \cdot k^2$ a lattice param.

$A = 10^{-38}\ J \cdot m^2$

Energies up to $ka = (2\pi^2)^{1/3}$ filled

Wanted: a) Effective mass m^* for electrons at $\mathcal{E}_F$

b) Number of conduction electrons per atom

Solution a) $\frac{1}{m^*} = \frac{1}{\hbar^2}\frac{\partial^2 \mathcal{E}}{\partial k^2} = \frac{1}{\hbar^2} \cdot 2A$

$$m^* = \frac{\hbar^2}{2A} = \frac{(1.05 \cdot 10^{-34}\ J\cdot s)^2}{2 \cdot 10^{-38}\ J \cdot m^2} \cdot \frac{m_e}{\underbrace{9.11 \cdot 10^{-31}\,kg}_{\text{el. mass}}}$$

$$= \underline{\underline{0.61 \cdot m_e}}$$

b) $k_F = (3\pi^2 n)^{1/3}$ where $n = \frac{N_{ions} \cdot Z}{V} = \frac{Z}{a^3}$

$$\Rightarrow k_F = \frac{(3\pi^2 Z)^{1/3}}{a}, \quad k_F a = (3\pi^2 Z)^{1/3}$$

but $k_F a = (2\pi^2)^{1/3}$ given

$$\Longrightarrow (3\pi^2 Z)^{1/3} = (2\pi^2)^{1/3}$$

$$Z = \frac{2\pi^2}{3\pi^2} = \underline{\underline{\frac{2}{3}}}$$

#7-4 a) Given: Tightbinding $\varepsilon(\bar{k}) = -\alpha - 2\gamma(\cos k_x a + \cos k_y a + \cos k_z a)$

a = lattice param.

Show that scalar effective mass m^* can be defined at Γ of the 1:st B.Z.

Calculate m^*.

Solution $\frac{1}{m^*} = \frac{1}{\hbar^2} \frac{\partial^2 \varepsilon}{\partial k^2}$ so is $\frac{\partial^2 \varepsilon}{\partial k^2}$ the same at Γ regardless of direction of $\bar{k}$?

Around Γ: $\cos k_x a \approx 1 - \frac{(k_x a)^2}{2}$ etc.
$(k=0)$

$$\Longrightarrow \varepsilon(\bar{k}) = -\alpha - 2\gamma\left[1 - \frac{\bar{k}^2 \cdot a^2}{2}\right] \rightarrow$$

$\varepsilon = \varepsilon(|\bar{k}|)$: m^* can be defined

Since $k_x^2 + k_y^2 + k_z^2 = k^2$

$$\Longrightarrow \frac{1}{m^*} = \frac{1}{\hbar^2} \cdot 2\gamma \cdot \frac{2 \cdot a^2}{2} = \frac{1}{\hbar^2} \cdot 2\gamma a^2$$

$$\boxed{m^* = \frac{\hbar^2}{2\gamma a^2}}$$ around Γ

b) Generally: $\left(\frac{1}{m^*}\right)_{\mu\nu} = \frac{1}{\hbar^2} \frac{\partial^2 \varepsilon(\bar{k})}{\partial k_\mu \partial k_\nu}$ $\mu, \nu \in (x, y, z)$

tensor

If scalar effective mass m^*: Tensor components?

Solution

$$\left.\begin{array}{l} \mu = \nu \} \left(\frac{1}{m^*}\right)_{xx} = \frac{1}{\hbar^2} \frac{\partial^2 \varepsilon}{\partial k_x^2} = \frac{1}{m^*} \\ \mu \neq \nu \} \left(\frac{1}{m^*}\right) = \frac{1}{\hbar^2} \frac{\partial^2 \varepsilon}{\partial k_x \partial k_y} = 0 \end{array}\right\} \left(\frac{1}{m^*}\right)_{\mu\nu} = \begin{pmatrix} 1/m^* & 0 & 0 \\ 0 & 1/m^* & 0 \\ 0 & 0 & 1/m^* \end{pmatrix}$$

#7-4 c) <u>Given:</u> Tightbinding, fcc, lattice param. a

$$\varepsilon(\bar{k}) = -\alpha - 8\gamma \cdot \cos\left(\frac{k_x a}{2}\right)\cos\left(\frac{k_y a}{2}\right)\cos\left(\frac{k_z a}{2}\right)$$

<u>Wanted:</u> Show if there is a scalar effective mass m^* at Γ of the B.Z. Calc. m^* in that case.

<u>Solution:</u> Calculate $\left(\frac{1}{m^*}\right)_{\mu\nu}$ and see if it is on the form

$$\begin{pmatrix} 1/m^* & 0 & 0 \\ 0 & 1/m^* & 0 \\ 0 & 0 & 1/m^* \end{pmatrix}$$

$$\left(\frac{1}{m^*}\right)_{xx} = \frac{1}{\hbar^2}\frac{\partial^2 \varepsilon}{\partial k_x^2} = \frac{1}{\hbar^2} 8\gamma \left(\frac{a}{2}\right)^2 \cdot \cos\left(\frac{k_x a}{2}\right)\cos\left(\frac{k_y a}{2}\right)\cos\left(\frac{k_z a}{2}\right)$$

$$\left(\frac{1}{m^*}\right)_{yy} = \left(\frac{1}{m^*}\right)_{zz} = \nearrow$$

$$\left(\frac{1}{m^*}\right)_{xy} = \frac{1}{\hbar^2}\frac{\partial^2 \varepsilon}{\partial k_x \partial k_y} = \frac{1}{\hbar^2}\frac{\partial}{\partial k_x}\left(8\gamma \cos\left(\frac{k_x a}{2}\right)\sin\left(\frac{k_y a}{2}\right)\cdot\frac{a}{2}\cos\left(\frac{k_z a}{2}\right)\right)$$

$$= -\frac{1}{\hbar^2}\cdot 8\gamma \cdot \left(\frac{a}{2}\right)^2 \sin\left(\frac{k_x a}{2}\right)\sin\left(\frac{k_y a}{2}\right)\cos\left(\frac{k_z a}{2}\right)$$

$$\bar{k} = 0 \text{ at } \Gamma \implies \left(\frac{1}{m^*}\right)_{xy} = 0$$

The same for xz, yz etc.

$$\implies \frac{1}{m^*}(\Gamma) = \frac{1}{\hbar^2} 8\gamma \cdot \left(\frac{a}{2}\right)^2 = \frac{1}{\hbar^2} 2\gamma a^2$$

$$\boxed{m^*(\Gamma) = \frac{\hbar^2}{2\gamma a^2}}$$

Yes, scalar effective mass at Γ.