Due to 25.11.2024. Please stick to the deadline so that I can post the solution on 26.11.24. To help you with the exam.

Problem

Consider a conductive material with a simple hexagonal crystal structure and primitive lattice vectors

$$\vec{a}_1 = a\hat{x}, \;\; \vec{a}_2 = \frac{a}{2}(\hat{x} + \sqrt{3}\hat{y}), \;\; \vec{a}_3 = a\hat{z}$$

Its conduction band fits well into a tight-binding model of electrons with a single isotropic atomic orbital per atom, and the extent of the overlap between orbitals is only relevant to first neighbors.

1. For this approximation, show that the shape of the conduction band at $\vec{k} \sim 0$ is given by

$$\epsilon(\vec{k}) = \varepsilon_0 + \gamma a^2 \left[\frac{3}{2}(k_x^2 + k_y^2) + k_z^2\right]$$

2. Obtain the inverse tensor of the effective mass.

3. To determine the value of γ, a cyclotron resonance experiment is performed, subjecting the solid to a uniform magnetic field $\vec{B} = B\hat{z}$ and an oscillating electric field $\vec{E}_e = E_e e^{i\omega t}\hat{x}$.

   (a) Write the semiclassical equations of motion in direct space. (Hint: The equation of motion in approx. semiclassical is Newton's law incorporating the effective mass.)

   (b) Supposing that these equations have the oscillating solutions in the plane perpendicular to the magnetic field of the form

   $$x = x_0 e^{i\omega t}, \;\; y = y_0 e^{i\omega t},$$

   determine x_0 and y_0 function of band parameters.

   (c) Determine the value of γ knowing that resonance is observed for a value of the frequency of the oscillating electric field, ω_r.

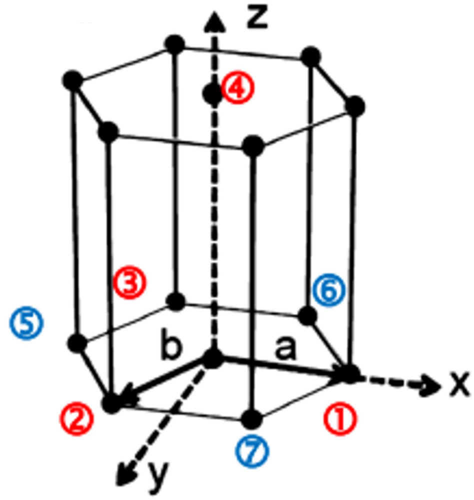


Figure 1: hexagonal crystal structure

Hint: In the tight-binding model, the band energy restricted to the nearest neighbors only, can be written as (Chapter 5, Omar):

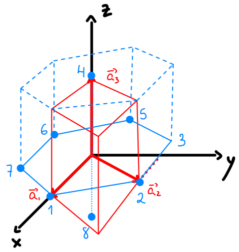
$$\epsilon(\vec{k}) = \varepsilon_0 - \alpha - \sum_n \gamma_n e^{-i\vec{k}\cdot\vec{\rho}}$$

In a hexagonal crystal structure (see Figure) there are 8 nearest neighbors in the positions:
$\vec{\rho}_1 = \vec{a}_1 = -\vec{\rho}_5$
$\vec{\rho}_2 = \vec{a}_2 = -\vec{\rho}_6$
$\vec{\rho}_3 = \vec{a}_2 - \vec{a}_1 = -\vec{\rho}_7$
$\vec{\rho}_4 = \vec{a}_3 = -\vec{\rho}_8$

1. $\vec{a}_1 = a\hat{x}$

$\vec{a}_2 = \frac{a}{2}(\hat{x} + \sqrt{3}\,\hat{y})$

$\vec{a}_3 = a\hat{z}$



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In the tight binding model with just a single isotropic atomic orbital per atom,

$$\varepsilon(\vec{k}) = \varepsilon_0' - \alpha - \sum_n \gamma_n e^{-i\vec{k}\vec{\rho}_n}$$

Every first neighbor is at the same distance, a, from the atom in the origin we consider when calculating the energy, so

$$\gamma_n \equiv \gamma \ , \ \forall n$$

Then, plugging the $\vec{\rho}_n$ on the expression for $\varepsilon(\vec{k})$, we get:

$$\varepsilon(\vec{k}) = \varepsilon_0 - \alpha - \gamma\Big[e^{-ik_xa} + e^{ik_xa} + e^{-i\frac{1}{2}(k_x+\sqrt{3}k_y)a} + e^{i\frac{1}{2}(k_x+\sqrt{3}k_y)a}$$
$$+ e^{-i\frac{1}{2}(-k_x+\sqrt{3}k_y)a} + e^{i\frac{1}{2}(-k_x+\sqrt{3}k_y)a} + e^{-ik_za} + e^{ik_za}\Big]$$
$$= \varepsilon_0' - \alpha - \gamma\Big[2\cos(k_xa) + 4\cos\left(\tfrac{1}{2}k_xa\right)\cos\left(\tfrac{\sqrt{3}}{2}k_ya\right) + 2\cos(k_za)\Big]$$

At $\vec{k} \sim 0$, $\cos(x) \sim 1 - \frac{x^2}{2}$:

$$\varepsilon(\vec{k}) \approx \varepsilon_0' - \alpha - \gamma\Big[2 - (k_xa)^2 + \left(2 - \left(\tfrac{1}{2}k_xa\right)^2\right)\left(2 - \left(\tfrac{\sqrt{3}}{2}k_ya\right)^2\right) + 2 - (k_za)^2\Big]$$

Dropping $k_x^2k_y^2$ $\approx \varepsilon_0' - \alpha - \gamma\left[8 - a^2\left(\frac{3}{2}k_x^2 + \frac{3}{2}k_y^2 + k_z^2\right)\right]$

Defining a new energy constant $\varepsilon_0 \equiv \varepsilon_0' - \alpha - 8\gamma$, we finally have:

$$\varepsilon(\vec{k}) = \varepsilon_0 + \gamma a^2\left[\frac{3}{2}(k_x^2 + k_y^2) + k_z^2\right]$$

2. The inverse tensor of the effective mass is defined as $\left[M^{-1}(\vec{k})\right]_{ij} = \frac{1}{\hbar^2}\frac{\partial^2 \varepsilon(\vec{k})}{\partial k_i \partial k_j}$

We compute the different elements:

$$M^{-1}_{xx} = \frac{1}{\hbar^2}\frac{\partial^2 \varepsilon}{\partial k_x^2} = \frac{3\gamma a^2}{\hbar^2} \qquad M^{-1}_{yy} = \frac{1}{\hbar^2}\frac{\partial^2 \varepsilon}{\partial k_y^2} = \frac{3\gamma a^2}{\hbar^2} \qquad M^{-1}_{zz} = \frac{1}{\hbar^2}\frac{\partial^2 \varepsilon}{\partial k_z^2} = \frac{2\gamma a^2}{\hbar^2}$$

$$M^{-1}_{xy} = M^{-1}_{yx} = M^{-1}_{xz} = M^{-1}_{zx} = M^{-1}_{yz} = M^{-1}_{zy} = 0$$

The tensor is then

$$M^{-1}(\vec{k}) = \gamma \frac{a^2}{\hbar^2}\begin{bmatrix} 3 & 0 & 0 \\ 0 & 3 & 0 \\ 0 & 0 & 2 \end{bmatrix}$$

3. $\vec{B} = B\hat{z}$, $\vec{E} = E e^{i\omega t}\hat{x}$

a) Semiclassical equation of motion.

$$m\frac{dv}{dt} = -e\vec{E} - e\vec{v}\times\vec{B} \longrightarrow \frac{d^2\vec{r}}{dt^2} = -eM^{-1}\left(\vec{E} + \frac{d\vec{r}}{dt}\times\vec{B}\right)$$

b) We have $\vec{r} = \begin{bmatrix} x_0 e^{i\omega t} \\ y_0 e^{i\omega t} \\ 0 \end{bmatrix}$

$$\underbrace{\begin{bmatrix} x_0 e^{i\omega t} \\ y_0 e^{i\omega t} \\ 0 \end{bmatrix} \times \begin{bmatrix} 0 \\ 0 \\ B \end{bmatrix} = \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ x_0 & y_0 & 0 \\ 0 & 0 & B \end{vmatrix} e^{i\omega t} = B\begin{bmatrix} y_0 e^{i\omega t} \\ -x_0 e^{i\omega t} \\ 0 \end{bmatrix}}$$

Using the equation on a),

$$-\omega^2\begin{bmatrix} x_0 e^{i\omega t} \\ y_0 e^{i\omega t} \\ 0 \end{bmatrix} = -e\gamma\frac{a^2}{\hbar^2}\begin{bmatrix} 3 & 0 & 0 \\ 0 & 3 & 0 \\ 0 & 0 & 2 \end{bmatrix}\left(\begin{bmatrix} E e^{i\omega t} \\ 0 \\ 0 \end{bmatrix} + i\omega B\begin{bmatrix} y_0 e^{i\omega t} \\ -x_0 e^{i\omega t} \\ 0 \end{bmatrix}\right)$$

$$\Rightarrow \begin{cases} \omega^2 x_0 = 3e\gamma\frac{a^2}{\hbar^2}(E + i\omega y_0) \\ \omega^2 y_0 = 3e\gamma\frac{a^2}{\hbar^2}(-i\omega B x_0) \end{cases} \xrightarrow[\frac{3e\gamma a^2}{\omega^2\hbar^2} \equiv C]{} \left.\begin{cases} x_0 = C(E + i\omega B y_0) \\ y_0 = -C i\omega B x_0 \end{cases}\right\} \Rightarrow x_0 = C(E + C\omega^2 B^2 x_0)$$

$$\Rightarrow x_0 = \frac{E}{1/C - C\omega^2 B^2}, \qquad y_0 = \frac{-i\omega B E}{1/C^2 - \omega^2 B^2}$$

$\frac{3e\gamma a^2}{\omega^2\hbar^2} \equiv C$

$$\hookrightarrow \Rightarrow x_0 = \frac{E}{\frac{\omega^2\hbar^2}{3e\gamma a^2} - \frac{3\gamma a^2}{\hbar^2}B^2}, \qquad y_0 = \frac{-iE}{\frac{\omega^3\hbar^4 B}{9e^2\gamma^2 a^4} - \omega B}$$

c) We have a resonance when the denominators above go to zero:

$$C^{-1} = \omega_r B \Rightarrow \frac{\omega_r \hbar^2}{3e\gamma a^2} = B \Rightarrow \gamma = \frac{\omega_r \hbar^2}{3ea^2 B}$$