Electronic Band Structure, Condensed Matter Physics 24/25

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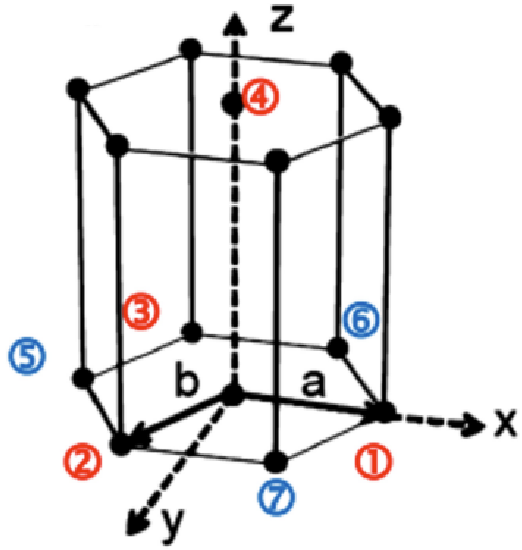
Problem

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

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

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.



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

$$\epsilon(\vec{k}) = \epsilon_0 - \alpha - \sum_n \gamma_n e^{-i\vec{k}\cdot\vec{\rho}_n}.$$

In a hexagonal crystal structure (see Figure), there are 8 nearest neighbors in the positions:

$$\vec{\rho}_1 = \vec{a}_1 = -\vec{\rho}_5, \quad \vec{\rho}_2 = \vec{a}_2 = -\vec{\rho}_6, \quad \vec{\rho}_3 = \vec{a}_2 - \vec{a}_1 = -\vec{\rho}_7, \quad \vec{\rho}_4 = \vec{a}_3 = -\vec{\rho}_8.$$

1. For this approximation, show that the shape of the conduction band at $\vec{k} \sim 0$ is given by: $\epsilon(\vec{k}) = \epsilon_0 + \gamma a^2 \left[\frac{3}{2}(k_x^2 + k_y^2) + k_z^2\right]$

Starting from the provided equation, for the band energy restricted to the nearest neighbors only, in the tight-binding model:

$$\epsilon(\vec{k}) = \epsilon_0 - \alpha - \sum_n \gamma_n e^{-i\vec{k}\cdot\vec{\rho}_n} = \epsilon_0 - \alpha - \gamma \underbrace{\sum_n e^{-i\vec{k}\cdot\vec{\rho}_n}}_{\equiv E} .$$

Where we extracted γ, since all neighbors are at the same distance $|\vec{a_1}| = |\vec{a_2}| = |\vec{a_3}| = a$.

Now we can plug all the given $\vec{\rho_i}$ into the term E, getting:

$$\begin{aligned} E &= e^{-ik_xa} + e^{ik_xa} + e^{-\frac{i}{2}(k_x+\sqrt{3}k_y)a} + e^{\frac{i}{2}(k_x+\sqrt{3}k_y)a} + e^{-\frac{i}{2}(-k_x+\sqrt{3}k_y)a} + e^{\frac{i}{2}(-k_x+\sqrt{3}k_y)a} + e^{-ik_za} + e^{ik_za} \\ &= \left(e^{ik_xa} + e^{-ik_xa}\right) + \left(e^{i\frac{a}{2}k_x} + e^{-i\frac{a}{2}k_x}\right)\left(e^{i\frac{a\sqrt{3}}{2}k_y} + e^{-i\frac{a\sqrt{3}}{2}k_y}\right) + \left(e^{ik_za} + e^{-ik_za}\right) = \\ &= 2\cos(k_xa) + 4\cos\left(\frac{1}{2}k_xa\right)\cos\left(\frac{\sqrt{3}}{2}k_ya\right) + 2\cos k_za \end{aligned}$$

which for $\vec{k} \sim 0$, since $\cos(x) \sim 1 - \frac{x^2}{2}$ for small x's, becomes:

$$\begin{aligned} E &= 2\left(1 - \frac{k_x^2a^2}{2}\right) + 4\left(1 - \frac{k_x^2a^2}{8}\right)\left(1 - \frac{3k_y^2a^2}{8}\right) + 2\left(1 - \frac{k_z^2a^2}{2}\right) = \\ &= 2 - k_x^2a^2 + 4\left(1 - \frac{k_x^2a^2}{8} - \frac{3k_y^2a^2}{8} + O[\vec{k}]^4\right) + 2 - k_z^2a^2 \approx \\ &\approx 8 - k_x^2a^2 - \frac{k_x^2a^2}{2} - \frac{3k_y^2a^2}{2} - k_z^2a^2 = 8 - \left(\frac{3}{2}k_x^2 + \frac{3}{2}k_y^2 + k_z^2\right)a^2 \end{aligned}$$

so finally coming back to the full expression, and defining $\epsilon_0' = \epsilon_0 - \alpha - \gamma 8$, we get:

$$\epsilon(\vec{k}) = \epsilon_0 - \alpha - \gamma 8 + \gamma\left(\frac{3}{2}k_x^2 + \frac{3}{2}k_y^2 + k_z^2\right)a^2 = \boxed{\epsilon_0' + \gamma a^2\left(\frac{3}{2}\left(k_x^2 + k_y^2\right) + k_z^2\right)}$$

2. Obtain the inverse tensor of the effective mass.

The inverse tensor of the effective mass, is the Hessian matrix in the reciprocal space of $\epsilon(\vec{k})$, so we just need to do the derivatives respect both variables, like:

$$[M^{-1}(\vec{k})]_{ij} = \frac{1}{h^2}\left[\nabla_k\left(\nabla_k \epsilon(\vec{k})\right)\right]_{ij} = \frac{1}{h^2}\frac{\partial^2\epsilon(\vec{k})}{\partial k_i \partial k_j}$$

which for $\vec{k} \sim 0$, we can see from the approximation above, that will be 0 for all non-diagonal elements, since there are only k_i^2 terms. And for the diagonals we got:

$$\begin{cases} [M^{-1}_{\vec{k}\sim 0}]_{xx} = \frac{1}{h^2}\frac{\partial^2\epsilon(\vec{k})}{\partial k_x \partial k_x} = \frac{3\gamma a^2}{h^2} \\ [M^{-1}_{\vec{k}\sim 0}]_{yy} = \frac{1}{h^2}\frac{\partial^2\epsilon(\vec{k})}{\partial k_y \partial k_y} = \frac{3\gamma a^2}{h^2} \\ [M^{-1}_{\vec{k}\sim 0}]_{zz} = \frac{1}{h^2}\frac{\partial^2\epsilon(\vec{k})}{\partial k_z \partial k_z} = \frac{2\gamma a^2}{h^2} \end{cases} \quad \rightarrow \quad \boxed{M^{-1}_{\vec{k}\sim 0} = \frac{\gamma a^2}{h^2}\begin{pmatrix} 3 & 0 & 0 \\ 0 & 3 & 0 \\ 0 & 0 & 2 \end{pmatrix}}$$

But if we wanted to compute it for all ranges of $\vec{k}$, we need to take each term of E and derive it. The first and last ones are trivial, since only depend on one component:

$$2\cos\left(k_{x/z}a\right) \xrightarrow{\partial k^2_{x/z}} -2a^2\cos\left(k_{x/z}a\right)$$

But the middle term $4\cos\left(\frac{1}{2}k_x a\right)\cos\left(\frac{\sqrt{3}}{2}k_y a\right)$, is trickier since it will contribute to four terms of the matrix:

- $\partial k_x^2 \to -4\frac{a^2}{4}\cos\left(\frac{1}{2}k_x a\right)\cos\left(\frac{\sqrt{3}}{2}k_y a\right) = -a^2\cos\left(\frac{1}{2}k_x a\right)\cos\left(\frac{\sqrt{3}}{2}k_y a\right)$
- $\partial k_y^2 \to -4\frac{3a^2}{4}\cos\left(\frac{1}{2}k_x a\right)\cos\left(\frac{\sqrt{3}}{2}k_y a\right) = -3a^2\cos\left(\frac{1}{2}k_x a\right)\cos\left(\frac{\sqrt{3}}{2}k_y a\right)$
- $\partial k_x \partial k_y = \partial k_y \partial k_x \to 4\frac{\sqrt{3}a^2}{4}\sin\left(\frac{1}{2}k_x a\right)\sin\left(\frac{\sqrt{3}}{2}k_y a\right) = \sqrt{3}a^2\sin\left(\frac{1}{2}k_x a\right)\sin\left(\frac{\sqrt{3}}{2}k_y a\right)$

resulting in the full Hessian matrix of E, being the collection of this 6 computations:

$$H_E = \begin{bmatrix} -2a^2\cos(k_x a) - a^2\cos\left(\frac{1}{2}k_x a\right)\cos\left(\frac{\sqrt{3}}{2}k_y a\right) & \sqrt{3}a^2\sin\left(\frac{1}{2}k_x a\right)\sin\left(\frac{\sqrt{3}}{2}k_y a\right) & 0 \\ \sqrt{3}a^2\sin\left(\frac{1}{2}k_x a\right)\sin\left(\frac{\sqrt{3}}{2}k_y a\right) & -3a^2\cos\left(\frac{1}{2}k_x a\right)\cos\left(\frac{\sqrt{3}}{2}k_y a\right) & 0 \\ 0 & 0 & -2a^2\cos(k_z a) \end{bmatrix}$$

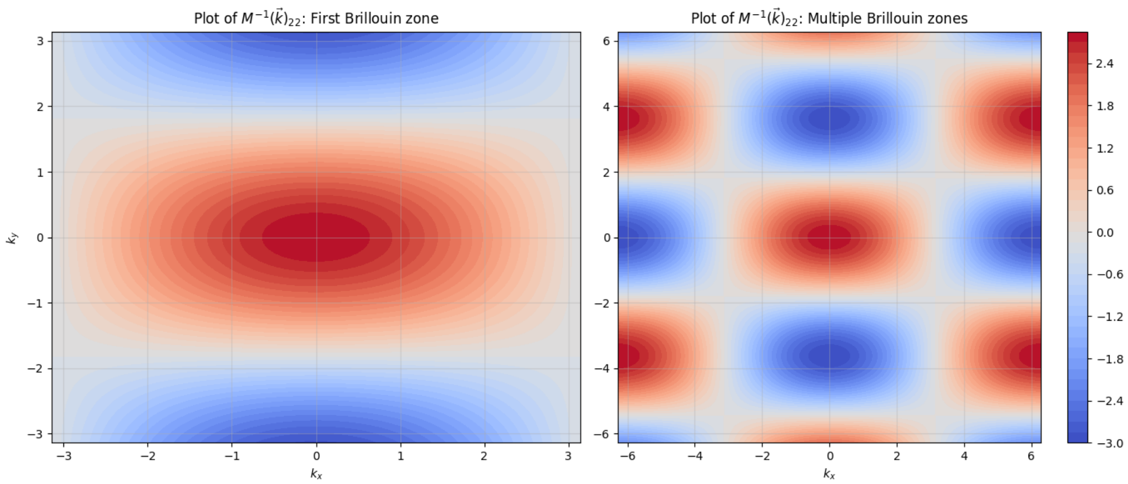
with finally:

$$\boxed{M^{-1}(\vec{k}) = \frac{\gamma a^2}{h^2}\begin{bmatrix} 2\cos(k_x a) + \cos\left(\frac{1}{2}k_x a\right)\cos\left(\frac{\sqrt{3}}{2}k_y a\right) & -\sqrt{3}\sin\left(\frac{1}{2}k_x a\right)\sin\left(\frac{\sqrt{3}}{2}k_y a\right) & 0 \\ -\sqrt{3}\sin\left(\frac{1}{2}k_x a\right)\sin\left(\frac{\sqrt{3}}{2}k_y a\right) & 3\cos\left(\frac{1}{2}k_x a\right)\cos\left(\frac{\sqrt{3}}{2}k_y a\right) & 0 \\ 0 & 0 & 2\cos(k_z a) \end{bmatrix}}$$

from where it's easy to see, changing the $cos(x) \sim 1$ and $sin(x) \sim 0$, that we retrieve the same matrix from above for $\vec{k} \sim 0$, but this time, we can also keep higher orders, getting:

$$M^{-1}(\vec{k})_{\vec{k}\sim 0} = \frac{\gamma a^2}{h^2}\begin{bmatrix} \boxed{3} - 2(k_x a)^2 + \frac{3(k_y a)^2}{8} & -\frac{3}{4}k_x k_y & 0 \\ -\frac{3}{4}k_x k_y & \boxed{3} - \frac{3(k_x a)^2}{8} - \frac{9(k_y a)^2}{8} & 0 \\ 0 & 0 & \boxed{2} - (k_z a)^2 \end{bmatrix}.$$

And finally, we can also plot a random coordinate, like $[M^{-1}(\vec{k})]_{yy}$ for example, which for $\gamma = a = h = 1$, should $\in [-3, 3]$:



where we see the same behaviour of the 1D case in the campus reference, having valleys and hills with divergences between them, but this time in 2D (doing a 1D slice, you retrieve the web plot). Also notice that we can explicitly see the periodicity of the reciprocal space!

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 the semiclassical approximation is Newton's law incorporating the effective mass.

Starting from Newton's law, we can pass the mass to the other side, getting:

$$m\ddot{\vec{r}} = -e\left(\vec{E} - +\dot{\vec{r}} \times \vec{B}\right) \rightarrow \boxed{\ddot{\vec{r}} = -eM^{-1}\left(\vec{E} + \dot{\vec{r}} \times \vec{B}\right)}$$

(b) Supposing that these equations have oscillating solutions in the plane perpendicular to the magnetic field of the form: $x = x_0 e^{i\omega t}, \quad y = y_0 e^{i\omega t}$, determine x_0 and y_0 as a function of band parameters.

Plugging our given solutions $\vec{r} = \left(x_0 e^{i\omega t}, \quad y_0 e^{i\omega t}, \quad 0\right)$, into the E.o.M., we have:

$$\underbrace{-\omega^2 \begin{pmatrix} x_0 e^{i\omega t} \\ y_0 e^{i\omega t} \\ 0 \end{pmatrix}}_{\ddot{\vec{r}}} = -e\underbrace{\gamma \frac{a^2}{h^2}\begin{pmatrix} 3 & 0 & 0 \\ 0 & 3 & 0 \\ 0 & 0 & 2 \end{pmatrix}}_{M^{-1}} \left(\underbrace{\begin{pmatrix} E_e e^{i\omega t} \\ 0 \\ 0 \end{pmatrix}}_{\vec{E}} + \underbrace{i\omega \begin{pmatrix} x_0 e^{i\omega t} \\ y_0 e^{i\omega t} \\ 0 \end{pmatrix}}_{\dot{\vec{r}}} \times \underbrace{\begin{pmatrix} 0 \\ 0 \\ B \end{pmatrix}}_{\vec{B}} \right)$$

resulting in:

$$\omega^2 \begin{pmatrix} x_0 \\ y_0 \\ 0 \end{pmatrix} = e\gamma \frac{3a^2}{h^2} \begin{pmatrix} E_e + i\omega y_0 B \\ -i\omega x_0 B \\ 0 \end{pmatrix} \rightarrow \begin{cases} \omega^2 x_0 = e\gamma \frac{3a^2}{h^2}(E_e + i\omega y_0 B) \\ \omega^2 y_0 = ie\gamma \frac{3a^2}{h^2}\omega x_0 B \end{cases}$$

from where it is trivial to solve the bottom equation for y_0, and substituting it in the first equation, and simplifying terms, results in:

$$\boxed{\begin{cases} x_0 = C\frac{E_e}{\omega^2 - C^2B^2} \\ y_0 = \frac{C^2}{i\omega}\frac{E_e}{\omega^2 - C^2B^2} \end{cases} \quad \text{with} \quad C = e\gamma\frac{3a^2}{h^2}}$$

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

And finally, the resonance will occur when the denominators go to zero:

$$\omega_r^2 = C^2B^2 = e^2\gamma^2 9\frac{a^4}{h^4}B^2 \rightarrow \boxed{\gamma = \frac{h^2}{3ea^2B}\omega_r}$$