PHYS 563 HW#8

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Problem [1]

(a)

① $\gamma > 0$, $-2\gamma < 0$

$\because \cos(t)$ has max / min at $t = 0 / \pi$

$\therefore \mathcal{E}(\vec{k}) = (-2\gamma)[\cos(k_x a) + \cos(k_y a)]$

has min / max at $(k_x, k_y) = (0,0) / (\pm\frac{\pi}{a}, \pm\frac{\pi}{a})$

$\Rightarrow$ Bottom : Γ-point $(0,0)$

Top : Four corners of 1st BZ $(\pm\frac{\pi}{a}, \pm\frac{\pi}{a})$

② $\gamma < 0$, $-2\gamma > 0$

The opposite of ①

$\Rightarrow$ Bottom : Four corners $(\pm\frac{\pi}{a}, \pm\frac{\pi}{a})$

Top : Γ-point $(0, 0)$

(b) $$(M^{-1})_{ij} = \frac{1}{\hbar^2}\frac{\partial^2 \mathcal{E}(\vec{k})}{\partial k_i \partial k_j} \quad (\text{A\&M } 12.29)$$

$$= \frac{-2\gamma}{\hbar^2}\begin{bmatrix} -a^2\cos(k_x a) & 0 \\ 0 & -a^2\cos(k_y a)\end{bmatrix}$$

$$= \frac{2\gamma a^2}{\hbar^2}\begin{bmatrix} \cos(k_x a) & 0 \\ 0 & \cos(k_y a)\end{bmatrix} \quad (1 = x,\ 2 = y)$$

$$\Rightarrow (M(\vec{k}))_{ij} = \frac{\hbar^2}{2\gamma a^2}\begin{bmatrix} \sec(k_x a) & 0 \\ 0 & \sec(k_y a)\end{bmatrix}$$

For $\gamma > 0$, Bottom is at $(0,0)$

① Top is at $(\frac{\pi}{a}, \frac{\pi}{a})$

At Bottom $(0,0)$

$$\left(M(\vec{k}=(0,0))\right)_{ij} = \frac{\hbar^2}{2\gamma a^2}\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

And all element are positive

② At Top $(\frac{\pi}{a}, \frac{\pi}{a})$

$$\left(M(\vec{k}=(\frac{\pi}{a}, \frac{\pi}{a}))\right)_{ij} = \frac{\hbar^2}{2\gamma a^2}\begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix}$$

all elements are negative.

$\Rightarrow$ The same conclusion can also be found for $\gamma < 0$ case that

$M > 0$ for bottom $(= (\frac{\pi}{a}, \frac{\pi}{a})$ for $\gamma < 0)$

&

$M < 0$ for top $(= (0,0)$ for $\gamma < 0)$

Problem [2]

$$\mathcal{E}(\vec{k}) = -2\gamma\left[\cos(k_x a) + \cos(k_y a) + \cos(k_z a)\right]$$

$$\left(M^{-1}(\vec{k})\right)_{ij} = \frac{1}{\hbar^2}\frac{\partial^2 \mathcal{E}(\vec{k})}{\partial k_i \partial k_j} \quad (1=x,\ 2=y,\ 3=z)$$

$$= \frac{-2\gamma}{\hbar^2}\begin{bmatrix} -a^2\cos(k_x a) & 0 & 0 \\ 0 & -a^2\cos(k_y a) & 0 \\ 0 & 0 & -a^2\cos(k_z a) \end{bmatrix}$$

$$= \frac{2\gamma a^2}{\hbar^2}\begin{bmatrix} \cos(k_x a) & 0 & 0 \\ 0 & \cos(k_y a) & 0 \\ 0 & 0 & \cos(k_z a) \end{bmatrix}$$

$$\Rightarrow \left(M(\vec{k})\right)_{ij} = \frac{\hbar^2}{2\gamma a^2}\begin{bmatrix} \sec(k_x a) & 0 & 0 \\ 0 & \sec(k_y a) & 0 \\ 0 & 0 & \sec(k_z a) \end{bmatrix}$$

(1)

For $\vec{k} = (0, 0, 0)$,

$$\left(M(\vec{k})\right)_{ij} = \frac{\hbar^2}{2\gamma a^2}\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

②

And for $\vec{k} = \left(\frac{\pi}{a}, \frac{\pi}{a}, \frac{\pi}{a}\right)$

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