HW # 5 Solutions

3. (A) FOR $P \ll 1$ AND $k = 0$,

EQ. 21b BECOMES

$$\frac{P}{Ka} \sin Ka + \cos Ka = 1$$

NOW YOU MIGHT SAY, WE TAKE $P = 0$ WHICH $\Rightarrow$ $Ka = 0$. THIS DOES NOT GIVE A "GAP." THE GAP IS SMALL ($\sim P$) SO WE HAVE TO BE MORE CAREFUL

TAKE Ka SMALL (IT WILL BE $\sim P$) AND EXPAND $\frac{\sin Ka}{Ka}$ AND $\cos Ka$ TO ORDER $(Ka)^2$

$$\cos Ka \approx 1 - \frac{1}{2}(Ka)^2$$

$$\frac{\sin Ka}{Ka} \approx 1 - \frac{1}{6}(Ka)^2$$

(ACTUALLY, $K \sim P^x$ i.e. SOME POWER OF P, IN THIS CASE $x = \frac{1}{2}$, BUT WE CAN STILL DROP SECOND TERM IN $\frac{\sin x}{x}$)

SINCE $Ka \sim P$, WE CAN DROP $\frac{1}{6}(Ka)^2$ TERM IN $\frac{\sin Ka}{Ka}$

SINCE THAT WILL BE 3RD ORDER IN P, WE ARE LEFT WITH

$$P + 1 - \frac{1}{2}(Ka)^2 = 1$$

OR

$$\boxed{K \approx \sqrt{2P}/a}$$

SINCE $P = \frac{mAa^2}{2\hbar^2}$ (AFTER EQ. 43 IN TEXT)

$$\Rightarrow \boxed{K \approx \sqrt{\frac{mA}{\hbar^2}}}$$

THE ENERGY IS

$$\boxed{\mathcal{E} = \frac{\hbar^2 K^2}{2m} = \frac{\hbar^2 P}{ma^2} = \frac{A}{2}}$$

(THE GAP IS RELATED TO $U_G/2$)

$\sin(\alpha+\beta) = \sin\alpha\cos\beta + \sin\beta\cos\alpha$

$\cos(\alpha+\beta) = \cos\alpha\cos\beta + \sin\alpha\sin\beta$

(B) @ $k = \pi/a$

$\Rightarrow$

$$P\,\frac{\sin Ka}{Ka} + \cos Ka = -1$$

EXPAND $Ka \approx (\pi + \delta)$

$$\sin(\pi+\delta) = -\sin\delta \approx -\delta$$

$$\cos(\pi+\delta) = -\cos\delta \approx -1 + \frac{\delta^2}{2}$$

($Ka \approx \pi$ IN DENOMINATOR)

SO $$\frac{P}{\pi}(-\delta) + \frac{\delta^2}{2} = 0$$

$\Rightarrow$ $\delta_1 = 0$ OR

$\delta_2 = 2P/\pi$

(THESE ARE THE TWO BANDS)

THE GAP IS THE ENERGY DIFFERENCE

$$E_1 = \frac{\hbar^2 K_1^2}{2m} \qquad K_1 = \frac{\pi + \overset{0}{\delta_1}}{a}$$

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

$$E_2 = \frac{\hbar^2 K_2^2}{2m} = \frac{\hbar^2}{2ma^2}(\pi + \delta_2)^2$$

$$\approx \frac{\hbar^2}{2ma^2}\left(\pi^2 + 2\pi\delta_2\right)$$

SO THE GAP IS

$$\boxed{E_{GAP} = E_2 - E_1 = \frac{\hbar^2}{ma^2}\pi\delta_2 = \frac{2\hbar^2}{ma^2}P = 2A = 2U_G}$$

6. THE FOURIER TRANSFORM OF S.E.:

$$(\lambda_k - \epsilon) C_k + \sum_G U_G C_{k-G} = 0$$

WITH $\lambda_k = \frac{\hbar^2 k^2}{2m}$

HERE $U(x,y) = -4U \cos\frac{2\pi x}{a} \cos\frac{2\pi y}{a}$

FOR 2-D SQUARE LATTICE

$$\underbrace{\vec{a}_1 = a\hat{x}, \quad \vec{a}_2 = a\hat{y},}_{D.L.} \quad \underbrace{\vec{b}_1 = \frac{2\pi}{a}\hat{x}, \quad \vec{b}_2 = \frac{2\pi}{a}\hat{y}}_{R.L.}$$

SO RL VECTORS ARE

$$\vec{G} = n_1 \frac{2\pi}{a}\hat{x} + n_2 \frac{2\pi}{a}\hat{y} \qquad n_1, n_2 \in \mathbb{Z}$$

NOW FOR THE POTENTIAL,

USE $\cos\alpha \cos\beta = \frac{1}{2}\left(\cos(\alpha+\beta) + \cos(\alpha-\beta)\right)$

SO $U(x,y) = -2U\left\{\cos\left(\frac{2\pi x}{a} + \frac{2\pi y}{a}\right) + \cos\left(\frac{2\pi x}{a} - \frac{2\pi y}{a}\right)\right\}$

WHEN WE FOURIER TRANSFORM THE POTENTIAL, WE HAVE

$$U_{\vec{G}} = \begin{cases} -U & \text{FOR } \vec{G} = \pm\left(\frac{2\pi}{a}\hat{x} + \frac{2\pi}{a}\hat{y}\right) \\ & \text{OR } \vec{G} = \pm\left(\frac{2\pi}{a}\hat{x} - \frac{2\pi}{a}\hat{y}\right) \\ 0 & \text{ALL OTHER } \vec{G} \end{cases}$$

FOR THE BAND STRUCTURE AT $\vec{k} = \frac{\pi}{a}\hat{x} + \frac{\pi}{a}\hat{y}$

POSSIBLE POINTS THAT CAN COUPLE TO $C_{\vec{k}}$ ARE AT

① $\vec{k}_1 = \vec{k} + \left(\frac{2\pi}{a}\hat{x} + \frac{2\pi}{a}\hat{y}\right) = \frac{3\pi}{a}(\hat{x} + \hat{y})$

② $\vec{k}_2 = \vec{k} - \left(-\frac{2\pi}{a}\hat{x} - \frac{2\pi}{a}\hat{y}\right) = -\frac{\pi}{a}(\hat{x} + \hat{y})$

③ $\vec{k}_3 = \vec{k} + \left(\frac{2\pi}{a}\hat{x} - \frac{2\pi}{a}\hat{y}\right) = \frac{3\pi}{a}\hat{x} - \frac{\pi}{a}\hat{y}$

④ $\vec{k}_4 = \vec{k} - \left(\frac{2\pi}{a}\hat{x} - \frac{2\pi}{a}\hat{y}\right) = -\frac{\pi}{a}\hat{x} + \frac{3\pi}{a}\hat{y}$

THE ENERGY @ $\vec{k}_2$ IS THE SAME AS THE ENERGY @ $\vec{k}$ SO WE ONLY CONSIDER THAT COUPLING.

LET $\lambda = \lambda_{\vec{k}} = \lambda_{\vec{k}_2} = \frac{\hbar^2}{2m}(k^2)$

THE FOURIER TRANSFORMED S.E BECOMES

$$(\lambda-\varepsilon)C_{\frac{\pi}{a},\frac{\pi}{a}} - U C_{-\frac{\pi}{a},-\frac{\pi}{a}} = 0$$

$$-U C_{\frac{\pi}{a},\frac{\pi}{a}} + (\lambda-\varepsilon)C_{-\frac{\pi}{a},-\frac{\pi}{a}} = 0$$

$$\Rightarrow \begin{vmatrix} \lambda-\varepsilon & -U \\ -U & \lambda-\varepsilon \end{vmatrix} = 0$$

OR $(\lambda-\varepsilon)^2 - U^2 = 0$

$$(\lambda-\varepsilon) = \pm U$$

OR $\boxed{\varepsilon = \lambda \pm U}$

AND $\boxed{\varepsilon_{GAP} = 2U}$