Condensed Matter physics (phy 771)
HW #5 - Solution
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① problem 7.2 Marder:

$$[T_R, T_{R'}]\,\psi(\vec r) = (T_R T_{R'} - T_{R'} T_R)\,\psi(\vec r)$$
$$= T_R\,\psi(\vec r+\vec R') - T_{R'}\,\psi(\vec r+\vec R)$$
$$= \psi(\vec r+\vec R+\vec R') - \psi(\vec r+\vec R'+\vec R) = 0$$

so $T_R, T_{R'}$ commute with each other

and
$$[T_R, H(\vec r)]\,\psi(\vec r) = T_R\, H(\vec r)\psi(\vec r) - H(\vec r)\, T_R\,\psi(\vec r)$$
$$= H(\vec r+\vec R)\,\psi(\vec r+\vec R) - H(\vec r)\,\psi(\vec r+\vec R)$$
$$= H(\vec r)\,\psi(\vec r+\vec R) - H(\vec r)\,\psi(\vec r+\vec R) = 0$$

H is invariant under translational symmetry
$H(\vec r+\vec R) = H(\vec r)$ $\Rightarrow$ so T_R, H commute

- another way of proving $[T_R, H] = 0$ is

$$[T_R, H] = [e^{i\vec k\cdot\vec R}, H] = [e^{\frac{i\vec P\cdot\vec R}{\hbar}}, \frac{P^2}{2m} + U(\vec r)]$$

Now $[e^{\frac{i\vec P\cdot\vec R}{\hbar}}, \frac{P^2}{2m}] = 0$ as $[x, f(x)] = 0$, and

$$[T_R, U(\vec r)]\,\psi(\vec r) = T_R\big(U(\vec r)\psi(\vec r)\big) - U(\vec r)\, T_R\,\psi(\vec r)$$
$$= U(\vec r+\vec R)\,\psi(\vec r+\vec R) - U(\vec r)\,\psi(\vec r+\vec R)$$

$U(\vec r+\vec R) = U(\vec R)$

$$= U(\vec r)\,\psi(\vec r+\vec R) - U(\vec r)\,\psi(\vec r+\vec R) = 0$$
$$\Rightarrow [T_R, H] = 0$$

② for real potential $U(\vec{r})$, show that $U_K^* = U_{-K}$

$$U_K = \frac{1}{\Omega}\int_\Omega d^3\vec{r}\, U(\vec{r})\, e^{-i\vec{K}\cdot\vec{r}}$$, and

$$U_K^* = \frac{1}{\Omega}\int_\Omega d^3\vec{r}\, U^*(\vec{r})\, e^{i\vec{K}\cdot\vec{r}}$$, but $U(\vec{r})$ is real $\Rightarrow$ $U^* = U$

$$= \frac{1}{\Omega}\int d^3\vec{r}\, U(\vec{r})\, e^{-i(-\vec{K}\cdot\vec{r})} = U_{-K}$$

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③ let $\vec{K} = K_x\hat{i} + K_y\hat{j} + K_z\hat{k}$, $\vec{r} = x\hat{i} + y\hat{j} + z\hat{k}$

$$\int_\Omega d^3\vec{r}\, e^{i\vec{K}\cdot\vec{r}} = \frac{\int_V d^3\vec{r}\, e^{i\vec{K}\cdot\vec{r}}}{N}$$; where $V = N\Omega$

Ω: volume of unit cell

V: volume of crystal

N: # of unit cells

$$= \frac{1}{N}\int_V d^3\vec{r}\, e^{i\vec{K}\cdot\vec{r}}$$

$$= \frac{1}{N}\int_V dx\,dy\,dz\, e^{iK_x x}\, e^{iK_y y}\, e^{iK_z z}$$

$$= \frac{1}{N}\int_0^{L_x} dx\, e^{iK_x x}\int_0^{L_y} dy\, e^{iK_y y}\int_0^{L_z} dz\, e^{iK_z z}$$

$$= \frac{1}{N}\left(L_x \delta_{K_x,0}\right)\left(L_y \delta_{K_y,0}\right)\left(L_z \delta_{K_z,0}\right)$$

$$= \frac{L_x L_y L_z}{N}\delta_{\vec{K},0} = \frac{V}{N}\delta_{\vec{K},0} = \Omega\,\delta_{\vec{K},0}$$

$=$ zero, as $\vec{K}$ is nonvanishing vector ($\vec{K} \neq 0$)

(4)

$$U(x) = 2V_0 \cos^2\left(\frac{\pi}{a}x\right) \; ; \quad \text{using } \cos^2 x = \frac{1+\cos 2x}{2}$$

$$= \underbrace{V_0}_{\text{constant term}} + \underbrace{V_0 \cos\left(\frac{2\pi}{a}x\right)}_{\text{Periodic term}} = V_0\left(1+\cos\left(\frac{2\pi}{a}x\right)\right)$$

Note: the constant term V_0 uniformly shift all energies and it does not contribute to gap formation and does not affect the eigenstates

a) $$U_K(x) = \frac{1}{a}\int_0^a dx\, U(x)\, e^{-iKx}$$

$$K=0 \Rightarrow U_0 = \frac{1}{a}\int_0^a V_0\left(1+\cos\frac{2\pi}{a}x\right)dx$$

$$= \frac{V_0}{a}\left[\int_0^a 1\,dx + \underbrace{\int_0^a \cos\frac{2\pi}{a}x\,dx}_{\text{Zero! integration over full Period } \frac{2\pi}{2\pi/a}=a}\right]$$

$$= \frac{V_0}{a}\cdot a = V_0$$

$$K = \frac{2\pi}{a}$$

$$U_{\frac{2\pi}{a}} = \frac{1}{a}\int_0^a dx\, V_0\left(1+\cos\frac{2\pi}{a}x\right)e^{-i\frac{2\pi}{a}x} \; ;$$

$$= \frac{V_0}{a}\left[\underbrace{\int_0^a dx\, e^{-i\frac{2\pi}{a}x}}_{\text{Zero! int over full Period (a)}} + \int_0^a dx\, \cos\left(\frac{2\pi}{a}x\right)e^{-i\frac{2\pi}{a}x}\right] \quad \text{using } \cos x = \frac{e^{ix}+e^{-ix}}{2}$$

$$= \frac{V_0}{a}\int_0^a dx\left[\frac{e^{i\frac{2\pi}{a}x}+e^{-i\frac{2\pi}{a}x}}{2}\right]e^{-i\frac{2\pi}{a}x} = \frac{V_0}{2a}\int_0^a dx\left(1+e^{-i\frac{4\pi}{a}x}\right)$$

$$= \frac{V_0}{2a}\left[a - \frac{a}{i4\pi}\left(\underbrace{e^{-i4\pi}}_{1}-1\right)\right] = \frac{V_0}{2a}\left[a-0\right] = \frac{V_0}{2} \equiv U_{-\frac{2\pi}{a}}$$

$$U_{\frac{4\pi}{a}} = \frac{1}{a}\int_0^a dx\, V_0 \left(1+\cos\frac{2\pi}{a}x\right) e^{-i\frac{4\pi}{a}x}$$

$$= \frac{V_0}{a}\left[\underbrace{\int_0^a e^{-i\frac{4\pi}{a}x}dx}_{\mathrm{I}} + \underbrace{\int_0^a dx\, e^{-i\frac{4\pi}{a}x}\cos\frac{2\pi}{a}x}_{\mathrm{II}}\right]$$

$$\mathrm{I} = \int_0^a e^{-i\frac{4\pi}{a}x}dx = \frac{-a\, e^{-i\frac{4\pi}{a}x}}{i4\pi}\Big|_0^a = \frac{-a}{4\pi i}\left[\underbrace{e^{-i4\pi}}_{1} - 1\right]$$

$$= \frac{-a}{4\pi i}\left[1-1\right] = \text{zero}$$

$$\mathrm{II} = \int_0^a dx\, e^{-i\frac{4\pi}{a}x}\cos\left(\frac{2\pi}{a}\right)x = \int_0^a dx\, e^{-i\frac{4\pi}{a}x}\left[\frac{e^{i\frac{2\pi}{a}x} + e^{-i\frac{2\pi}{a}x}}{2}\right]$$

$$= \frac{1}{2}\underbrace{\int_0^a dx\, e^{-i\frac{4\pi}{a}x} e^{i\frac{2\pi}{a}x}}_{\text{zero due to orthogonality of plane waves}} + \frac{1}{2}\int_0^a dx\, e^{-i\frac{4\pi}{a}x} e^{-i\frac{2\pi}{a}x}$$

$$\int_0^a e^{ikx}e^{-ik'x}dx = a\,\delta_{k,k'}$$

$$= \frac{1}{2}\int_0^a dx\, e^{-i\frac{6\pi}{a}x} = \text{zero}$$

$\Rightarrow U_{\frac{4\pi}{a}} = U_{-\frac{4\pi}{a}} = 0$; similarly for all other higher Fourier components, all of them vanish

$$\therefore\ U_k(x) = \begin{cases} V_0 & ;\ k=0 \\ \frac{V_0}{2} & ;\ k = \pm\frac{2\pi}{a} \\ 0 & ;\ \text{otherwise} \end{cases}$$

Note that, we can find the non-vanishing Fourier components using

$$U(\vec{r}) = \sum_{K} U_K e^{i\vec{K}\cdot\vec{r}} \Rightarrow U(x) = \sum_{K} U_K e^{iKx} \quad ; \quad K = \frac{2\pi}{a} n$$

$n = 0, \pm 1, \pm 2, \cdots$

$$\Rightarrow U(x) = \sum_{n} U_{\frac{2\pi}{a}n} e^{i\frac{2\pi}{a}nx}$$

$$= U_0 + U_{\frac{2\pi}{a}} e^{i\frac{2\pi}{a}x} + U_{-\frac{2\pi}{a}} e^{-i\frac{2\pi}{a}x} +$$

$$U_{\frac{4\pi}{a}} e^{i\frac{4\pi}{a}x} + U_{-\frac{4\pi}{a}} e^{-i\frac{4\pi}{a}x} + U_{\frac{6\pi}{a}} e^{i\frac{6\pi}{a}x} + U_{-\frac{6\pi}{a}} e^{-i\frac{6\pi}{a}x}$$

$$+ \cdots \quad \text{--(1)}$$

and using

$$U(x) = V_0 + V_0 \cos \frac{2\pi}{a} x$$

$$= V_0 + V_0 \frac{e^{i\frac{2\pi}{a}x} + e^{-i\frac{2\pi}{a}x}}{2}$$

$$= V_0 + \frac{V_0}{2} e^{i\frac{2\pi}{a}x} + \frac{V_0}{2} e^{-i\frac{2\pi}{a}x} \quad \text{--- (2)}$$

compare eqns (1) and (2) to find

$U_0 = V_0$, $U_{+\frac{2\pi}{a}} = \frac{V_0}{2}$, $U_{-\frac{2\pi}{a}} = \frac{V_0}{2}$ and the rest components vanish, i.e

$$U_{\pm\frac{4\pi}{a}} = U_{\pm\frac{6\pi}{a}} = \cdots = 0$$

b) E_g can be found by mixing $K_1 = 0$ $(n_1 = 0)$ with $K_2 = -\frac{2\pi}{a}$ $(n_2 = -1)$

from eq^n 7.4 in our lecture notes, we have

$$\begin{bmatrix} \frac{\hbar^2}{2m}\left(k + \frac{2\pi}{a} n_1\right)^2 + U_0 - \mathcal{E} & U_{K_2 - K_1} \\ U^*_{K_2 - K_1} & \frac{\hbar^2}{2m}\left(k + \frac{2\pi}{a} n_2\right)^2 + U_0 - \mathcal{E} \end{bmatrix} \begin{bmatrix} \psi(k - K_1) \\ \psi(k - K_2) \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

using $k = \pi/a$; $U_0 = V_0$; $n_1 = 0$, $n_2 = -1$,

and $U_{K_2 - K_1} = U_{-\frac{2\pi}{a}} = U_{\frac{2\pi}{a}} = \frac{V_0}{2}$, we have

$$\begin{bmatrix} \frac{\hbar^2 \pi^2}{2ma^2} + V_0 - \mathcal{E} & \frac{V_0}{2} \\ \frac{V_0}{2} & \frac{\hbar^2 \pi^2}{2ma^2} + V_0 - \mathcal{E} \end{bmatrix} \begin{bmatrix} \psi(\pi/a) \\ \psi(-\pi/a) \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \quad \cdots (1)$$

$\Rightarrow$ has non-trivial solution if

$$\begin{vmatrix} \frac{\hbar^2 \pi^2}{2ma^2} + V_0 - \mathcal{E} & \frac{V_0}{2} \\ \frac{V_0}{2} & \frac{\hbar^2 \pi^2}{2ma^2} + V_0 - \mathcal{E} \end{vmatrix} = 0$$

$$\Rightarrow \left(\frac{\hbar^2 \pi^2}{2ma^2} + V_0 - \mathcal{E}\right)^2 - \frac{V_0^2}{4} = 0 \quad \Rightarrow \frac{\hbar^2 \pi^2}{2ma^2} + V_0 - \mathcal{E} = \pm \frac{V_0}{2}$$

$$\Rightarrow \mathcal{E} = \frac{\hbar^2 \pi^2}{2ma^2} + V_0 \pm \frac{V_0}{2} \quad \Rightarrow \mathcal{E}_+ = \frac{\hbar^2 \pi^2}{2ma^2} + \frac{3}{2} V_0$$

$$\mathcal{E}_- = \frac{\hbar^2 \pi^2}{2ma^2} + \frac{1}{2} V_0$$

$$\Rightarrow E_g = \Delta\mathcal{E} = \mathcal{E}_+ - \mathcal{E}_- = \frac{3}{2} V_0 - \frac{1}{2} V_0$$

$$= V_0 \equiv E_g(-\pi/a)$$

to find E_g at k-value outside 1^{st} B.Z, fold it into the 1^{st} B.Z by addition/subtraction of suitable reciprocal lattice vector

at $k = \frac{5\pi}{a}$ folds into $\frac{5\pi}{a} - \frac{4\pi}{a} = \pi/a$

$$\Rightarrow E_g\left(\frac{5\pi}{a}\right) = E_g(\pi/a) = V_0$$

similarly $k = -\frac{5\pi}{a}$ folds into $-\frac{5\pi}{a} + \frac{4\pi}{a} = -\pi/a$

$$\Rightarrow E_g\left(-\frac{5\pi}{a}\right) = E_g(-\pi/a) = V_0$$

c) $$\psi(x) = \frac{1}{L}\sum_{K} \psi(k-K)\, e^{i(k-K)x} = \frac{1}{L}\sum_{\substack{n=0\\n=-1}} \psi\left(k+\frac{2\pi}{a}n\right) e^{i\left(k+\frac{2\pi}{a}n\right)x}$$

at $k = \pi/a$

$$\psi(x) = \frac{1}{L}\left[\psi(\pi/a)\, e^{i\frac{\pi}{a}x} + \psi(-\pi/a)\, e^{-i\frac{\pi}{a}x}\right]$$

need to Determine $\psi(\pi/a)$ and $\psi(-\pi/a)$ for both $\mathcal{E}_+$ and $\mathcal{E}_-$

for $\mathcal{E}_+$ and using eqn(1), we have

$$\begin{bmatrix} \frac{\hbar^2\pi^2}{2ma^2} + V_0 - \mathcal{E}_+ & \frac{V_0}{2} \\ \frac{V_0}{2} & \frac{\hbar^2\pi^2}{2ma^2} + V_0 - \mathcal{E}_+ \end{bmatrix} \begin{bmatrix} \psi(\pi/a) \\ \psi(-\pi/a) \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

$$\begin{bmatrix} -\frac{V_0}{2} & \frac{V_0}{2} \\ \frac{V_0}{2} & -\frac{V_0}{2} \end{bmatrix} \begin{bmatrix} \psi(\pi/a) \\ \psi(-\pi/a) \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

$$\Rightarrow -\frac{V_0}{2}\psi(\pi/a) + \frac{V_0}{2}\psi(-\pi/a) = 0 \quad \Rightarrow \psi(-\pi/a) = \psi(\pi/a)$$

$\psi(\pi/a)$ is arbitrary, set it to 1

$\Rightarrow \psi(\pi/a) = 1$ and hence $\psi(-\pi/a) = 1$

$$\Rightarrow \psi^+(x) = \frac{1}{L}\left[e^{i\frac{\pi}{a}x} + e^{-i\frac{\pi}{a}x}\right] = \frac{2}{L}\cos\frac{\pi}{a}x$$

Normalize $\psi^+(x) = \frac{2A}{L}\cos\frac{\pi}{a}x$; A constant of normalization

$$\int_0^L |\psi^+|^2 dx = 1 \quad \Rightarrow \frac{4A^2}{L^2}\underbrace{\int_0^L \cos^2\frac{\pi}{a}x\, dx}_{L/2} = 1 \Rightarrow A = \sqrt{\frac{L}{2}}$$

$$\Rightarrow \psi^+(x) = \frac{2}{L}\sqrt{\frac{L}{2}}\cos\frac{\pi}{a}x$$

$$= \sqrt{\frac{2}{L}}\cos\frac{\pi}{a}x$$; this is a standing wave that gets reflected at $k = \pm\pi/a$

similarly for $\mathcal{E}_-$, we have

$$\begin{bmatrix} \frac{\hbar^2\pi^2}{2ma^2} + V_0 - \mathcal{E}_- & \frac{V_0}{2} \\ \frac{V_0}{2} & \frac{\hbar^2\pi^2}{2ma^2} + V_0 - \mathcal{E}_- \end{bmatrix} \begin{bmatrix} \psi(\pi/a) \\ \psi(-\pi/a) \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

$$\begin{bmatrix} \frac{V_0}{2} & \frac{V_0}{2} \\ \frac{V_0}{2} & \frac{V_0}{2} \end{bmatrix} \begin{bmatrix} \psi(\pi/a) \\ \psi(-\pi/a) \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

$$\Rightarrow \frac{V_0}{2}\psi(\pi/a) + \frac{V_0}{2}\psi(-\pi/a) = 0 \quad \Rightarrow \psi(-\pi/a) = -\psi(\pi/a)$$

$\psi(\pi/a)$ is arbitrary, set it to 1 $\Rightarrow \psi(\pi/a) = +1$

$\Rightarrow \psi(-\pi/a) = -1$

$$\Rightarrow \psi^-(x) = \frac{1}{L}\left\{e^{i\frac{\pi}{a}x} - e^{-i\frac{\pi}{a}x}\right\} = \frac{2i}{L}\sin\frac{\pi}{a}x$$

Normalize $\psi^-(x) = \frac{2iA}{L}\sin\frac{\pi}{a}x \Rightarrow A = \sqrt{\frac{L}{2}} \Rightarrow \psi^-(x) = \sqrt{\frac{2}{L}}\, i\sin\frac{\pi}{a}x$

again standing wave

⑤

$U(x) = 2V_0 \cos \frac{2\pi}{a}x$; the general solution of the band structure in the 1^{st} B.Z $[-\pi/a, \pi/a]$ is given by

$$E(k) = \frac{\hbar^2}{2m}\left[(k-\pi/a)^2 + \frac{\pi^2}{a^2}\right] \pm \sqrt{\left[\frac{\pi\hbar^2}{ma}(k-\pi/a)\right]^2 + V_0^2} \quad \text{---} (1)$$

critical points occurs when $\frac{dE}{dk} = 0$. To prove that $k = \pi/a$ is a critical point,

we need to expand first $E(k)$ near $k = \pi/a$ and then find the 1^{st} derivative

let $q = k - \pi/a \Rightarrow E(q) = \frac{\hbar^2}{2m}\left(q^2 + \frac{\pi^2}{a^2}\right) \pm \sqrt{\left(\frac{\hbar^2\pi q}{ma}\right)^2 + V_0^2}$ ...(2)

$$E(q) = \frac{\hbar^2}{2m}\left(q^2 + \frac{\pi^2}{a^2}\right) \pm V_0\left[1 + \left(\frac{\hbar^2\pi q}{maV_0}\right)^2\right]^{1/2}$$; now when

$q \ll 1$ (i.e $k \approx \pi/a$), expand the squre root as

$$E(q) = \frac{\hbar^2 q^2}{2m} + \frac{\hbar^2\pi^2}{2ma^2} \pm V_0\left[1 + \frac{1}{2}\frac{\hbar^4\pi^2 q^2}{m^2a^2V_0^2}\right]$$; $(1+x)^{1/2} \approx 1 + \frac{1}{2}x$ when $x \ll 1$

$$= \underbrace{\frac{\hbar^2\pi^2}{2ma^2} \pm V_0}_{E_{edge}} + \frac{\hbar^2 q^2}{2m} \pm \frac{\hbar^4\pi^2 q^2}{2m^2a^2V_0} \quad \text{---} (3)$$

$$E(q) = E_{edge} + \frac{\hbar^2 q^2}{2m} \pm \frac{\hbar^4\pi^2 q^2}{2m^2a^2V_0} \quad \text{---} (4)$$

$$\frac{dE}{dk} = \frac{dE}{dq}\frac{dq}{dk} = \frac{dE}{dq} \Rightarrow$$

$$\frac{dE}{dq} = \frac{\hbar^2}{m}q \pm \frac{\hbar^4\pi^2 q}{m^2a^2V_0}, \Rightarrow \left.\frac{dE}{dq}\right|_{q=0} = 0 \text{ i.e } \left.\frac{dE}{dk}\right|_{k=\pi/a} = 0$$

so at $k=\pi/a$, $E(k)$ is extreme, exhibiting Van Hove singularities.

Now from eq^n(4), it can be written as

$$E = E_{edge} + \frac{\hbar^2 q^2}{2}\left(\frac{1}{m} \pm \frac{\hbar^2\pi^2}{m^2a^2V_0}\right) = E_{edge} + \frac{\hbar^2 q^2}{2m_\pm}, \text{ where}$$

$$m_\pm = \left(\frac{1}{m} \pm \frac{\hbar^2\pi^2}{m^2a^2V_0}\right)^{-1};$$ are effective masses in the upper and lower bands, respectively.

$$\therefore E = E_{edge} + \frac{\hbar^2 q^2}{2m_\pm}, \text{ solve for } q = \pm\sqrt{\frac{2m_\pm}{\hbar^2}(E - E_{edge})}$$

$$D(E) = \frac{1}{\pi}\frac{1}{\left|\frac{dE}{dk}\right|} = \frac{1}{\pi}\left|\frac{dk}{dE}\right| = \frac{1}{\pi}\left|\frac{dq}{dE}\right| \quad \cdots (5)$$

; $m_\pm$ are both positive

$$\frac{dq}{dE} = \pm\frac{1}{2}\left(\frac{2m_\pm}{\hbar^2}(E-E_{edge})\right)^{-1/2}\cdot\frac{2m_\pm}{\hbar^2}$$

$$= \pm\frac{1}{2}\left(\frac{2m_\pm}{\hbar^2}\right)^{1/2}\frac{1}{\sqrt{E-E_{edge}}}$$

$$\Rightarrow \left|\frac{dq}{dE}\right| = \frac{1}{2}\left(\frac{2m_\pm}{\hbar^2}\right)^{1/2}\frac{1}{\sqrt{|E-E_{edge}|}};$$ absolute value has been added to make sure that $E - E_{edge} > 0$ must be positive

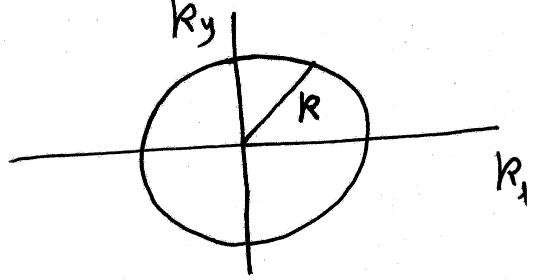
$$\Rightarrow D(E) = \frac{1}{2\pi}\left(\frac{2m_\pm}{\hbar^2}\right)^{1/2}\frac{1}{\sqrt{|E-E_{edge}|}}$$

$$\sim \frac{1}{\sqrt{|E-E_{edge}|}};$$ we see that at $E = E_{edge} = \frac{\hbar^2\pi^2}{2ma^2} \pm V_0$, $D(E)$ diverges

⑥

$E(k_x, k_y) = \frac{\hbar^2}{2m}(k_x^2 + k_y^2) = C$; this a circular contour with radius $k = \sqrt{2mC}/\hbar$ and literally called a surface.

ⓐ The tangent vector $\vec{A}$ is in the direction of $\hat{\theta}$ when using polar coordinates, so let $k_x = k\cos\theta$ and $k_y = k\sin\theta$



$$\vec{A} = \frac{d\vec{k}}{d\theta} = \left(\frac{dk_x}{d\theta}, \frac{dk_y}{d\theta}\right) = (-k\sin\theta, k\cos\theta) = (-k_y, k_x)$$

ⓑ $\vec{\nabla}_k E = \left(\frac{\partial}{\partial k_x}\hat{i} + \frac{\partial}{\partial k_y}\hat{j}\right)E = \frac{\hbar^2}{m}(k_x, k_y)$

ⓒ $\vec{\nabla}_k E$ is normal to the surface if $(\vec{\nabla}_k E)\cdot\vec{A} = \text{zero}$

$$\Rightarrow \frac{\hbar^2}{m}(k_x, k_y)\cdot(-k_y, k_x) = \frac{\hbar^2}{2m}\left[-k_x k_y + k_x k_y\right] = \text{zero}$$

ⓓ the critical points occur when $\vec{\nabla}_k E = 0$

$\Rightarrow \frac{\hbar^2}{m}(k_x, k_y) = 0$ when $(k_x, k_y) = (0,0) \Rightarrow$ one critical point

to determine the type of this critical point, we find the Hessian matrix H at $(0,0)$

$$H = \begin{bmatrix} \frac{\partial^2 E}{\partial k_x^2} & \frac{\partial^2 E}{\partial k_x \partial k_y} \\ \frac{\partial^2 E}{\partial k_y \partial k_x} & \frac{\partial^2 E}{\partial k_y^2} \end{bmatrix}$$

; $\frac{\partial^2 E}{\partial k_x^2} = \frac{\partial^2 E}{\partial k_y^2} = \frac{\hbar^2}{m}$, and

$$\frac{\partial^2 E}{\partial k_x \partial k_y} = \frac{\partial}{\partial k_x}\left(\frac{\partial E}{\partial k_y}\right) = \frac{\partial}{\partial k_x}\left(\frac{\hbar^2}{m}k_y\right) = 0 \equiv \frac{\partial^2 E}{\partial k_y \partial k_x}$$

$$\Rightarrow H = \begin{bmatrix} \frac{\hbar^2}{m} & 0 \\ 0 & \frac{\hbar^2}{m} \end{bmatrix}$$, we see that H is diagonal with positive eigenvalues $\left(\frac{\hbar^2}{m}\right) \Rightarrow$ Eenergy is minimum at $(0,0)$ i.e E_{min}, so at $E=0$, the DOS starts at $D(E)=0$ and becomes constant for $E>0$, so No Van Hove singularities. Van Hove singularities in 2D usually occur at saddle points, (2D square lattice for example with $E(k_x,k_y)=\frac{\hbar^2}{2m}(k_x^2-k_y^2)$, resulting in logarithmic divergence in $D(E)$.

Note added
if all eigenvalues of the H matrix are negative, then the critical point would be E_{max}, and if eigenvalues are mixed (indifinite: contains both positive and negative), then the critical point is saddle point

⑦

$$E(k_x,k_y) = E_0 - \frac{\hbar^2}{2m}(k_x^2 - k_y^2),$$

critical points occur where $\vec{\nabla}_{\vec{k}} E = 0$

$$\vec{\nabla}_{\vec{k}} E = -\frac{\hbar^2}{2m}(2k_x, -2k_y).$$ This is equal zero at $(0,0)$

so the critical point is $(k_x, k_y) = (0,0)$.

$$H = \begin{bmatrix} \frac{\partial^2 E}{\partial k_x^2} & \frac{\partial^2 E}{\partial k_x \partial k_y} \\ \frac{\partial^2 E}{\partial k_y \partial k_x} & \frac{\partial^2 E}{\partial k_y^2} \end{bmatrix} = \begin{bmatrix} -\frac{\hbar^2}{2m} & 0 \\ 0 & \frac{\hbar^2}{2m} \end{bmatrix} = \frac{\hbar^2}{2m}\begin{bmatrix} -1 & 0 \\ 0 & +1 \end{bmatrix}$$

since the eigenvalues of H have opposite signs, the critical point is saddle point and the energy at the saddle point reads $E = E_0$

Now $$D(E) = \int \frac{d\vec{k}^2}{(2\pi)^2}\,\delta(E - E(k)) = \frac{1}{(2\pi)^2}\int dk_x dk_y\, \delta\left(E - E_0 + \frac{\hbar^2}{2m}(k_x^2 - k_y^2)\right)$$

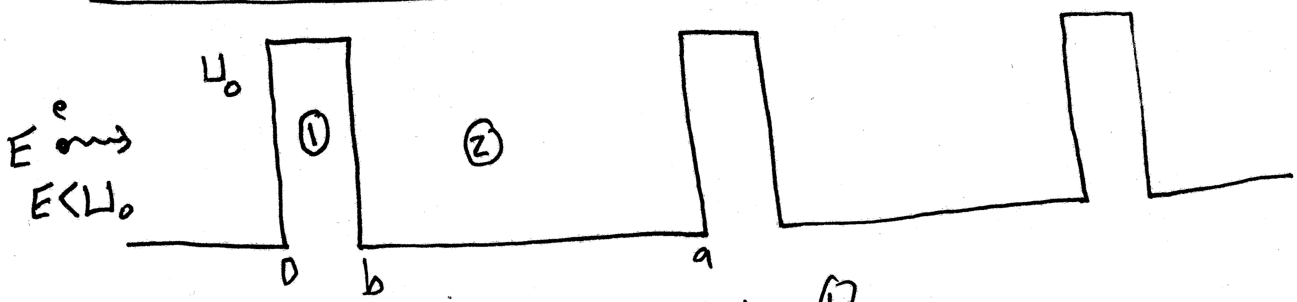
change variables let $x = k_x\sqrt{\frac{\hbar^2}{2m}}$ and $y = k_y\sqrt{\frac{\hbar^2}{2m}}$ $\Rightarrow$

$$D(E) = \frac{2m}{(2\pi)^2\hbar^2}\int \delta(E - E_0 + (x^2 - y^2))\,dx\,dy,$$ calculating this integral is not an easy task, the result reads

$$\approx -\ln|E - E_0|$$ in the proximity of $E = E_0$

we see that at $E = E_0$ diverges ∞

⑧ problem 7.5 Marder: (1D Kronig-Penney model)



$$U(x) = \begin{cases} U_0, & 0<x<b \rightarrow \text{region ①} \\ 0, & b<x<a \rightarrow \text{region ②} \end{cases}$$

in region ① shrodinger eqn reads

$$-\frac{\hbar^2}{2m}\psi_1''(x) + U_0\psi_1(x) = E\psi_1(x) \Rightarrow \psi_1'' - \frac{2m}{\hbar^2}(U_0 - E)\psi_1 = 0$$

$$\Rightarrow \text{let } \beta^2 = \frac{2m}{\hbar^2}(U_0 - E) \Rightarrow \psi_1'' - \beta^2\psi_1 = 0 \Rightarrow \psi_1(x) = Ae^{\beta x} + Be^{-\beta x}$$

in region ② $-\frac{\hbar^2}{2m}\psi_2''(x) = E\psi_2(x) \Rightarrow \psi_1'' + \frac{2m}{\hbar^2}E\psi_1 = 0$

$$\Rightarrow \psi_1'' + \alpha^2\psi_1 = 0, \text{ where } \alpha^2 = \frac{2m}{\hbar^2}E \Rightarrow \psi_2(x) = Ce^{i\alpha x} + De^{-i\alpha x}$$

Boundary conditions:

① at $x=b$ $\psi_1(b) = \psi_2(b) \Rightarrow Ae^{\beta b} + Be^{-\beta b} = Ce^{i\alpha b} + De^{-i\alpha b}$

$$\Rightarrow Ae^{\beta b} + Be^{-\beta b} - Ce^{i\alpha b} - De^{-i\alpha b} = 0 \quad \text{---- ①}$$

② at $x=b$ $\psi_1'(b) = \psi_2'(b)$

$$A\beta e^{\beta b} - B\beta e^{-\beta b} = i\alpha Ce^{i\alpha b} - i\alpha De^{-i\alpha b}$$

$$\Rightarrow A\beta e^{\beta b} - B\beta e^{-\beta b} - i\alpha Ce^{i\alpha b} + i\alpha De^{-i\alpha b} = 0 \quad \text{---- ②}$$

③ from Bloch theorem $\psi_2(a) = e^{ika}\psi_1(0)$; k: wave number

$$Ce^{i\alpha a} + De^{-i\alpha a} = e^{ika}(A+B)$$

$$\Rightarrow Ae^{ika} + Be^{ika} - Ce^{i\alpha a} - De^{-i\alpha a} = 0 \quad \text{---- ③}$$

(4) from Bloch theorem at $x=a$, $\psi_2'(a) = e^{ika}\psi_1'(0)$

$$i\alpha C e^{i\alpha a} - i\alpha D e^{-i\alpha a} = e^{ika}(A\beta - B\beta)$$

$$\Rightarrow A\beta e^{ika} - B\beta e^{ika} - i\alpha C e^{i\alpha a} + i\alpha D e^{-i\alpha a} = 0 \quad \cdots (4)$$

equations (1) ... (4) can be written in matrix form as

$$\begin{bmatrix} e^{\beta b} & e^{-\beta b} & -e^{i\alpha b} & -e^{-i\alpha b} \\ \beta e^{\beta b} & -\beta e^{-\beta b} & -i\alpha e^{i\alpha b} & i\alpha e^{-i\alpha b} \\ e^{ika} & e^{ika} & -e^{i\alpha a} & -e^{-i\alpha a} \\ \beta e^{ika} & -\beta e^{ika} & -i\alpha e^{i\alpha a} & i\alpha e^{-i\alpha a} \end{bmatrix} \begin{bmatrix} A \\ B \\ C \\ D \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} \quad \cdots (5)$$

the above four eqns have a non-trivial solution when the determinent of the coefficients A, B, C, D vanishs, After Lengthy math, we arrive at the dispersion relation

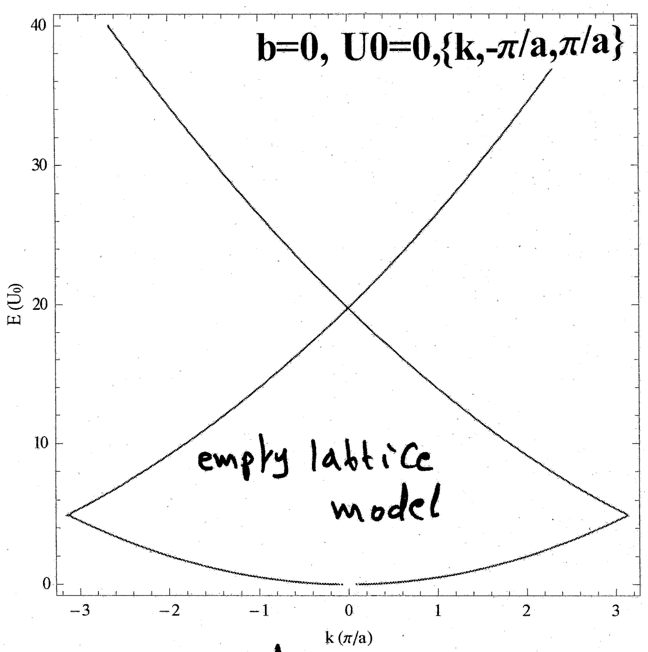
$$\cos ka = \overbrace{\cosh(\beta b)\cos(\alpha(a-b))}^{\text{term 1}} + \overbrace{\frac{\beta^2 - \alpha^2}{2\alpha\beta}\sinh(\beta b)\sin(\alpha(a-b))}^{\text{term 2}} \quad \cdots (6)$$

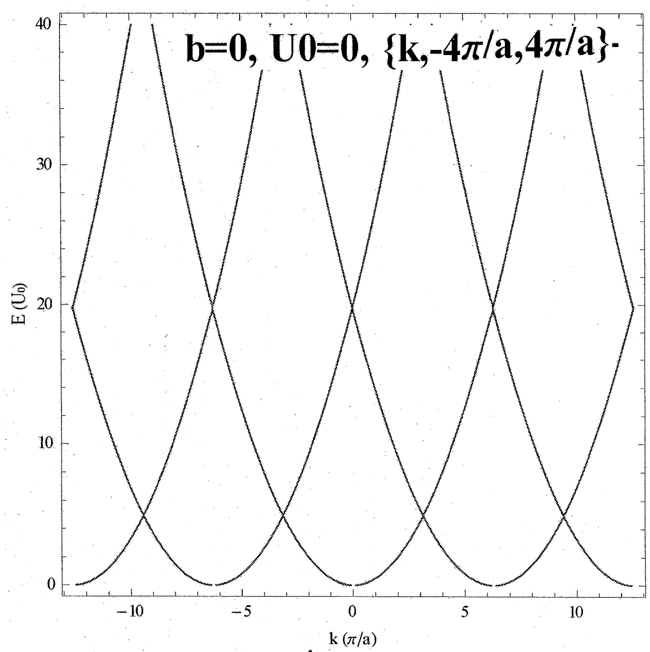
now α and β depend on E and I need to solve for $E(k)$. it is very hard to obtaine an expression for $E(k)$ algebrically, instead, we can solve the equation numerrcally.

define $f(E,k) = \cos ka - (\text{term 1} + \text{term 2})$, so we run over k from $[-\pi/a, \pi/a]$ and at each value of k, we find the root E that makes $f(E,k) = 0$ satisfied.

To make calculations easy, set $\hbar = 1$, $m = 1$, $a = 1$, and then play with b and V_0 (change width and height of Barrier) and see the effect.

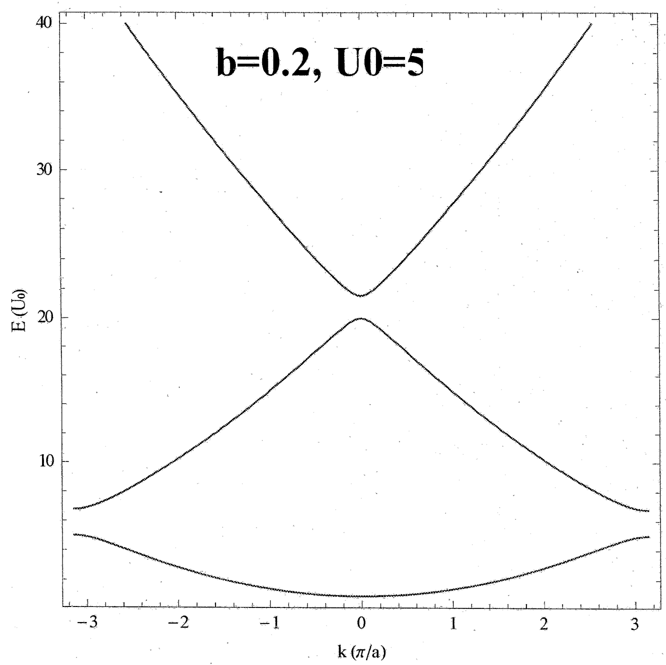
```
In[1812]:= (*Clear all previous definitions*)ClearAll["Global`*"];
  (*Parameters*)ħ = 1; m = 1; a = 1; b = 0.0; U0 = 0.0;
  (*Change width b and hieght of barrier U0 and see the effect*)

  (*Dispersion relation for E<U0*)
  dispersion[E_, k_] := Module[{β = Sqrt[2 m * (U0 - E)] / ħ, α = Sqrt[2 m * E] / ħ, term1, term2},
    term1 = Cosh[β * b] * Cos[α * (a - b)];
    term2 = ((β^2 - α^2) / (2 β * α)) * Sinh[β * b] * Sin[α * (a - b)];
    Cos[k * a] - (term1 + term2)]

  (*Plot band structure*)
  ContourPlot[dispersion[E, k] == 0, {k, -π / a, π / a}, {E, 0, 25}, FrameLabel → {"k (π/a)", "E (U□)"},
   PlotRange → All, PlotPoints → 50, MaxRecursion → 3] (*you can change to extended zone by changing the
   interval such as from {k,-2π/a,2π/a}*)
```

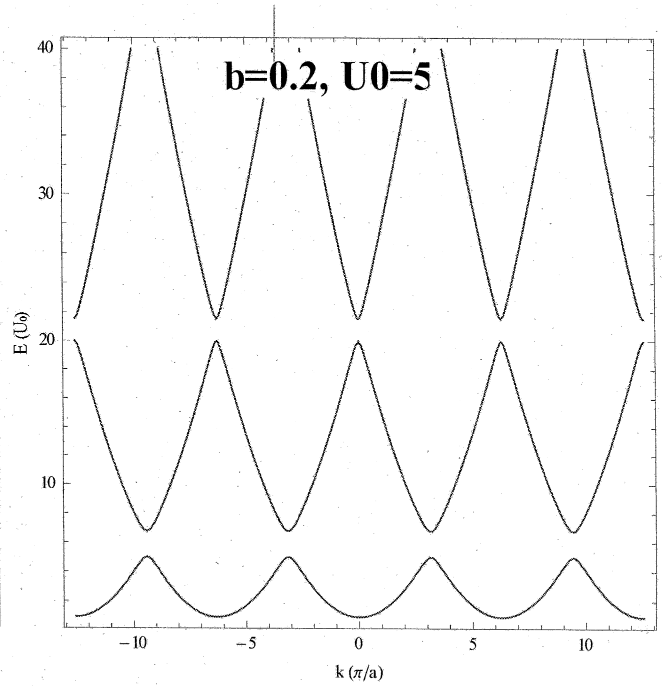




reduced zone

Extended zone





Now from eq^n (6)

$$\cos ka = \cosh(\beta b)\cos(\alpha(a-b)) + \frac{\beta^2-\alpha^2}{2\alpha\beta}\sinh(\beta b)\sin(\alpha(a-b)),$$ and

in the limit $b \to 0$ and $U_0 \to \infty$, we have

$\cosh(\beta b) \approx 1$, $\sinh \beta b \approx \beta b$, $\cos(\alpha(a-b)) = \cos\alpha a$, $\sin(\alpha(a-b)) = \sin\alpha a$

then eq^n (6) reduces to

$$\cos ka = \cos\alpha a + \frac{\beta^2 b}{2\alpha}\sin\alpha a$$, where I used $\beta^2-\alpha^2 \approx \beta^2$ as $\beta^2 \gg \alpha^2$ since $U_0 \to \infty$

$$\cos ka = \cos\alpha a + \frac{\beta^2 b}{2\alpha}\frac{a}{a}\sin\alpha a$$

$$\cos ka = \cos\alpha a + \frac{\beta^2 b a}{2}\frac{\sin\alpha a}{\alpha a}$$; let $W_0 = \frac{\beta^2 b a}{2}$ $\Rightarrow$

$$\boxed{\cos ka = \cos\alpha a + \frac{W_0}{\alpha a}\sin\alpha a}$$

```
(*the following code is for the limit when b goes to 0 and U0 goes to infinity*)
(*Clear all previous definitions*)ClearAll["Global`*"];
(*Parameters*)ħ = 1; m = 1; a = 1; W0 = 0.5; (*Change width b and hieght of barrier U0 and see the effect*)

(*Dispersion relation for E<U0*)
dispersion[E_, k_] := Module[{α = Sqrt[2 m * E] / ħ, term1, term2}, term1 = Cos[α * a];
  term2 = ((W0) / (α * a)) * Sin[α * a];
  Cos[k * a] - (term1 + term2)]

(*Plot band structure*)
ContourPlot[dispersion[E, k] == 0, {k, -π / a, π / a}, {E, 0, 30}, FrameLabel → {"k ", "E "}, PlotRange → All,
 PlotPoints → 50, MaxRecursion → 3]
 (*you can change to extended zone by changing the interval such as from {k,-2π/a,2π/a}*)
```