# Periodic Potential in 1D :

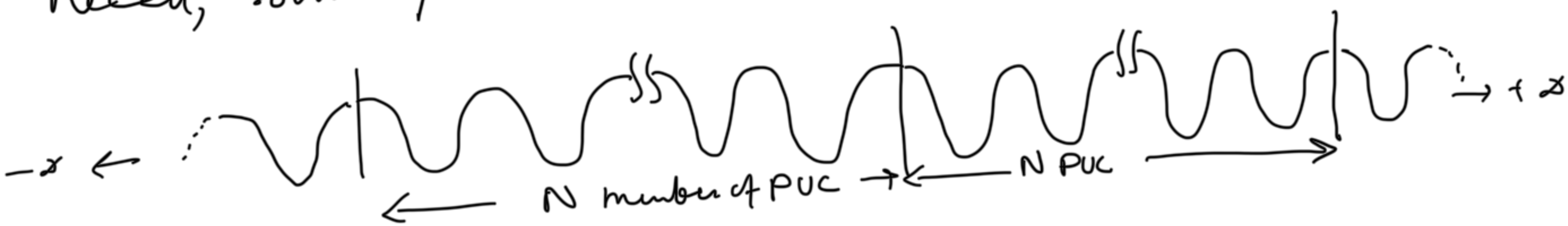
$$V(x) = V(x + Na) \; ; \; N = \pm 1, \pm 2, \pm 3, \ldots$$


1 smallest periodic unit → primitive unit cell. (PUC)

Unit cell : Multiple of PUC : a valid periodic unit.

In this simple 1D case we will refer PUC "loosely" as unit cell.

Recall, Sommerfeld model : Born - von Karman PBC

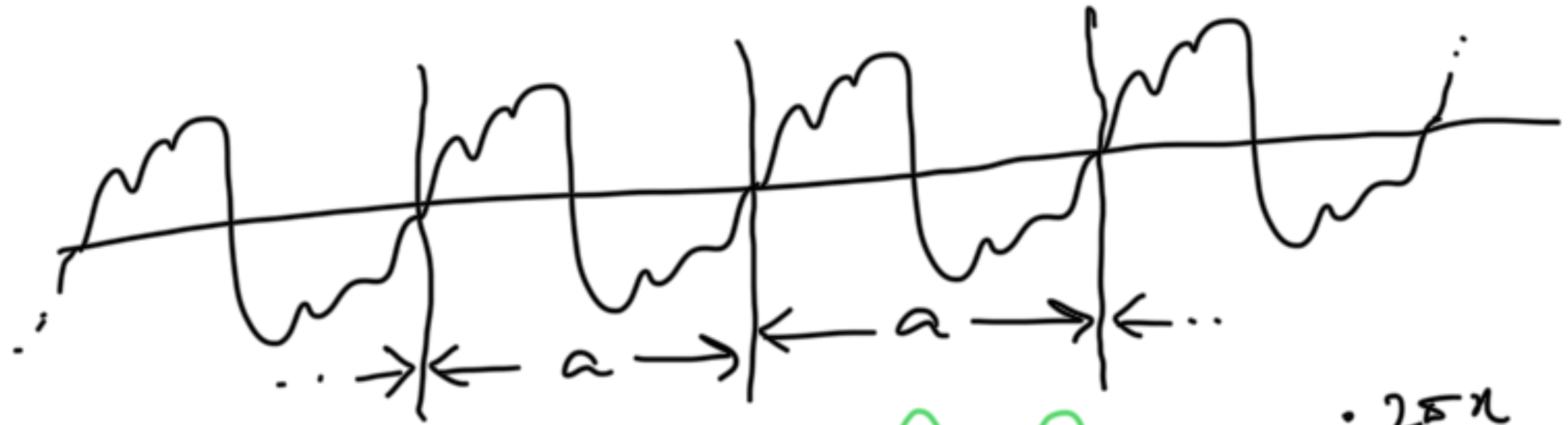


Recall, $f(x') = f(x'+a)$ and $\left.\dfrac{d^n}{dx^n} f(x)\right|_{x=x'} = \left.\dfrac{d^n}{dx^n} f(x)\right|_{x=x'+a}$

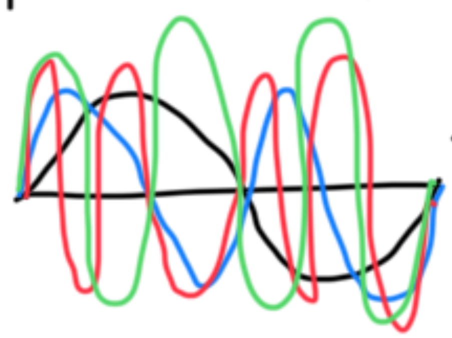
$x'$ is a value of $x$

$$\Rightarrow f(x) = \sum_n c_n e^{i n \frac{2\pi}{a} x}$$

Ex



$\Rightarrow$



$$= c_1 e^{i \frac{2\pi x}{a}} + c_2 e^{i 2\times\frac{2\pi}{a} x} + c_3 e^{i 3\times\frac{2\pi}{a} x} + c_4 e^{i 4\times\frac{2\pi}{a} x} + \cdots$$

BvK PBC $\quad \psi(x) = \psi(x + Na)$

$$\Rightarrow \psi(x) = \sum_n C_n e^{i n \frac{2\pi}{Na} x} = \sum_q C_q e^{i q x}, \quad q \in \{q_n\}, \boxed{q_n = n\frac{2\pi}{Na}}$$

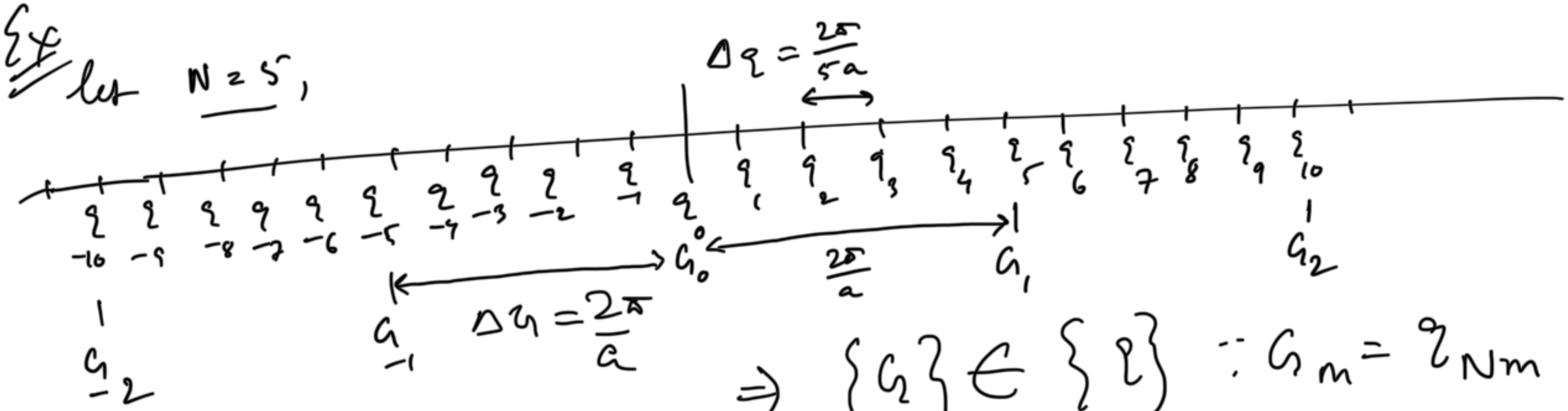
$n = 0, \pm 1, \pm 2, \cdots \pm \infty$

Periodic potential! $\quad V(x) = V(x+a)$

$$\Rightarrow V(x) = \sum_m V_m e^{i m \frac{2\pi}{a} x} = \sum_G V_G e^{i G x}$$

where $G \in \{G_m\}$, $\boxed{G_m = m\frac{2\pi}{a}}$, $m = 0, \pm 1, \pm 2, \cdots, \pm \infty$

Ex let $N = 5$,




$$\Rightarrow \{G\} \in \{q\} \quad \because G_m = q_{Nm}$$

$$\therefore \hat{H}\Psi = E\Psi$$

$$\Rightarrow -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\sum_q C_q e^{iqx} + \sum_G V_G e^{iGx}\sum_q C_q e^{iqx} = E\sum_q C_q e^{iqx}$$

$$\Rightarrow \sum_q C_q\left(\frac{\hbar^2 q^2}{2m}\right)e^{iqx} + \sum_G\sum_q V_G C_q e^{i(G+q)x} = E\sum_q C_q e^{iqx}$$

$$K_q = \frac{\hbar^2 q^2}{2m}$$

$$\Rightarrow \sum_q C_q\left\{K_q - E\right\}e^{iqx} + \sum_G V_G \sum_q C_q e^{i(\underbrace{G+q}_{q'})x} = 0$$

$$\Rightarrow \sum_q C_q\left\{K_q - E\right\}e^{iqx} + \sum_G V_G \sum_{q'-G} C_{q'-G}\, e^{iq'x} = 0,$$

$$-\infty \longleftarrow G_0' \longrightarrow +\infty$$

$$-\infty \longleftarrow G \neq 0 \longrightarrow +\infty$$

Note: $\sum_{q'-G}^{\infty} \equiv \sum_{q'}^{\infty}$ since $\{q\} \in \{q'\}$

Not equivalent if range of $q$ is finite.

$$\Rightarrow \sum_q C_q \{K_q - E\} e^{iqx} + \sum_G V_G \sum_{q'} C_{q'-G} e^{iq'x} = 0 ;$$

$$\Rightarrow \sum_q e^{iqx} \left[ \{K_q - E\} C_q + \sum_G V_G C_{q-G} \right] = 0$$

within BvK PBC (periodicity of $Na$) $\int_0^{Na} e^{-iqx} e^{iq'x} dx = Na\,\delta_{qq'}$

$$\therefore \int_0^{Na} e^{-iq'x} \sum_n e^{iqx} \left[ \{K_q - E\} C_q + \sum_G V_G C_{q-G} \right] = 0$$

$$\Rightarrow \left[ \{K_{q'} - E\} C_{q'} + \sum_G V_G C_{q'-G} \right] = 0 \quad \text{— for each } q'$$

$\underline{\underline{\text{Note}}}$ that this equation $\underline{\text{does NOT}}$ involve all $C_q$ coefficients. Recall, $q' \in \{q_n\}$; $q_n = n\frac{2\pi}{Na}$, $n = 0, \pm 1, \pm 2, \cdots, \pm\infty$

The equation involves $\underline{\text{only}}$ $\{C_{q+G}\}$ where $G \in \{G_m\}$, $G_m = m\frac{2\pi}{a}$; $m = 0, \pm 1, \pm 2, \cdots, \pm\infty$

Other equations involving the same set of coeffs:

$$\left\{ K_{q'+G'} - E \right\} C_{q'+G'} + \sum_{G} V_G \, C_{q'+G'-G} = 0$$

$$G' \in \{G_m\}$$

We can therefore regroup the equations as:

$\underline{N=5}$

$q_1 + G$

$\vdots$

$\left\{ K_{q_{-10}} - E \right\} C_{q_{-10}} + \sum_{G} V_G \, C_{q_{-10}-G} = 0$

$-9$

$-8$

$-7$

$-6$

$-5$

$-4$

$-3$

$-2$

$-1$

$0$

$1$

$2$

$3$

$\rightarrow$

$-10$, $-5$, $0$, $5$, $10$ — $q_0 + G$ — Set of simultaneous eqns. for coefficients $\{C_{q_0+G}\}$; $G \in \{G_m\}$

No common $C_q$

$-9$, $-4$, $1$, $6$, $11$ — $q_1 + G$ — Set of simultaneous eqns for coeffs $\{C_{q_1+G}\}$.

$-8$, $-3$, $2$ — $q_2 + G$

**Note**: Each set

4
5
6
7
8
9
10
11
12
13
⋮

7
12
⋮
⋮
-7
-2 $\quad q_3 + G$
3
8
13
⋮

of equations <u>uniquely</u> indentified by a $q$ in the range:

$$G_0 \leq q < G_1$$

since $C_{q+G_1} \in \{C_{q+G}\}$.

The range of the unique identifier $q$ can be generalized to $q' + G_0 \leq q < q' + G_1$ for $q' \in \{q_n\}$. and since the length of the range is $G_1 - G_0 = \frac{2\pi}{a}$ and $\Delta q = \frac{2\pi}{Na}$; we <u>must</u> have $N$ unique values of $q$ for each of which a set of simultaneous eqn to be solved.

$\therefore$ <u>Unique set of $q$</u> can thus be chosen as:

$$\boxed{q_n = q' + n\frac{2\pi}{Na}, \quad n = 0, 2, \cdots, (N-1); \; q' \in \{q_n\}}$$

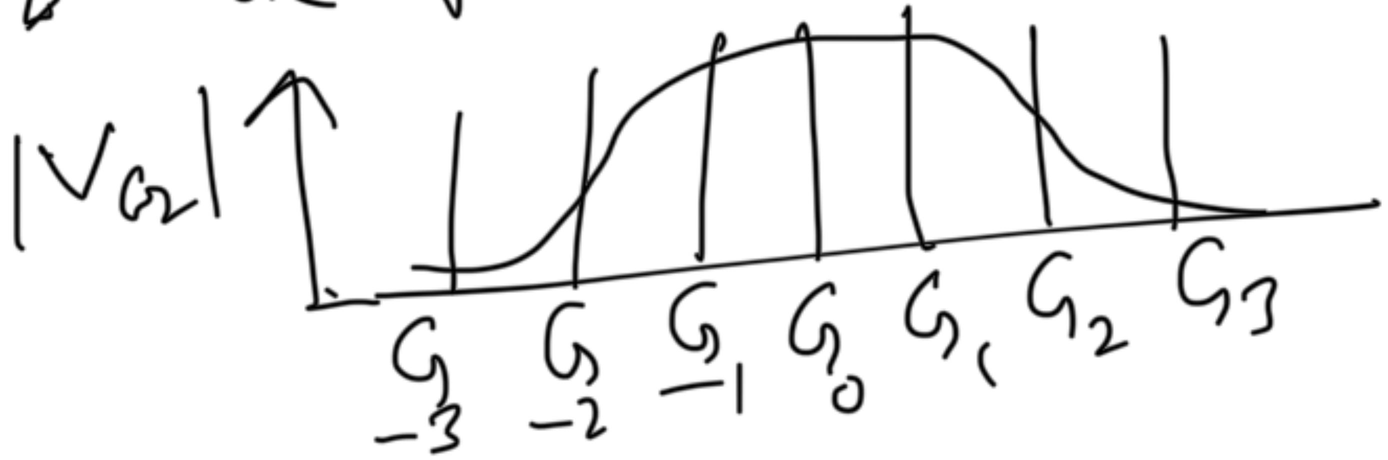
Simultaneous equations for coeffs $\{C_{q'+G}\}$:

$$
\begin{array}{ccccccccc}
\cdots & -3 & -2 & -1 & 0 & 1 & 2 & 3 & \cdots
\end{array}
$$

$$
\Rightarrow
\begin{pmatrix}
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
\cdots & V_{-G_2} & V_{-G_1} & \left[\frac{\hbar^2(q'+G_1)^2}{2m} - E + V_{G_0}\right] & V_{G_1} & V_{G_2} & V_{G_3} & V_{G_4} \; \cdots \\
\cdots & V_{-G_3} & V_{-G_2} & V_{-G_1} & \left[\frac{\hbar^2 q'^2}{2m} - E + V_{G_0}\right] & V_{G_1} & V_{G_2} & V_{G_3} \; \cdots \\
 & & & & V_{-G_1} & \left[\frac{\hbar^2(q'-G_1)^2}{2m} - E + V_{G_0}\right] & V_{G_1} & V_{G_2} \; \cdots \\
\cdots & V_{G_{-4}} & V_{G_{-3}} & V_{-G_2} & & & & \\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots
\end{pmatrix}
\begin{pmatrix}
\vdots \\
C_{q'+G_2} \\
C_{q'+G_1} \\
C_{q'} \\
C_{q'-G_1} \\
C_{q'-G_2} \\
\vdots
\end{pmatrix}
= 0
$$

Realistically, $V_G$ is set to zero above certain $|G|$ for smooth enough $V(x)$.

In class we considered $V_G = 0$ for $|G| > |G_2|$ which is ok if the Fourier transform of $V(x)$ is

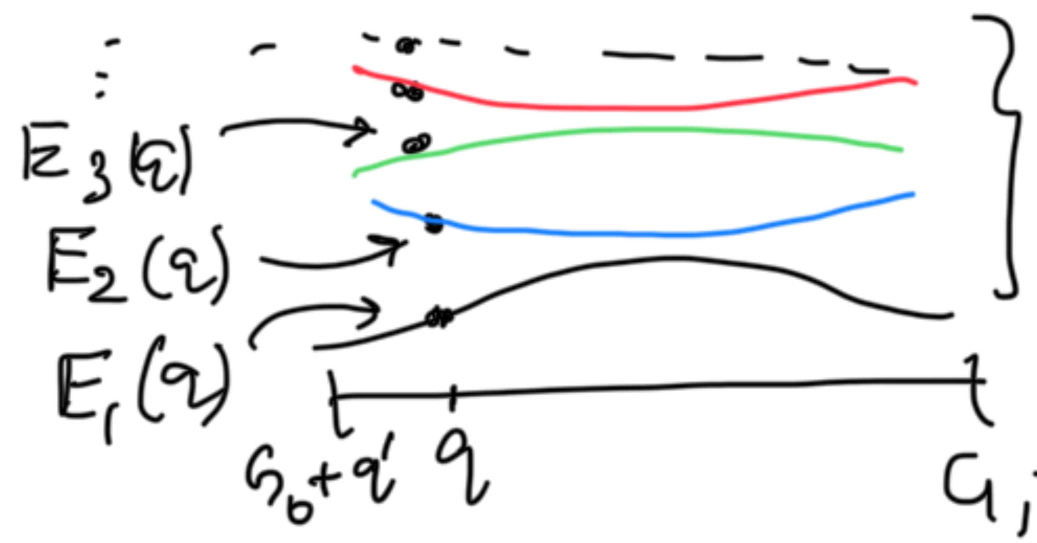



We get a band-diagonal matrix with two bands above and below the diagonal.

The size of the matrix will depend on our choice of limiting $|C_{q'-G}| \neq 0$ for $|G| \leq |G_M|$ implying the size of the H matrix to $(2M+1) \times (2M+1)$.

Diagonalising the H matrix for each unique $q$ we obtain $2M+1$ number of energy eigenvalues for each $q$

$\Rightarrow$

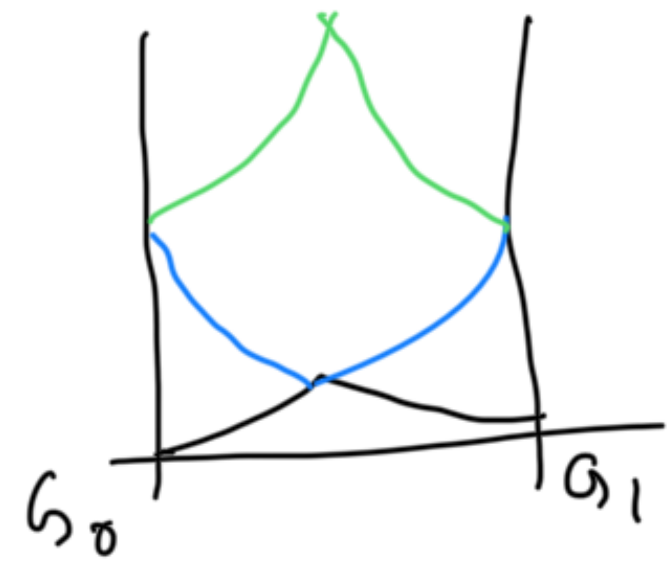



$2M+1$ bands formed by $2M+1$ eigenvalues at each $q$ in the range $q'+G_0 \leq q < q'+G_1$

Introduce band index $j$ : $\{\psi_{qj}\}$

$\Rightarrow$ $(2M+1)$ number of orthonormal states with real eigenvalues $\{E_{qj}\}$

If $V(x) \to 0$ $\Rightarrow$ Diagonal matrix. $\Rightarrow$ Free electron bands




See separate note.

<u>In summary</u>: (Bloch formalism)

with $V(x) = V(x + la)$; $l = \pm 1, \pm 2, \dots$

and $N$ unit cell in the BVK cell, we have $N$ unique sets of orthonormal solutions for $\Psi$ identified by $N$ unique values of $q$:

$$q_n = q' + \frac{n 2\pi}{Na}; \quad n = 0, 1, 2, \dots, N-1; \quad q' \in \{q_n\}$$

such that:

$$\Psi_q = \sum_G C_{q+G} e^{i(q+G)x}$$

$$= e^{iqx} \sum_G C_{q+G} e^{iGx}$$

$$\boxed{\Psi_q(x) = e^{iqx} \underline{U_q(x)} \qquad U_q(x) = U_q(x + la)}$$

cell periodic $\qquad l = \pm 1, \pm 2, \dots$

Bloch Theorem

Note: $U_q(x)$ is periodic in $a$ because $\{e^{iGx}\}$ are periodic in $a, \frac{a}{2}, \frac{a}{3}, \frac{a}{4}, \ldots$

<u>what is $q$?</u>

Note that if $V(x) = 0 \Rightarrow \{V_G\} = 0 \Rightarrow$ Each of $\{C_{q+G}\}$ individual plane wave

$\Rightarrow \psi_q(x) \to e^{iqx} \to$ should be plane wave $\Rightarrow q \equiv k \Rightarrow \hbar k \to$ momentum

In presence of $V(x)$ : $\hbar q \to$ "crystal momentum"

<u>Note:</u>

$$U_{q+G}(x) = \sum_{G'} C_{(q+G)+G'}\, e^{iG'x}$$

$$= \sum_{G''} C_{q+G''}\, e^{i(G''-G)x} \quad ; \quad G'' = G + G'$$

$$= e^{-iGx} \sum_{G''} C_{q+G''}\, e^{iG''x}$$

$$\boxed{U_{q+G}(x) = e^{-iGx}\, u_q(x)}$$

$$\Rightarrow \quad \psi_{q+G}(x) = e^{i(q+G)x}\, u_{q+G}(x)$$

$$= e^{i(q+G)x}\, e^{-iGx}\, u_q(x)$$

$$= e^{iqx}\, u_q(x) = \psi_q(x)$$

$$\Rightarrow \boxed{\psi_{q+G}(x) = \psi_q(x)}$$ periodicity in $q$ space

Orthonormality of Bloch state: (We will write band index and write $q$ as $k$ hence forth.)

$$\psi_q \equiv \psi_{nk}(x) = e^{ikx}\, \underbrace{u_{nk}(x)}_{\text{cell periodic}}$$

$n$ band index

$k$ allowed wavevector

$$\langle u_{nk} | u_{mk} \rangle = \int_0^a u^*_{nk}(x)\, u_{mk}(x)\, dx$$

$$= \int_0^a \sum_G C^{n*}_{k+G} e^{\ldots} \sum_{G'} C_{k+G'} e^{\ldots} dx$$

$$= \sum_G \sum_{G'} C^{n*}_{k+G} C^{m}_{k+G'} \int_0^a e^{-iGx} e^{iG'x} dx$$

$$= \sum_G \sum_{G'} C^{n*}_{k+G} C^{m}_{k+G'} \; a\,\delta_{GG'}$$

$$= a \sum_G C^{n*}_{k+G} C^{m}_{k+G} = a\,\delta_{nm}$$

$$\therefore \boxed{u_{nk} = \frac{1}{\sqrt{a}} \sum_G C_{k+G} e^{iGx}} \rightarrow \langle u_{nk} | u_{mk} \rangle = \delta_{nm}$$

Note however that $\langle u_{nk} | u_{mk'} \rangle$ can be non zero

$$\langle \psi_{nk} | \psi_{mk'} \rangle$$

$$= \int_0^{Na} e^{-ikx} u^*_{nk}(x) e^{ik'x} u_{mk'}(x)\, dx$$

$$= \sum^{N} \int_0^a e^{-ik(x+ja)} u^*_{nk}(x+ja) e^{ik'(x+ja)} u_{mk'}(x+ja)\, dx$$

$$= \sum_{j}^{N} e^{-ikja} e^{ik'ja} \int_0^a u^*_{nk}(x)\, u_{mk'}(x)\, dx$$

$$= N\, \delta_{kk'} \langle u_{nk} | u_{mk'} \rangle$$

If $k = k'$: $\langle \psi_{nk} | \psi_{mk} \rangle = N\, \delta_{kk'}$

$$\therefore \boxed{\psi_{nk}(x) = \frac{1}{\sqrt{N}} e^{ikx} u_{nk}(x)} \Rightarrow \langle \psi_{nk} | \psi_{mk'} \rangle = \delta_{nm} \delta_{kk'}$$