Band gap

Recall, $(K_{q+G'} - E) C_{q+G'} + \sum_G V_G \, C_{q+G'-G} = 0$ —— (A)

let us see how plane wave $e^{i(q+G')x}$ would mix with other plane waves as cell periodic V is switched on.

$C_{q+G'}$ would decrease from 1 but will remain in the order of 1 if $|V|$ is small, $E \sim K_{q+G'}$

$C_{q+G''}\big|_{G'' \neq G'}$ would increase from zero but $\ll 1$.

~~let~~ let us see how $C_{q+G''}\big|_{G'' \neq G'}$ evolves.:

$$(K_{q+G''} - E) C_{q+G''} + \sum_G V_G C_{q+G''-G} = 0$$

$$\Rightarrow (E - K_{q+G''})\, C_{q+G''} = \underbrace{V_{G''-G'} \, \frac{C_{q+G'}}{\sim 1}}_{\text{is linear}} + \sum_{G \neq G''-G'} V_G \, C_{q+G''-G} \quad \text{--- (B)}$$

$\therefore$ Leading order of $V_{G''-G'}$ in $C_{q+G''}\big|_{G''\neq G'}$

$\therefore$ Leading " " " " the second term of (B) is $|V_{G''-G'}||V_G|$, $G \neq G''-G'$

For small V we thus neglect the second term.

$$\therefore (E - K_{q+G''})\, C_{q+G''} \approx V_{G''-G'} C_{q+G'}$$

$$\Rightarrow C_{q+G''} \approx \frac{V_{G''-G'} C_{q+G'}}{E - K_{q+G''}} \approx \frac{V_{G''-G'} \, C_{q+G'}}{K_{q+G'} - K_{q+G''}} \quad \text{--- (C)}$$

Recall (A): $(E - K_{q+G'})\, C_{q+G'} = \sum_G V_G \, \underset{\sim}{C_{q+G'-G}}$

Substituting $C_{q+G'-G}$ from (C) by setting $G'' = G'-G$

$$= V_0 C_{q+G'} + \sum_{G \neq 0} V_G \left(\frac{V_{-G} \, C_{q+G'}}{K_{q+G'} - K_{q+G'-G}} \right)$$

$$\Rightarrow E_{q+G'} \approx V_0 + K_{q+G'} + \sum_{G\neq 0} \frac{V_G V_{-G}}{K_{q+G'} - K_{q+G'-G}}$$

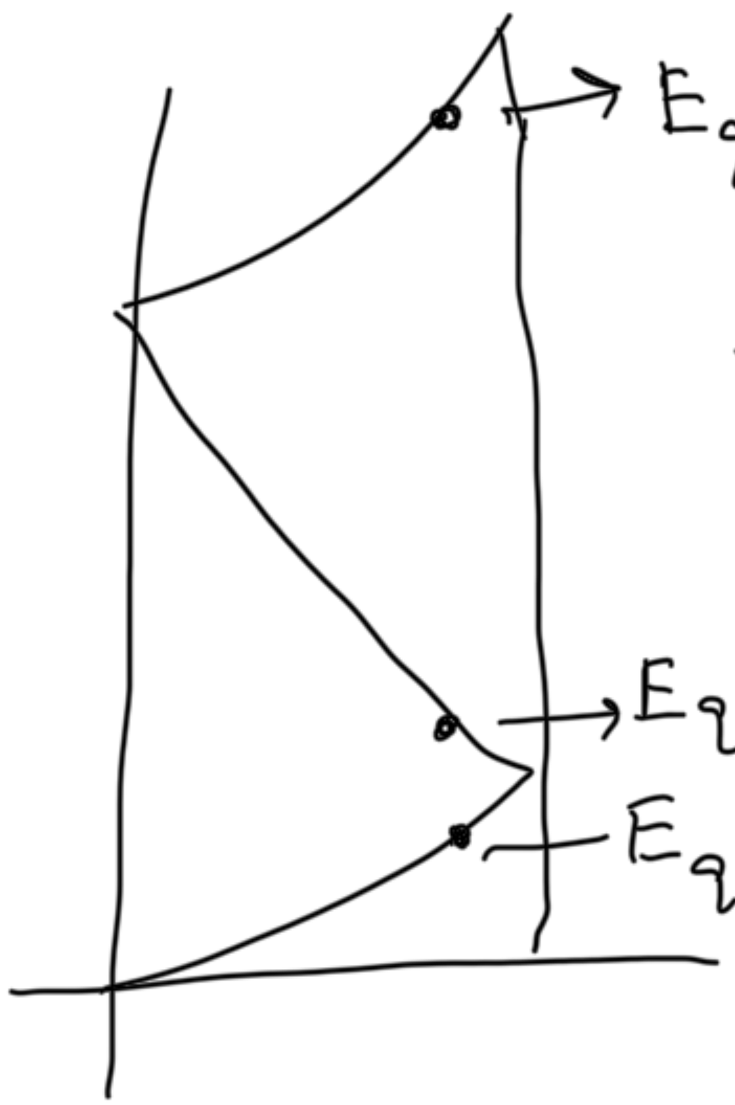
$\downarrow$

E_{qn} Correspond n to G' as per the free electron B St.

For the example we are doing in class: $V(x) = V_0 \cos\frac{2\pi x}{a}$

$V_{G_0} = 0,\ V_{G_{\pm 1}} = V_0/2$

$$\therefore E_{q+G'} \approx K_{q+G'} + \frac{V_0^2/4}{K_{q+G'} - K_{q+G'-G_1}} + \frac{V_0^2/4}{K_{q+G'} - K_{q+G'+G_1}}$$



$E_{q3} \to G' = G_1$

$E_{q+G'} \to E_{qn}$ see

$E_{q2} \Rightarrow G' = -G_1 \Rightarrow E_{q2} = k_{q-G_1} + \underbrace{\frac{V_0^2/4}{k_{q-G_1} - k_{q-G_2}}}_{-ve} + \underbrace{\frac{V_0^2/4}{K_{q-G_1} - k_q}}_{+ve}$

$E_{q1} \to G' = G_0 \Rightarrow E_{q1} = K_q + \underbrace{\frac{V_0^2/4}{k_q - K_{q-G_1}}}_{-ve} + \underbrace{\frac{V_0^2/4}{k_q - K_{q+G_1}}}_{-ve}$

$$E_{q_2} = K_{q-G_1} + C + D$$

$$E_{q_1} = K_q + A + B$$

Note $\boxed{\begin{array}{l} A > 0,\ B > 0 \Rightarrow E_{q_1} \Downarrow \\ \left.\begin{array}{l} C < 0,\ D > 0 \\ \text{but } |C| < |D| \end{array}\right\} \Rightarrow E_{q_2} \uparrow \end{array}}$

Note that as n increases the denominator increases

$\Rightarrow$ gap decreases.

Check yourself what happens close to $q = 0$

Note that you can not use the above approximate expressions at degenerate points like $q = 0, \frac{\pi}{a}$ as the denominator can go to zero. You can study only close to those points.

Now let us see in terms of the matrix representation in the $\{ e^{i(q+G)x} \}$ basis with $\{ G = 0, \pm 1, \pm 2 \}$ leading to 5 lowest solutions for ψ_q.

$$
\begin{bmatrix}
K_{q-G_2} & V_0/2 & 0 & 0 & 0 \\
V_0/2 & K_{q-G_1} & V_0/2 & 0 & 0 \\
0 & V_0/2 & K_q & V_0/2 & 0 \\
0 & 0 & V_0/2 & K_{q+G_1} & V_0/2 \\
0 & 0 & 0 & V_0/2 & K_{q+G_2}
\end{bmatrix}
\begin{bmatrix}
C_{q-G_2} \\ C_{q-G_1} \\ C_q \\ C_{q+G_1} \\ C_{q+G_2}
\end{bmatrix}
= E
\begin{bmatrix}
C_{q-G_2} \\ C_{q-G_1} \\ C_q \\ C_{q+G_1} \\ C_{q+G_2}
\end{bmatrix}
$$

$$\underline{\underline{h}}_q \, \underline{\psi}_q = E \, \underline{\psi}_q$$

If you consider $V_0 = 0$ then we have planewave solution:
$\begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \\ 0 \end{bmatrix} \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \\ 0 \end{bmatrix} \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}$ with energies K_{q-G_2}, K_{q-G_1}, K_q, K_{q+G_1}, K_{q+G_2} respectively.

Now switch on $V(x)$ with $V_0 \ll K_{\frac{\pi}{a}}$

However, infinitesimally close to $\frac{\pi}{a}$: $|V_0| \sim |K_q - K_{q-G_1}|$

Recall, 2nd order perturbation theory.

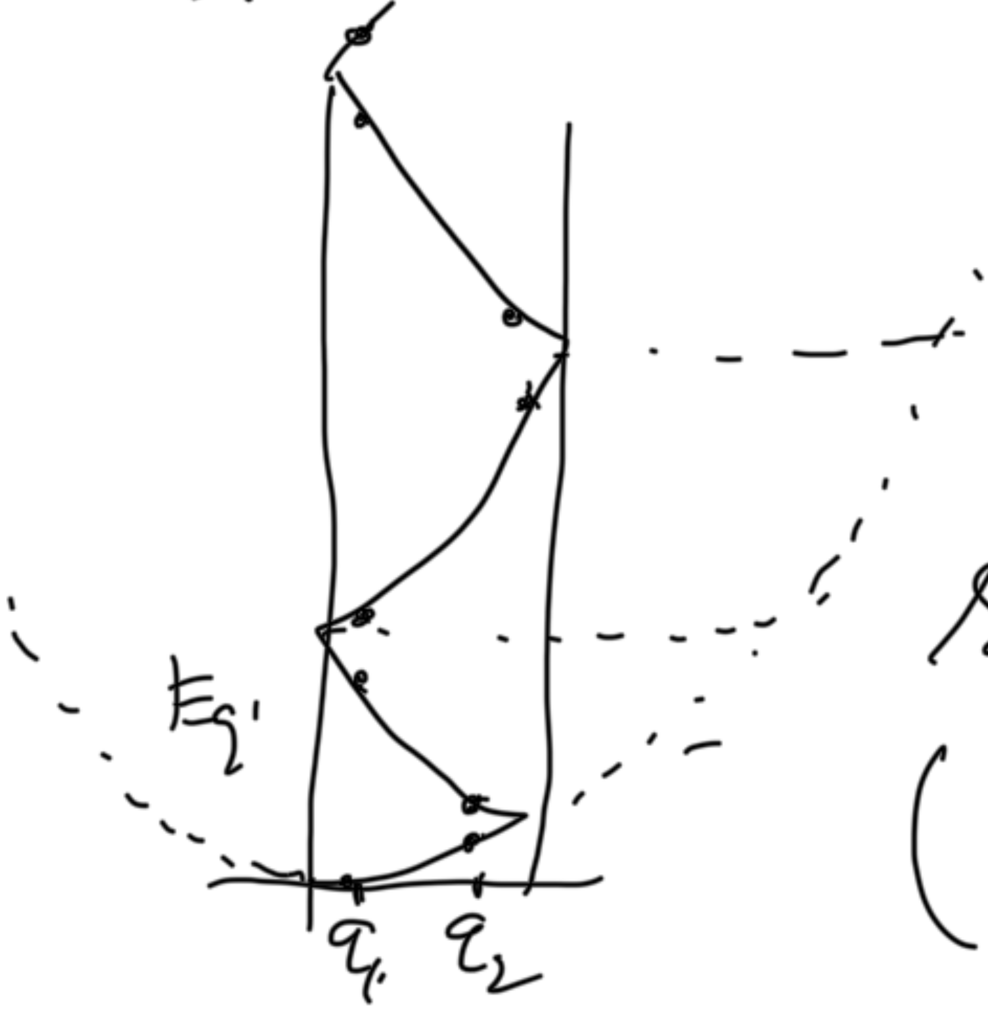
$$\Psi_n = \Psi_n^{(0)} + \sum_{n \neq m} \frac{H'_{nm}}{(E_n^0 - E_m^0)} \phi_m^0 + \cdots$$

∴ The mixing of two unperturbed eigenstates is proportional to $\dfrac{|V_{G_{n-m}}|}{|E_n^0 - E_m^0|}$.

∴ Since $|V_0| \sim |K_q - K_{q-G_1}|$ at $k = \frac{\pi}{a} \pm 0^+$

only e^{iqx} and $e^{i(q-G_1)x}$ would mix substantially.

Note that mixing will happen mainly at $q = 0, \frac{\pi}{a}, \frac{2\pi}{a}, \frac{3\pi}{a} \ldots$ since at these q values two bands come closer.



$$q_1 \to 0^+ \; ; \; q_2 \to \frac{\pi}{a} - 0^+$$

$$(E_{q_2 2} - E_{q_2 1}) < (E_{q_2 4} - E_{q_2 3}) < (E_{q_2 6} - E_{q_2 5}) < \cdots$$

Similarly

$$(E_{q_1 3} - E_{q_1 2}) < (E_{q_1 5} - E_{q_1 4}) < \cdots$$

$\therefore$ Mixing will be increasingly weaker as we go higher in band index.

$\therefore$ To obtain the correction to energies of bands 1 and 2 at $q = \pi/a$ it is sufficient to diagonalize H in the basis of e^{iqx} and $e^{i(q-G_1)x}$ since they would only mix dominantly.

$\therefore$

$$\begin{bmatrix} K_{q-G_1} & V_0/2 \\ V_0/2 & K_q \end{bmatrix} \begin{bmatrix} C_{q-G_1} \\ C_q \end{bmatrix} = E \begin{bmatrix} C_{q-G_1} \\ C_q \end{bmatrix}$$

$$\Rightarrow (K_{q-G_1} - E)(K_q - E) - \frac{V_0^2}{4} = 0$$

$$\Rightarrow K_{q-G_1} K_q - E\left(K_{q-G_1} + K_q\right) + E^2 - \frac{V_0^2}{4} = 0$$

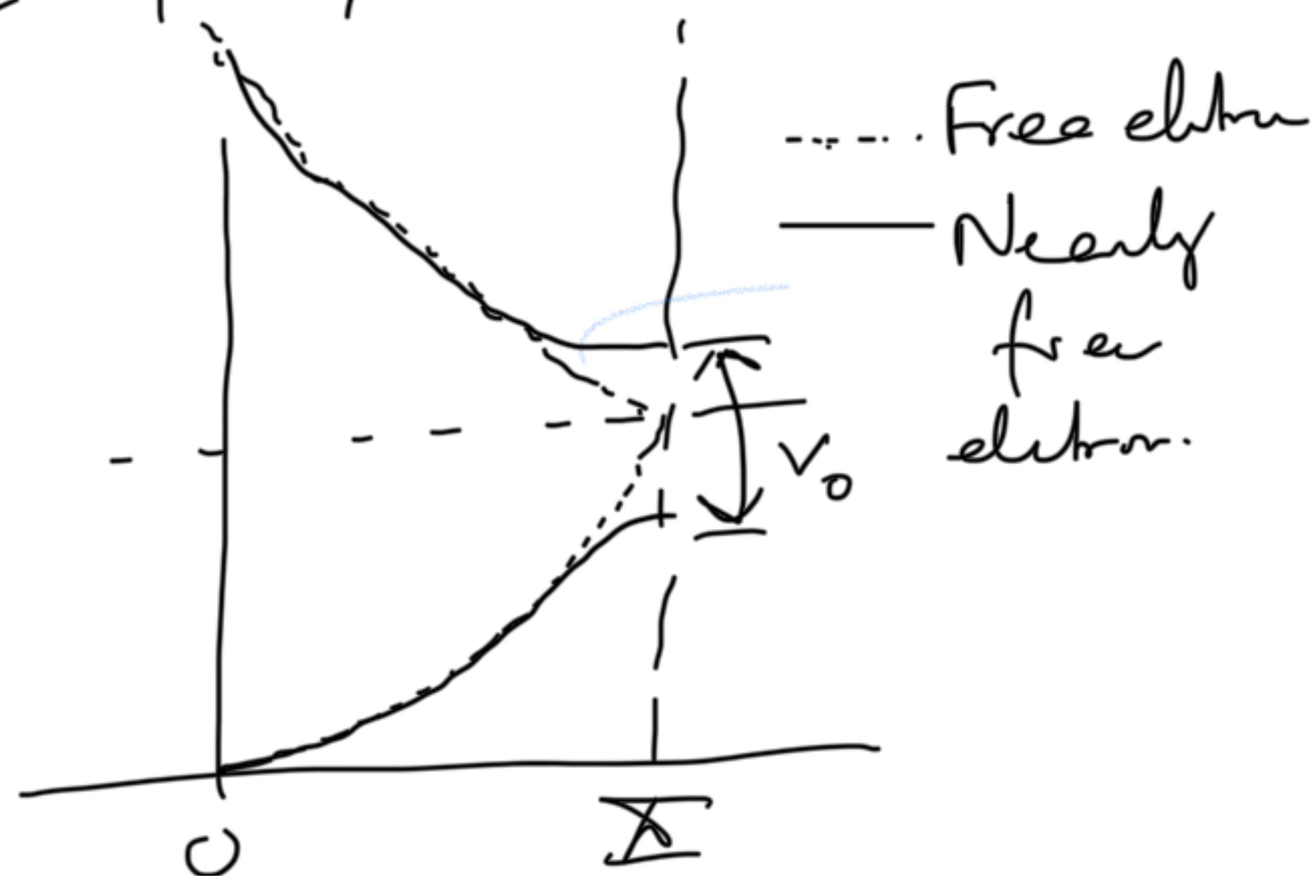
$$\Rightarrow E = \frac{1}{2}\left(K_{q-G_1} + K_q\right) \pm \frac{1}{2}\sqrt{\left(K_{q-G_1} + K_q\right)^2 - 4\left(K_{q-G_1} K_q - \frac{V_0^2}{4}\right)}$$

$\therefore$ For $q = \frac{\pi}{a}$:

$$E = K_{\frac{\pi}{a}} \pm \frac{1}{2} + \sqrt{V_0^2}$$

$$= K_{\frac{\pi}{a}} \pm V_0/2$$

$\Rightarrow$



Convince yourself that $\left.\frac{\partial E}{\partial q}\right|_{q=\frac{\pi}{a}} = 0$

To get the gap between bands 2 and 3 at $q=0$ diagonalise:

$$\begin{bmatrix} K_{q-G_1} & V_0/2 & 0 \\ V_0/2 & K_q & V_0/2 \\ 0 & V_0/2 & K_{q+G_1} \end{bmatrix}$$