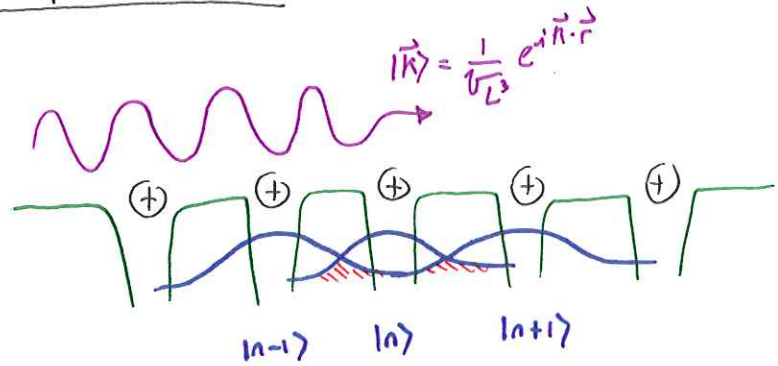
Physics 410/510 — Solid State Physics
Spring 2015
Monday, week 8:

Electrons in a periodic potential:



$$\hat{H}\psi = E\psi \qquad \hat{H} = \frac{\hat{\vec{P}}^2}{2m} + V(\vec{r})$$

$$= H_0 + V(\vec{r})$$

$\hookrightarrow V(\vec{r}+\vec{R}) = V(\vec{r})$ $\quad \vec{R} \in$ Lattice vectors

$$|\vec{k}\rangle = \frac{1}{\sqrt{L^3}} e^{i\vec{k}\cdot\vec{r}} \qquad H_0|\vec{k}\rangle = \frac{\hbar^2\vec{k}^2}{2m}|\vec{k}\rangle$$

Treat $V(\vec{r})$ as perturbation,

$$E = E_0 + \underbrace{E_1 + E_2}_{\text{a function of } \langle\vec{k}'|V|\vec{k}\rangle}$$

$$= \frac{\hbar^2\vec{k}^2}{2m}$$

The matrix elements $\langle \vec{k}' | V(\vec{r}) | \vec{k} \rangle$ are used in calculating E_i's. These elements are:

$$V_{\vec{k}',\vec{k}} = \langle \vec{k}' | V | \vec{k} \rangle = \frac{1}{L^3} \int_{\text{crystal}} e^{-i\vec{k}'\cdot\vec{r}} V(\vec{r}) e^{i\vec{k}\cdot\vec{r}} \, d\vec{r}$$

$$= \frac{1}{L^3} \int e^{i(\vec{k}-\vec{k}')\cdot\vec{r}} V(\vec{r}) \, d\vec{r}$$

$$= \frac{1}{L^3} \sum_{\vec{R}} \int_{\text{unit cell}} e^{i(\vec{k}-\vec{k}')\cdot(\vec{x}+\vec{R})} V(\vec{x}+\vec{R}) \, d\vec{x}$$

$$= \frac{1}{L^3} \sum_{\vec{R}} e^{-i(\vec{k}'-\vec{k})\cdot\vec{R}} \int_{\text{unit cell}} V(\vec{x}) e^{i(\vec{k}-\vec{k}')\cdot\vec{x}} \, d\vec{x}$$

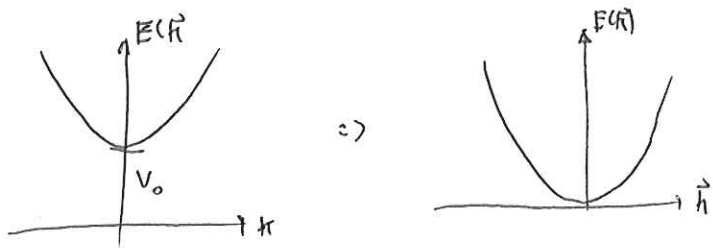
$$= 0 \quad \text{unless } \boxed{\vec{k}'-\vec{k} = \vec{G}} \quad \text{Also } \boxed{V_{\vec{k}'-\vec{k}}}$$

To first order (nondegenerate)

$$E(\vec{k}) = E_0(\vec{k}) + \underbrace{\langle \vec{k} | V | \vec{k} \rangle}_{V_0 = \frac{1}{L^3}\int V(\vec{r}) d\vec{r}}$$

[Constant for all $\vec{k}$]

This just shifts all energies by V_0. We can ignore this, and set it to zero.



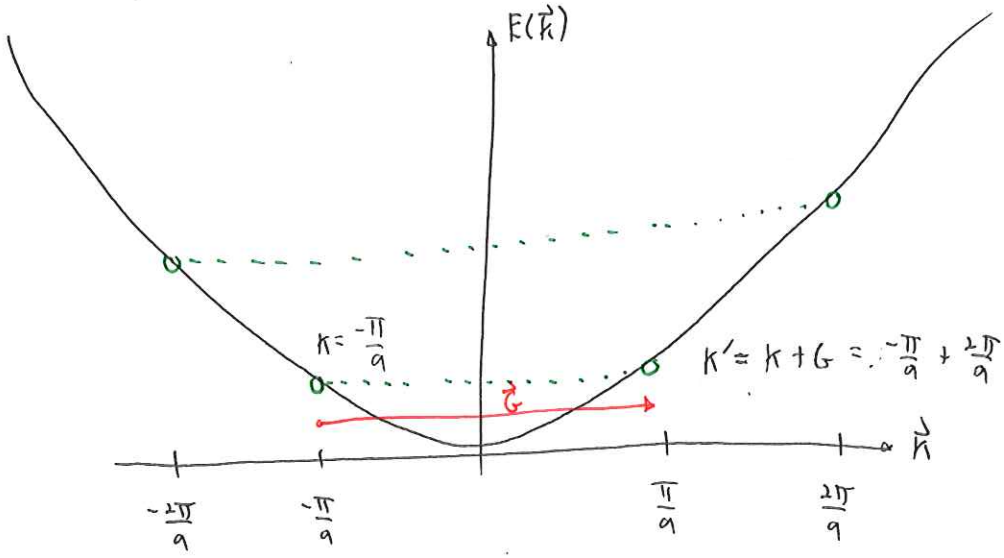
Just redefine $V'(\vec{r}) = V(\vec{r}) - V_0$

To second order (nondegenerate)

$$\boxed{E(\vec{k}) = E_0(\vec{k}) + \sum_{\substack{\vec{k}'=\vec{k}+\vec{G} \\ \vec{G}\neq 0}} \frac{|\langle \vec{k}' | V | \vec{k} \rangle|^2}{E_0(\vec{k}) - E_0(\vec{k}')}}$$

The nondegenerate pert. theory works well if $E_0(\vec{k}) \neq \vec{E}_0(\vec{k}')$, or if $E_0(\vec{k}) \not\sim \vec{E}_0(\vec{k}')$.

However, there are certain values of $\vec{k}'$ & $\vec{k}$ that do have the same energy (or close to it):



Also need $\vec{k}' = \vec{k} + \vec{G}$ for some $\vec{G}$, or else $\langle \vec{k}' | V | \vec{k} \rangle = 0$

Here, for example,

$$\boxed{E(k) = E(k')}$$

Note also that $\langle k' | V | k \rangle = \langle k + G | V | k \rangle$

so $\neq 0$

since $\boxed{k' = k + G}$

Note all cases where 2° Energy fails are near or at the BZ Edges!!

<u>To solve for approximate energies, we need degenerate perturbation theory.</u>

Here we need to diagonalize H_{mn}: The components are:

$$\langle \vec{k} | H | \vec{k} \rangle = E_0(\vec{k})$$

$$\langle \vec{k}' | H | \vec{k}' \rangle = E_0(\vec{k})$$

$$\langle \vec{k} | H | \vec{k}' \rangle = V_{\vec{k}-\vec{k}'} = V^*_{\vec{G}} = V_{-\vec{G}} \quad (\text{since } V(\vec{r}) \in \mathbb{R})$$

$$\langle \vec{k}' | H | \vec{k} \rangle = V_{\vec{k}'-\vec{k}} = V_{\vec{G}}$$

Note: $\langle \vec{k} | H_0 | \vec{k}' \rangle = \frac{\hbar^2 \vec{k}^2}{2m} \langle \vec{k} | \vec{k}' \rangle = 0$

Fourier Coefficients of $V(\vec{r}) = \sum_{\vec{G}} V_{\vec{G}} e^{i\vec{G}\cdot\vec{r}}$

In this subspace, we write

$$|\psi\rangle = \alpha|\vec{k}\rangle + \beta|\vec{k}'\rangle$$
$$= \alpha|\vec{k}\rangle + \beta|\vec{k}+\vec{G}\rangle$$

Then

$$\begin{pmatrix} E_0(\vec{k}) & V_{\vec{G}}^* \\ V_{\vec{G}} & E_0(\vec{k}+\vec{G}) \end{pmatrix}\begin{pmatrix} \alpha \\ \beta \end{pmatrix} = E\begin{pmatrix} \alpha \\ \beta \end{pmatrix} \longrightarrow \begin{pmatrix} E_0(\vec{k})-E & V_{\vec{G}}^* \\ V_{\vec{G}} & E_0(\vec{k}+\vec{G})-E \end{pmatrix}\begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \vec{0}$$

The characteristic equation is,

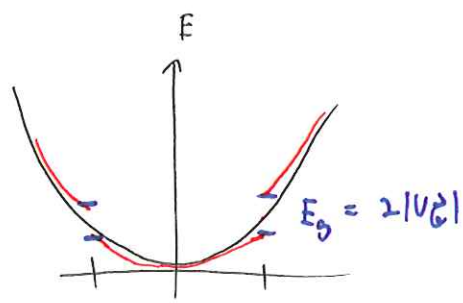
$$\boxed{\left(E_0(\vec{k})-E\right)\left(E_0(\vec{k}+\vec{G})-E\right) - |V_{\vec{G}}|^2 = 0} \qquad (*)$$

<u>$\vec{k}$ on BZ edge (zone boundary)</u>:

$E_0(\vec{k}) = E_0(\vec{k}+\vec{G})$, then

$$\left(E_0(\vec{k})-E\right)^2 = |V_{\vec{G}}|^2$$

$$\Rightarrow \boxed{\begin{aligned} E &= E_0(\vec{k}) \pm |V_{\vec{G}}| \\ &= \frac{\hbar^2\vec{k}^2}{2m} \pm |V_{\vec{G}}| \end{aligned}}$$



Thus a gap opens up at the zone boundary & the wave functions are some linear combination of $|\vec{k}\rangle$ & $|\vec{k}'\rangle$:

$$|\psi_\pm\rangle = \frac{1}{\sqrt{2}}\left(|\vec{k}\rangle \pm |\vec{k}'\rangle\right)$$

In 1D,

$$|k\rangle = e^{ikx} = e^{+i\frac{\pi}{a}x}$$

$$|k'\rangle = e^{ik'x} = e^{-ikx}$$

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

$$\Rightarrow \quad |\psi_+\rangle = e^{i\frac{\pi}{a}x} + e^{-i\frac{\pi}{a}x} \propto \cos\left(\frac{\pi}{a}x\right)$$

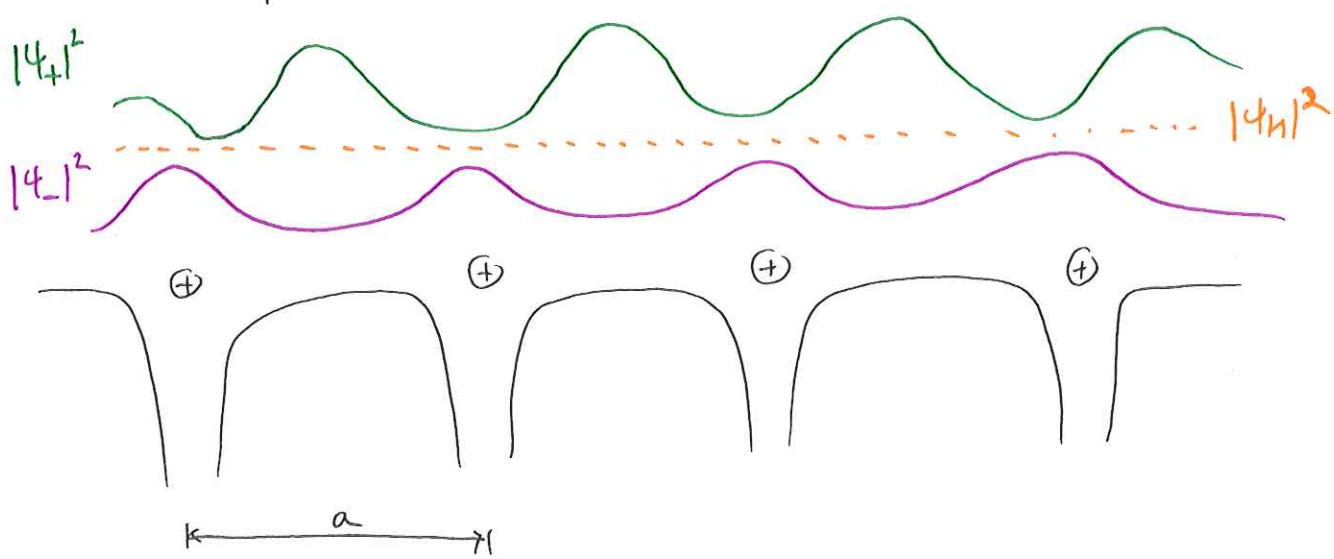
$$|\psi_-\rangle = e^{i\frac{\pi}{a}x} - e^{-i\frac{\pi}{a}x} \propto \sin\left(\frac{\pi}{a}x\right)$$

So

$$|\psi_+|^2 \propto \cos^2\left(\frac{\pi}{a}x\right)$$

$$|\psi_-|^2 \propto \sin^2\left(\frac{\pi}{a}x\right)$$

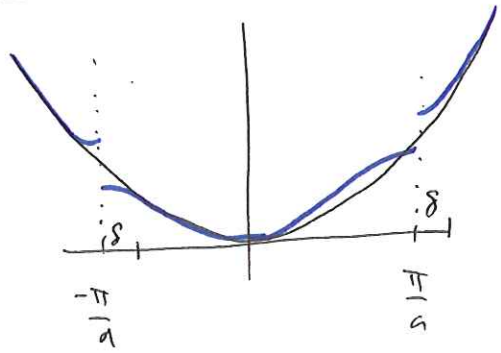
$$|\psi_k|^2 = |\psi_{-k}|^2 \propto 1$$



The $|\psi_-|^2$ charge distribution piles charge over the positive ion cores, so it has a lower energy than either the $|\psi_+|^2$ or the $|\psi_k|^2$!! For a similar reason, the $|\psi_+|^2$ has a higher energy than the plane wave. Note that these wave functions are "Standing Waves."

One way to interpret the standing wave is the Bragg condition. The plane waves with $\vec{k} \in [\text{BZ edge}]$ <u>cannot propagate</u>, but are instead scattered in the crystal to form standing waves!!

<u>$\vec{k}$ close to the BZ edge:</u>



$$E_0\left(\frac{n\pi}{a} + \delta\right) = \frac{\hbar^2}{2m}\left(\left(\frac{n\pi}{a}\right)^2 + \frac{2n\pi}{a}\delta + \delta^2\right) \qquad n \in \mathbb{Z}$$

$$E_0\left(-\frac{n\pi}{a} + \delta\right) = \frac{\hbar^2}{2m}\left(\left(\frac{n\pi}{a}\right)^2 - \frac{2n\pi}{a}\delta + \delta^2\right)$$

Our characteristic eq. (✱) gives:

$$\left(\frac{\hbar^2}{2m}\left[\left(\frac{n\pi}{a}\right)^2 + \delta^2\right] - E + \frac{\hbar^2}{2m}\cdot\frac{2\pi n}{a}\delta\right)\left(\frac{\hbar^2}{2m}\left[\left(\frac{n\pi}{a}\right)^2 + \delta^2\right] - E - \frac{\hbar^2}{2m}\cdot\frac{2\pi n}{a}\delta\right)$$

$$- |V_G|^2 = 0$$

or

$$\left(\frac{\hbar^2}{2m}\left[\left(\frac{n\pi}{a}\right)^2 + \delta^2\right] - E\right)^2 = \left(\frac{\hbar^2}{2m}\cdot\frac{2\pi n}{a}\delta\right)^2 + |V_G|^2$$

$$E_\pm = \frac{\hbar^2}{2m}\left[\left(\frac{n\pi}{a}\right)^2 + \delta^2\right] \pm \sqrt{\left(\frac{\hbar^2}{2m}\cdot\frac{2\pi n}{a}\delta\right)^2 + |V_G|^2}$$

& w/ $\delta \to 0$:

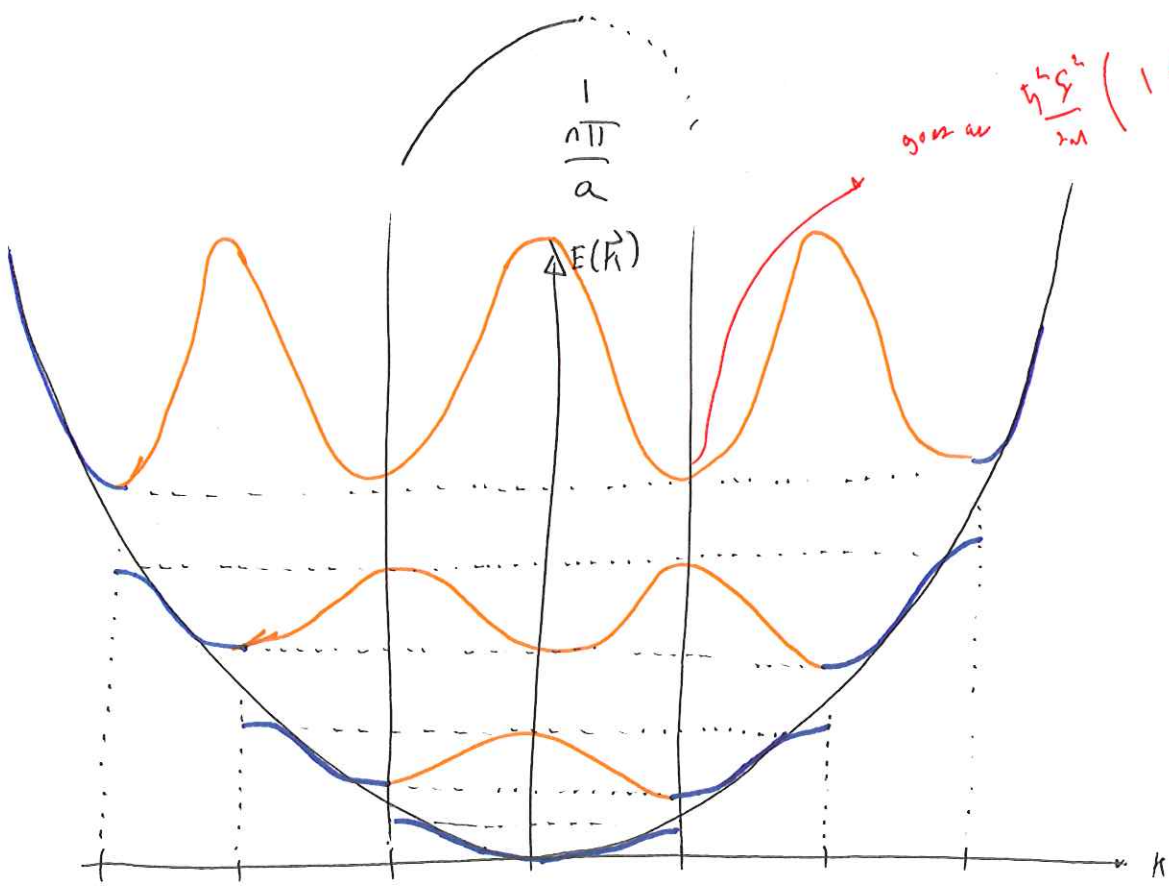
$$|V_G| \cdot \sqrt{\left(\frac{\hbar^2}{2m} \cdot \frac{2\pi n}{a} \delta\right)^2 / |V_G|^2 + 1} \approx |V_G| \cdot \left(1 + \frac{1}{2} \frac{1}{|V_G|^2} \left(\frac{\hbar^2}{2m} \frac{2\pi n}{a} \delta\right)^2\right)$$

so

$$E_\pm = \overbrace{\frac{\hbar^2}{2m}\left(\frac{n\pi}{a}\right)^2 \pm |V_G|}^{C_\pm} + \overbrace{\frac{\hbar^2 \delta^2}{2m}\left[1 \pm \frac{\hbar^2}{m}\left(\frac{\pi n}{a}\right)^2 \cdot \frac{1}{|V_G|}\right]}^{\frac{\hbar^2 \delta^2}{2m^*}}$$

For small perturbations, $\frac{\hbar^2}{m}\left(\frac{\pi n}{a}\right)^2 > |V_G| \Rightarrow$ > 1, so "$-$" solution will be concave down, & the "$+$" concave up:

sharper for higher BZ edges; n.



goes as $\frac{\hbar^2 \delta^2}{2m}\left(1 + \frac{\hbar^2}{m}\left(\frac{\pi \cdot 3}{a}\right)^2 \frac{1}{|V_G|}\right)$

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Wednesday, Week 8 :

Review: $|\vec{k}\rangle = \frac{1}{\sqrt{L^3}} e^{i\vec{k}\cdot\vec{r}}$

$$E = E_0 + \underbrace{E_1 + E_2 + \cdots}$$

$\langle \vec{k}'|V|\vec{k}\rangle = 0$ unless $\vec{k}' - \vec{k} = \vec{G}$

Use degenerate perturbation theory when $E(\vec{k}) \sim E(\vec{k}+\vec{G})$

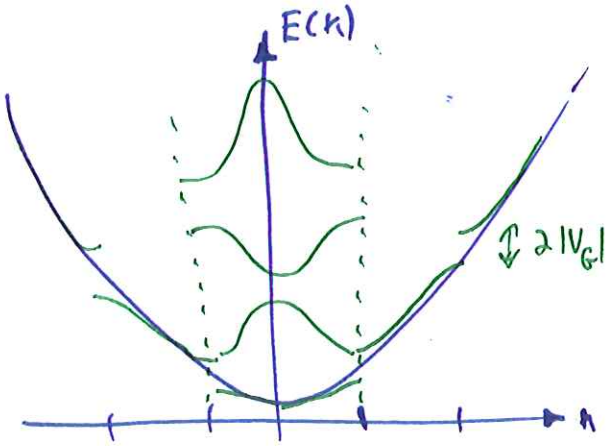
$$\left(E_0(\vec{k}) - E\right)\left(E_0(\vec{k}+\vec{G}) - E\right) - |V_{\vec{G}}|^2 = 0$$

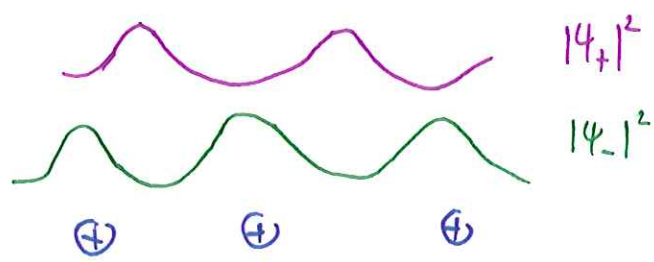
$\vec{k}$ @ zone boundary:

$$E_\pm = \underbrace{\frac{\hbar^2 \vec{k}^2}{2m} \pm |V_{\vec{G}}|}$$

$\vec{k}$ close to zone boundary:

$$E_\pm = C_\pm \pm \frac{\hbar^2 \delta^2}{2m^*} \quad \text{a} \quad m^* \equiv \overbrace{\left|\left[1 \pm \frac{\hbar^2}{m}\left(\frac{n\pi}{a}\right)^2 \frac{1}{|V_G|}\right]\right|}^{m}$$





$$E_\pm = C_\pm \pm \frac{\hbar \Omega^4}{2m^*_\pm}$$

$$m^*_\pm \equiv \left| \frac{m}{\left[1 \pm \frac{\hbar^2}{m}\left(\frac{n\pi}{a}\right)^2 \cdot \frac{1}{|V_G|} \right]} \right|$$

[effective mass]

Note that $|m^*_+| < |m^*_-|$, so m^*_+ electrons move faster under same force.

Now, what are the eigen wavefunctions of $H = \frac{\vec{p}^2}{2m} + V(\vec{r})$?

If $[A, H] = 0$ & $A|a\rangle = a|a\rangle$

$(AH - HA)|a\rangle = AH|a\rangle - HA|a\rangle$
$= AH|a\rangle - aH|a\rangle$
$= 0$

$\downarrow$

$A(H|a\rangle) = a(H|a\rangle)$

$\Rightarrow H|a\rangle = H_a|a\rangle$

$\Rightarrow |a\rangle$ also eigenfunction of H!!

We find another operator that commutes with H:

$$T_{\vec{R}} f(\vec{r}) \equiv f(\vec{r} + \vec{R})$$

[Translation Operator]

$$T_{\vec{R}} H\psi = H(\vec{r}+\vec{R})\psi(\vec{r}+\vec{R})$$
$$= H(\vec{r}) T_{\vec{R}} \psi(\vec{r})$$

$\Rightarrow T_{\vec{R}} H - H T_{\vec{R}} = 0$

- $H\psi = E\psi$, $T_{\vec{R}}\psi = C(\vec{R})\psi$
- $T_{\vec{R}} T_{\vec{R}'} \psi(\vec{r}) = T_{\vec{R}'} T_{\vec{R}} \psi(\vec{r}) = \psi(\vec{r} + \vec{R} + \vec{R}')$

$$T_{\vec{R}} T_{\vec{R}'} = T_{\vec{R}'} T_{\vec{R}} = T_{\vec{R}+\vec{R}'}$$

So
$$T_{\vec{R}} T_{\vec{R}'} \psi = C(\vec{R}) C(\vec{R}') \psi$$
$$= T_{\vec{R}'+\vec{R}} \psi$$
$$= C(\vec{R}+\vec{R}')\psi$$

$\Rightarrow C(\vec{R}+\vec{R}') = C(\vec{R})C(\vec{R}')$

For $\vec{a}_i$ primitive lattice vectors, $C(\vec{a}_i) = e^{i 2\pi x_i}$

$x_i \in \mathbb{C}$ is possible

for $\vec{R} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$

$$c(\vec{R}) = c(\vec{a}_1)^{n_1}\, c(\vec{a}_2)^{n_2}\, c(\vec{a}_3)^{n_3}$$

$$= e^{i(2\pi x_1 n_1 + 2\pi x_2 n_2 + 2\pi x_3 n_3)}$$

$$= e^{i\vec{K}\cdot\vec{R}} \qquad \vec{K} = x_1\vec{b}_1 + x_2\vec{b}_2 + x_3\vec{b}_3$$

where $\vec{a}_i \cdot \vec{b}_j = 2\pi\delta_{ij}$

So

$$T_{\vec{R}}\,\psi(\vec{r}) = e^{i\vec{K}\cdot\vec{R}}\,\psi(\vec{r})$$

We can choose eigenfunctions of $T_{\vec{R}}$ as

$$\boxed{\psi(\vec{r}) = e^{i\vec{K}\cdot\vec{r}}\, u_K(\vec{r})}$$

where $u_K(\vec{r}+\vec{R}) = u_{\vec{K}}(\vec{r})$, [Periodic function]

$$T_{\vec{R}}\,\psi_{\vec{K}}(\vec{r}) = T_{\vec{R}}\left(e^{i\vec{K}\cdot\vec{r}}\, u_{\vec{K}}(\vec{r})\right)$$

$$= e^{i\vec{K}\cdot(\vec{r}+\vec{R})}\, u_{\vec{K}}(\vec{r}+\vec{R})$$

$$= e^{i\vec{K}\cdot\vec{R}}\left(e^{i\vec{K}\cdot\vec{r}}\, u_{\vec{K}}(\vec{r})\right)$$

$$= e^{i\vec{K}\cdot\vec{R}}\,\psi_{\vec{K}}(\vec{r})$$

So $$\psi_{\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}}\, u_{\vec{k}}(\vec{r})$$

are Eigenfunctions of $H = \frac{\vec{p}^2}{2m} + V(\vec{r})$.

This is called <u>Bloch Theorem</u> & $\psi_{\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}}\, u_{\vec{k}}(\vec{r})$ are called <u>Bloch Functions</u>, <u>N.B.</u>: These eigenstates are almost plane waves → modified plane waves.

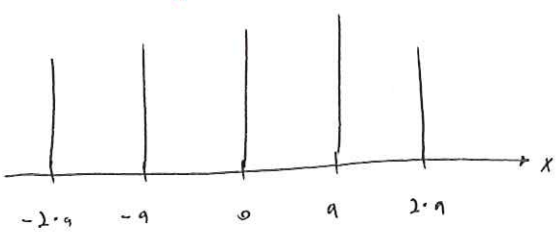
<u>What are $\vec{k}$ values?</u>

$$\psi_{\vec{k}}(x+Na) = \psi_k(x)$$
$$= e^{ik(x+Na)}\, u_k(x+Na)$$
$$= e^{ikNa}\left(e^{ikx}\, u_k(x)\right)$$

$$\Rightarrow \boxed{k = \frac{2\pi}{Na}\cdot n \quad n\in\mathbb{Z} \quad \& \quad k\in\mathbb{R}}$$

<u>Kronig - Penney (Dirac Comb):</u>

Find Solution here, $\psi_k(x)$, then $\psi_k(x+a) = \psi_k(x)e^{ik\cdot a}$.



$$\boxed{V(x) = \alpha \sum_{j=0}^{N-1} \delta(x - j\cdot a)}$$

Between Positive Dirac functions,

$$H\psi = \frac{-\hbar^2 d^2\psi}{2m\,dx^2} = E\psi$$

$$\psi(x) = A\sin(k_0 x) + B\cos(k_0 x) \qquad x\in[0,a]$$

$$k_0 \equiv \sqrt{\frac{2mE}{\hbar^2}}$$

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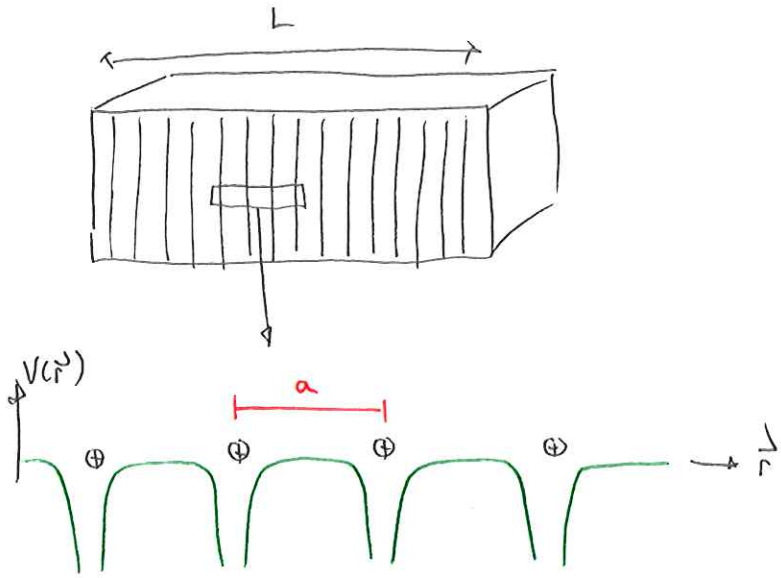
Friday, Week 8:

Review:



$$H = \frac{\vec{P}^2}{2M} + V(\vec{r}) \qquad T_{\vec{R}} \; : \; T_{\vec{R}} f(\vec{r}) = f(\vec{r} + \vec{R})$$

$$[H, T] = 0 \quad \Rightarrow \quad \text{Eigenstates of } T \Rightarrow \text{Eigenstates of } H.$$

showed eigenvalues of $T_{\vec{R}}$ are :

$$c(\vec{R}) = e^{i\vec{K}\cdot\vec{R}} \quad \text{where} \quad \vec{K} = \sum_i x_i \vec{b}_i \qquad \vec{a}_i \cdot \vec{b}_j = 2\pi$$

$$\vec{R} = \sum_i n_i \vec{a}_i$$

So $\quad T_{\vec{R}} \psi = c(\vec{R}) \psi$

$\therefore$ Eigenstates are Bloch Functions : $\boxed{\psi_{\vec{K}}(\vec{r}) = e^{i\vec{K}\cdot\vec{r}} \underbrace{u_{\vec{K}}(\vec{r})}}$

$$u_{\vec{K}}(\vec{r} + \vec{R}) = u_{\vec{K}}(\vec{r})$$

So $\quad \boxed{\psi_{\vec{K}}(\vec{r} + \vec{R}) = e^{i\vec{K}\cdot\vec{R}} \psi_{\vec{K}}(\vec{r})}$

Applying periodic boundary conditions, we see

$$\vec{K} = \begin{pmatrix} \frac{2\pi}{L_x} n_x \\ \frac{2\pi}{L_y} n_y \\ \frac{2\pi}{L_z} n_z \end{pmatrix} \qquad n_i \in \mathbb{Z}$$

Then because any ψ must be periodic over L:

$$\psi(\vec{r}) = \sum_{\vec{k}} A_{\vec{k}} e^{i\vec{k}\cdot\vec{r}}$$

In 1D,

$$\psi(x) = \sum_{k} A_k e^{ikx} \qquad k = \frac{2\pi}{N\cdot a} n \quad n \in \mathbb{Z}$$

$$= \sum_{k \in 1^{\circ}BZ} \sum_{G} A_{k+G} e^{i(k+G)x}$$

$$= \sum_{k \in 1^{\circ}BZ} \underbrace{\left(e^{ikx} \sum_{G} A_{k+G} e^{iGx} \right)}_{\psi_k(x) = e^{ikx} u_k(x)}$$

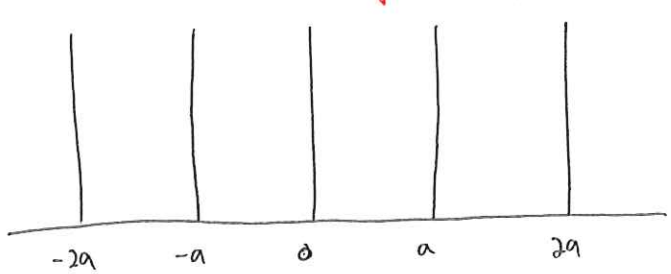
Bloch functions.

Therefore the eigenstates of H are Bloch functions which are label with $k \in 1^{\circ}BZ$.

Kronig-Penney (Dirac-Comb):

find solution here, $\psi_k(x)$

then here $\psi_k(x+a) = e^{ika}\psi_k(x)$



$$\boxed{H\psi = \frac{-\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi}$$

Between positive Dirac functions, so

$$\psi(x) = A\sin(k_0 x) + B\cos(k_0 x)$$

$$V(x) = \alpha \sum_{j=0}^{N-1} \delta(x - j\cdot a)$$

$$k_0 \equiv \sqrt{\frac{2mE}{\hbar^2}}$$

According to Bloch's theorem, the cell to the left gives:

$$\psi(x) = e^{-ika}\left[A\sin(k_0(x+a)) + B\cos(k_0(x+a))\right] \qquad x \in [-a, 0]$$

<u>Continuity of $\psi(x)$ @ $x=0$:</u>

$$\boxed{B = e^{-ika}\left[A\sin(k_0 a) + B\cos(k_0 a)\right]} \qquad (1)$$

$$\hookrightarrow \quad A\sin(k_0 a) = \left(e^{ika} - \cos(k_0 a)\right) B$$

$$\boxed{A = \frac{\left(e^{ika} - \cos(k_0 a)\right)}{\sin k_0 a} \cdot B} \qquad (1.1)$$

<u>Discontinuity of $\frac{d\psi}{dx}$ @ $x=0$:</u>

$$\int \left(H\psi = E\psi\right) dx$$

$$= -\frac{\hbar^2}{2m}\int_{-\epsilon}^{\epsilon} \frac{d^2\psi}{dx} dx + \int_{-\epsilon}^{\epsilon} V(x)\psi(x)\,dx = E\underbrace{\int_{-\epsilon}^{\epsilon}\psi(x)\,dx}_{0}$$

$$\Rightarrow \quad \left.\frac{d\psi}{dx}\right|_{-\epsilon}^{\epsilon} = \frac{2m}{\hbar^2}\int_{-\epsilon}^{\epsilon} \alpha\,\delta(x)\psi(x)\,dx$$

$$\boxed{\begin{aligned} &= \frac{2mB}{\hbar^2}\alpha \\ &= k_0 A - e^{-ika} k_0\left(A\cos(k_0 a) - B\sin(k_0 a)\right) \end{aligned}} \qquad (2)$$

Using 1.1 in 2 :

$$\frac{2m\alpha}{\hbar^2} B = k_0 \frac{\left(e^{ika} - \cos k_0 a\right)}{\sin k_0 a} B - e^{-ika} k_0 \left(\frac{\left(e^{ika} - \cos k_0 a\right)}{\sin k_0 a} \cos(k_0 a) B - B \sin k_0 a \right)$$

$$\downarrow$$

$$\frac{2m\alpha}{\hbar^2}\frac{\sin k_0 a}{k_0} = e^{ika} - \cos k_0 a - e^{-ika}\left(e^{ika}\cos k_0 a \underbrace{- \cos^2 k_0 a - \sin^2 k_0 a}_{-1} \right)$$

$$= \left(e^{ika} + e^{-ika}\right) - 2\cos k_0 a$$

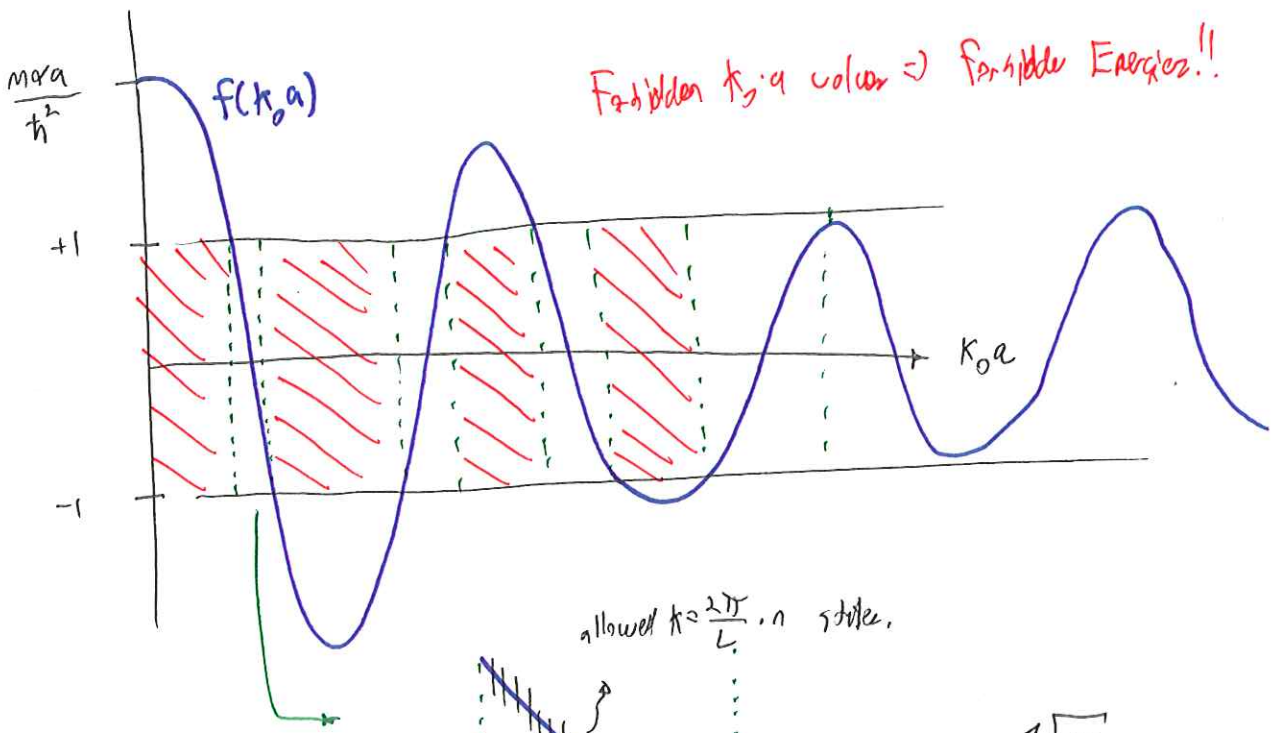
or

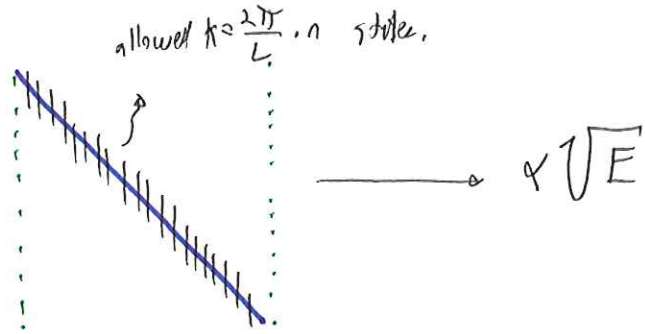
$$\boxed{\cos ka = \cos k_0 a + \frac{m\alpha a}{\hbar^2} \cdot \frac{\sin k_0 a}{k_0 a}} = f(k_0 a)$$

k-vector labeling

$k_0 = \sqrt{\frac{2mE}{\hbar^2}}$ from Sö Eq.

bloch function: $k = \frac{2\pi}{L} \cdot n$





Lowest energy states of allowable $k_0 a$.

$$\cos(ka) = \cos\left(\frac{2\pi n}{N \cdot a} \cdot a\right) = \cos\left(\frac{2\pi}{N} \cdot n\right)$$

can take on N discrete values.

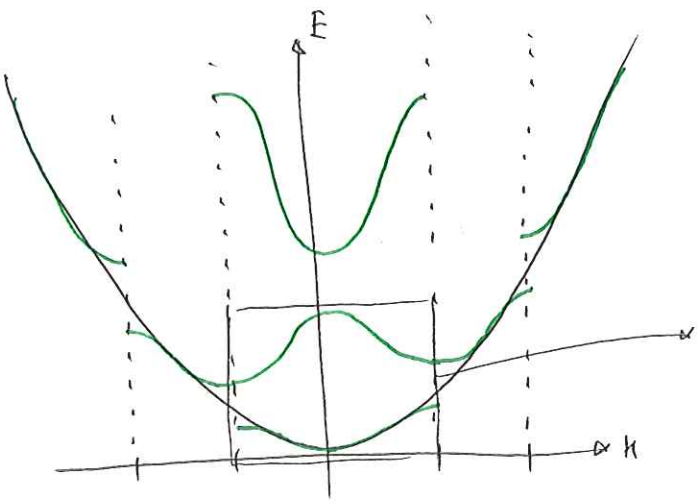
Remarks:

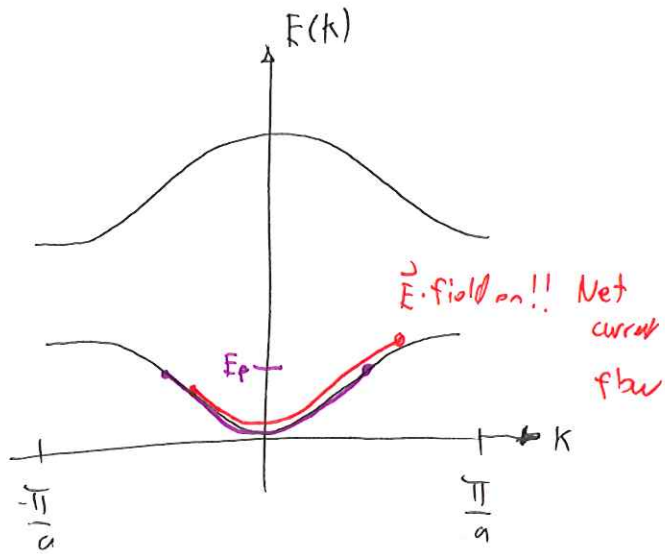
- As potential grows stronger ($q \to \infty$), band gaps also become larger.
- As $a \to 0$, band gaps disappear & material becomes metal;

  Metal → Insulator Transition!!
- Consistent w/ bandgap of $2|U_G|$ from Nearly Free Electron Model!!

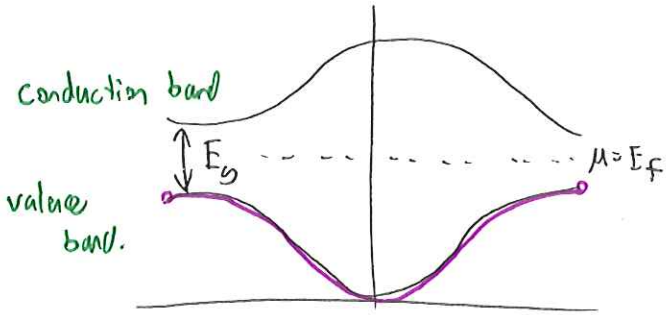
Insulators, Semiconductors & Metals:

Energy Bands in 1D:





Electrons can move freely to unfilled states. ⇒ 1 electron per unit cell.



Band insulator: electrons do Not respond to $\vec{E}$ field

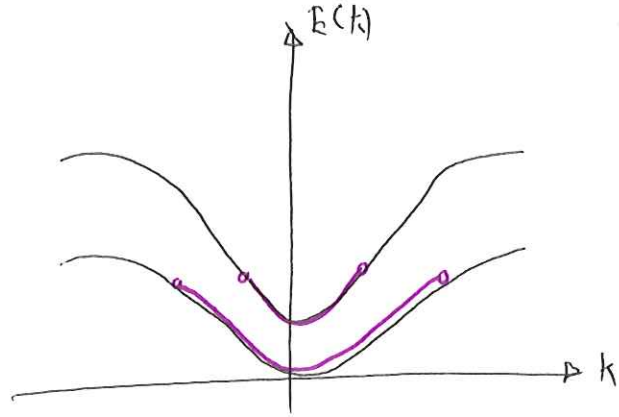
⇒ 2 electrons per unit cell.

- Rule of thumb: Even # e^- ⇒ Insulator / Semiconductor ; Odd # e^- ⇒ metal.

Even with divalent materials, metallic phases may exist;

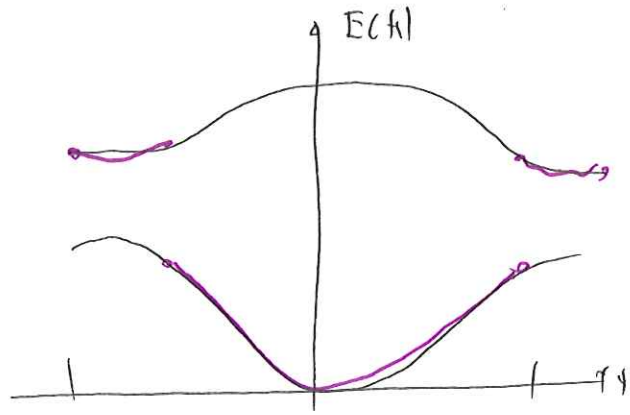
↳ & monovalent materials can be insulators !!

Mott insulators : NiO CoO. Here electron-electron interactions are strong.



Two partially filled bands ⇒ Metal

Also, at finite T, there will be current flow w/ applied $\vec{E}$ even in band insulators;



since $f(E,\mu,T) = \dfrac{1}{e^{(E-\mu)/kT} + 1}$

is nonzero for $E > \mu$ above $T > 0$. These electrons are thermally excited charge carriers. Usually if $E_g < 4eV$, then we call them

Semiconductors