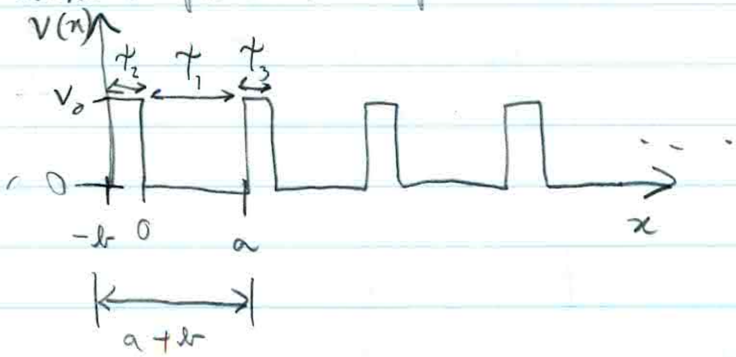
Lecture #2: Kronig–Penney model and Bloch's theorem

Kronig–Penney model

Consider a particle in the potential



$$\begin{cases} \psi_1(x) = A_1 e^{iKx} + B_1 e^{-iKx} & 0 < x < a \quad \text{with} \quad \boxed{\frac{\hbar^2 K^2}{2m} = E} \\ \psi_2(x) = A_2 e^{\kappa x} + B_2 e^{-\kappa x} & -b < x < 0, \quad \text{with} \quad \boxed{\frac{\hbar^2 \kappa^2}{2m} = (V_0 - E)} \end{cases}$$

Due to translation invariance (more later!) we may assume

$$\psi_3(x) = \psi_2(x)\, e^{ik\underbrace{X}_{X = (a+b) \text{ is the distance from } \psi_2}}, \quad a < x < a+b$$

Boundary conditions:

$$\begin{cases} \psi_1(0) = \psi_2(0) \\ \frac{\partial \psi_1}{\partial x}(0) = \frac{\partial \psi_2}{\partial x}(0) \\ \psi_1(a) = \psi_3(a) \\ \frac{\partial \psi_1(a)}{\partial x} = \frac{\partial \psi_3}{\partial x}(a) \end{cases}$$

Four unknowns: A_1, B_1, A_2, B_2

Four eqns $\Rightarrow$ $\underbrace{\begin{pmatrix} \end{pmatrix}}_{\det = 0} \begin{pmatrix} A_1 \\ B_1 \\ A_2 \\ B_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}$

From det = 0 ⇒

$$\left(\frac{\kappa^2 - K^2}{2\kappa K}\right)\sinh(\kappa b)\,\sin(Ka) + \cosh(\kappa b)\cos(Ka) = \cos\big(k(a+b)\big)$$

For simplicity,
Take $b \to 0$, $V_0 \to \infty$, with $V_0 b = \text{const}$. Hence $\kappa \approx \sqrt{\frac{2mV_0}{\hbar^2}}$

$$\kappa b \sim \sqrt{V_0}\, b = \sqrt{V_0 b}\,\sqrt{b} \to 0$$

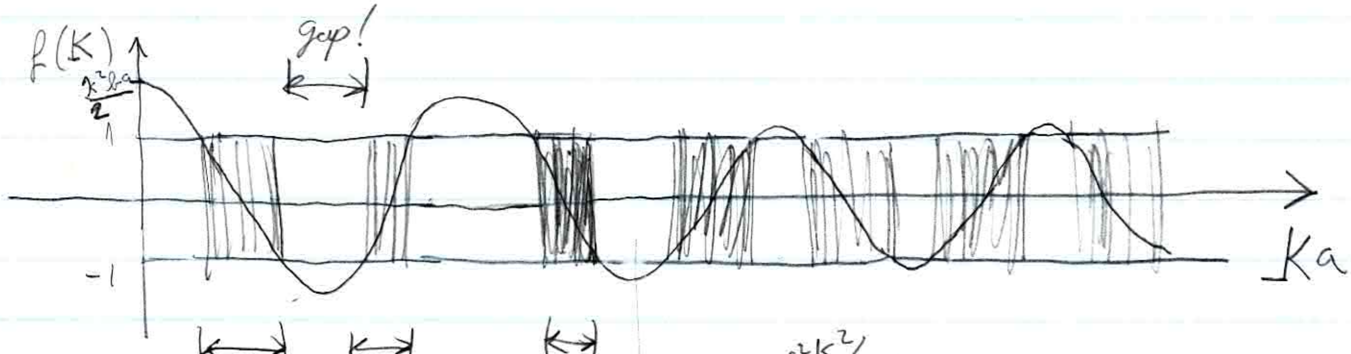
$$\kappa^2 b = \frac{2mV_0 b}{\hbar^2} = \text{const}$$

$$\Rightarrow \underbrace{\frac{\kappa^2 b - K^2 b}{2K}}\ \underbrace{\frac{\sinh(\kappa b)}{\kappa b}}_{\to 1}\sin(Ka) + \underbrace{\cosh(\kappa b)}_{\to 1}\cos(Ka) = \cos(k(a+\underset{\to 0}{b}))$$

$$\to \frac{\kappa^2 b}{2K} = \left(\frac{2mV_0}{\hbar^2}\right)\frac{b}{2K} = \frac{mV_0 b}{\hbar^2}\frac{1}{K}$$

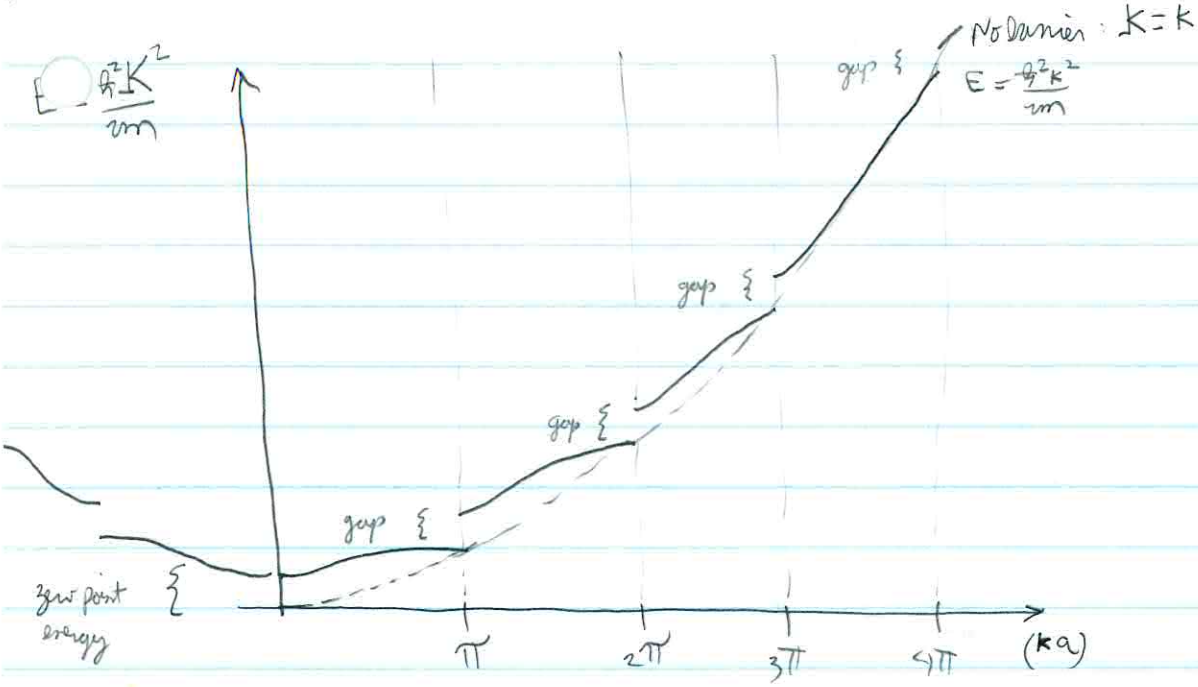
$$\underbrace{\boxed{\frac{mV_0 ba}{\hbar^2}\frac{\sin(Ka)}{(Ka)} + \cos(Ka) = \cos(ka)}}\quad (*)$$

$$f(Ka) = \cos(ka) \Rightarrow \text{Find } K = K(k) \text{ and } E = \frac{\hbar^2 K^2(k)}{2m} = E(k)$$



Real Solutions for K as a func of k only exist here!

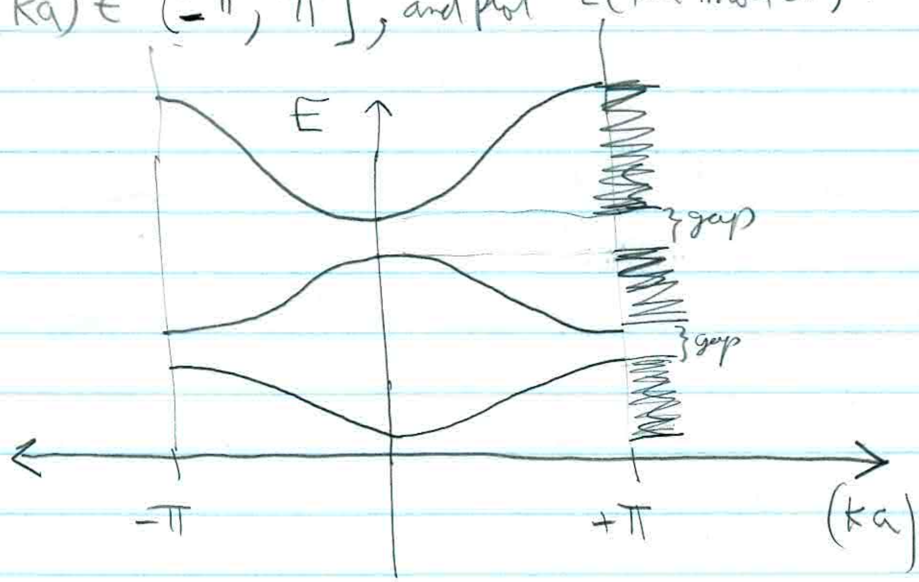
Here, in the gap, only complex solutions of k as a func of K exist ($\cos(ka) = \cosh(\kappa a) > 1$)



Gaps appear when $(ka) \approx n\pi$ $\quad n = 0, 1, 2, 3, \ldots$

"Extended zone scheme": Plot $E(ka)$ with ka larger than 2π.

Since the eqn determining band structure only depends on (ka) by a $\cos(ka)$, we can redefine (ka) as mod 2π. In other words, let's "fold" the bands into the interval $(ka) \in (-\pi, \pi]$, and plot $E(ka \bmod 2\pi)$:



(4)

Based on our calculations, we can think of the wave fnc as a plane wave with a period modulated by the single cell state: If $x = (x \bmod X) + (x \text{ div } X)X$

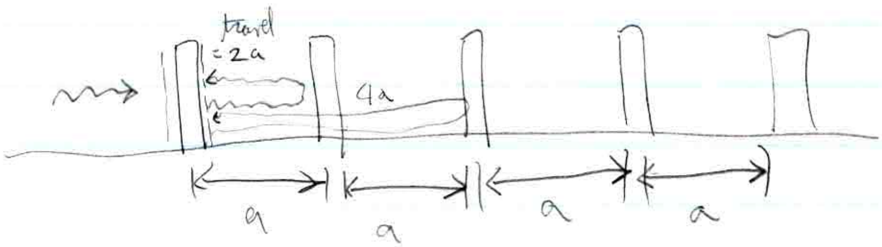
$$\psi(x) = \psi_{cell}(x \bmod \underbrace{X}_{\text{cell period}})\, e^{iK(x \text{ div } X)X}$$

↓ cell period

⇒ The "band structure" $E(K)$ is the "dispersion relation" for this plane wave.

- Why all gaps appear at $(Ka) = n\pi$?

Think of a wave travelling in the set of interfaces separated by a: we call this a "Bragg reflector".



If a wave gets reflected by one of the barriers, it travels a distance $2a$ before it reaches the next barrier. If the wavelength of the wave is

$\lambda_n = \frac{2a}{n}$, $n = 1, 2, 3, \ldots$, then the wave will be max at the barrier, i.e., it will add constructively: Waves with $K_n = \frac{2\pi}{\lambda_n} = \frac{2\pi}{\frac{2a}{n}} = \frac{n\pi}{a}$ will be perfectly reflected in an infinite system! (even if each partial reflection is quite small).

⇒ States with $K = n\pi$ cannot propagate as plane waves; They are "standing waves" (because reflections add coherently).

⇒ States within the gap are "evanescent waves", i.e., they have complex K.

Because waves at $k_n = \frac{n\pi}{a}$ are standing waves, their group velocity $\left(\frac{\partial E}{\partial k}\right)$ must be zero.

Indeed, we see this effect in the plots. To prove this, Consider $E = \frac{\hbar^2 K^2}{2m} \Rightarrow$

$$v_g = \frac{dE}{dk} = \frac{dE}{dK}\frac{dK}{dk} = \left(\frac{\hbar^2 K}{m}\right)\frac{dK}{dk} \propto \frac{dK}{dk}.$$

Take the derivative wrt k of Eq (*):

$$\frac{d}{dk}\left[\left(\frac{mV_0 ba}{\hbar^2}\right)\frac{\sin(Ka)}{Ka} + \cos(Ka)\right] = \frac{d}{dk}\left[\cos(ka)\right]$$

$$\frac{d}{dK}\left[\quad\right]\frac{dK}{dk} = -a\sin(ka)$$

$$\left[\frac{mV_0 ba^2}{\hbar^2}\frac{\cos(Ka)(Ka) - \sin(Ka)}{(Ka)^2} - a\sin(Ka)\right]\frac{dK}{dk} = -a\sin(ka)$$

$$\Rightarrow \left(\frac{dK}{dk}\right) = \frac{\sin(ka)}{\left\{\frac{mV_0 ba}{\hbar^2}\left[\frac{-\cos(Ka)(Ka) + \sin(Ka)}{(Ka)^2}\right] + \sin(Ka)\right\}}\Bigg|_{ka = n\pi} \propto \sin(n\pi) = 0 \, !$$

This prove that group velocity $v_g = \frac{dE}{dk} = 0$ at the band edges $\left(k = \frac{n\pi}{a}\right)$

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Let's also check two limits:

When $V_0 b \to \infty$, the wells are "isolated". In this case (*) becomes:

$$\frac{m V_0 b a}{\hbar^2} \sin(Ka) \approx 0 \Rightarrow Ka = N\pi$$

$$\Rightarrow E = \frac{\hbar^2}{2ma^2}(Ka)^2 = \frac{\hbar^2}{2ma^2}\pi^2 N^2$$ (discrete levels, as expected!)

When $V_0 b \to 0$ we have instead

Eq (*) $\Rightarrow \cos(Ka) = \cos(ka) \Rightarrow K = k \Rightarrow E = \frac{\hbar^2 k^2}{2m}$ as expected!

Bloch's theorem

Translation operator

$$T_{\vec{R}}\,\psi(\vec{r}) = \psi(\vec{r}+\vec{R}) = \psi(\vec{r}) + (\vec{R}\cdot\vec{\nabla})\psi(\vec{r}) + \dots = \sum_{n=0}^{\infty} \frac{(\vec{R}\cdot\vec{\nabla})^n}{n!}\psi(\vec{r}) = e^{\frac{i\vec{p}\cdot\vec{R}}{\hbar}}\psi(\vec{r}),$$

because $\vec{p} = \frac{\hbar}{i}\vec{\nabla}$. Therefore, $T_{\vec{R}} = e^{i\frac{\vec{p}\cdot\vec{R}}{\hbar}}$.

The Crystal Hamiltonian is given by

$$\mathcal{H} = \frac{p^2}{2m} + U(\vec{r}) = -\frac{\hbar^2}{2m}\nabla^2 + U(\vec{r})$$

with $U(\vec{r}+n\vec{a}) = U(\vec{r})$ the periodic crystal potential. We have

$$T_{\vec{R}}\,\mathcal{H}\,T^{+}_{\vec{R}} = e^{+i\frac{\vec{p}\cdot\vec{R}}{\hbar}}\frac{p^2}{2m}e^{-i\frac{\vec{p}\cdot\vec{R}}{\hbar}} + e^{+i\frac{\vec{p}\cdot\vec{R}}{\hbar}}U(\vec{r})e^{-i\frac{\vec{p}\cdot\vec{R}}{\hbar}} = \frac{p^2}{2m} + U(\vec{r}+\vec{R}) = \mathcal{H}, \text{ or } T_{\vec{R}}\mathcal{H} = \mathcal{H}T_R$$

$$\Rightarrow [T_R, \mathcal{H}] = 0.$$

Now, if $\psi(\vec{r})$ is a unique eigenstate of $T_{\vec{R}}$:

$$T_{\vec{R}}\,\psi(\vec{r}) = c_{\vec{R}}\,\psi(\vec{r}), \text{ and } T_R(\mathcal{H}\psi(\vec{r})) = \mathcal{H}(T_R\psi(\vec{r})) = c_{\vec{R}}(\mathcal{H}\psi(\vec{r})),$$

i.e. $\mathcal{H}\psi(\vec{r})$ is also an eigenstate of T_R with the same eigenvalue. Because $\psi(\vec{r})$ is unique, we must have $\mathcal{H}\psi(\vec{r}) \propto \psi(\vec{r}) \Rightarrow \mathcal{H}\psi(\vec{r}) = \epsilon\psi(\vec{r})$.
In other words, when $[\mathcal{H}, T] = 0$ we can diagonalize $\mathcal{H}$ and T simultaneously (this is a general theorem).

Let's find $c_{\vec{R}}$:

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

$$c_{\vec{R}+\vec{R}'}\,\psi(\vec{r}) = c_{\vec{R}}\,c_{\vec{R}'}\,\psi(\vec{r})$$

$$\boxed{c_{\vec{R}+\vec{R}'} = c_{\vec{R}}\,c_{\vec{R}'}}$$

And

$$1 = \langle \psi | \psi \rangle = \int d^3r\, \psi^*(\vec{r})\psi(\vec{r}) = \int d^3r\, \psi^*(\vec{r}+\vec{R})\psi(\vec{r}+\vec{R})$$

$$= C_R^* C_R \int d^3r\, \psi^*(\vec{r})\psi(\vec{r})$$

$$\boxed{\Rightarrow |C_{\vec{R}}|^2 = 1} \quad \text{or} \quad C_{\vec{R}} = e^{i\varphi_{\vec{R}}}$$

But $C_{\vec{R}+\vec{R}'} = C_{\vec{R}} C_{\vec{R}'} \Rightarrow \ln(C_{\vec{R}+\vec{R}'}) = \ln(C_{\vec{R}}) + \ln(C_{\vec{R}'})$

$\Rightarrow \varphi_{\vec{R}+\vec{R}'} = \varphi_{\vec{R}} + \varphi_{\vec{R}'}$ for all allowed translations $\vec{R}, \vec{R}'$.

$\Rightarrow \varphi_{\vec{R}} = \vec{k}\cdot\vec{R}$ for a real vector $\vec{k}$.

$$\Rightarrow \boxed{C_{\vec{R}} = e^{i\vec{k}\cdot\vec{R}}}.$$

Hence,

$$\begin{cases} H\psi_{nk}(\vec{r}) = E_{nk}\psi(\vec{r}) \\ \psi_{nk}(\vec{r}+\vec{R}) = e^{i\vec{k}\cdot\vec{R}}\psi_{nk}(\vec{r}) \end{cases}$$

↑ "Band index" ↑ "quasi-momentum" or "crystal momentum"

(The Bloch function ψ_{nk} is a simultaneous eigenstate of $T_{\vec{R}}$ and H).

Another way to write $\psi_{nk}(\vec{r})$:

$$e^{-i\vec{k}\cdot\vec{r}}\psi_{nk}(\vec{r}+\vec{R}) = e^{i\vec{k}\cdot\vec{R}} e^{-i\vec{k}\cdot\vec{r}}\psi_{nk}(\vec{r})$$

$$e^{-i\vec{k}\cdot(\vec{r}+\vec{R})}\psi_{nk}(\vec{r}+\vec{R}) = e^{-i\vec{k}\cdot\vec{r}}\psi_{nk}(\vec{r}) \Rightarrow e^{-i\vec{k}\cdot\vec{r}}\psi_{nk}(\vec{r}) \equiv \frac{u_{nk}(\vec{r})}{\sqrt{V}} \text{ is periodic, i.e.}$$

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

Bloch's theorem

$$\Rightarrow \boxed{\psi_{nk}(\vec{r}) = u_{nk}(\vec{r})\frac{e^{i\vec{k}\cdot\vec{r}}}{\sqrt{V}}} \quad \text{with } u_{nk}(\vec{r}+\vec{R}) = u_{nk}(\vec{r})$$

$$\int_{\vec{r}\in\Omega_{cell}} d^3r\, |u_{nk}(\vec{r})|^2 = 1$$

$u_{nk}(\vec{r})$ is called the "cell function".