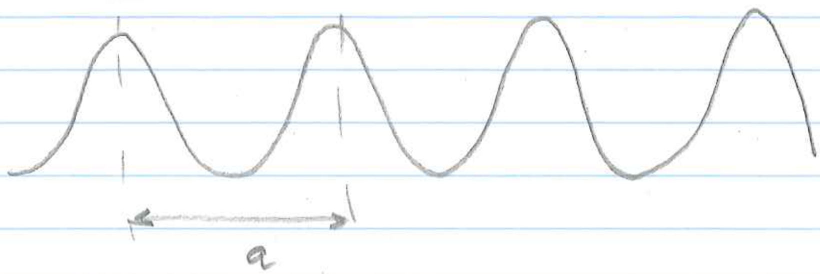
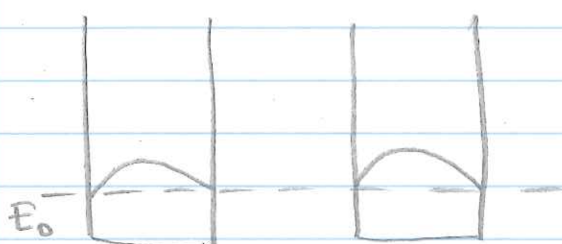
Lattice translation

Consider a periodic potential $V(x+a) = V(x)$



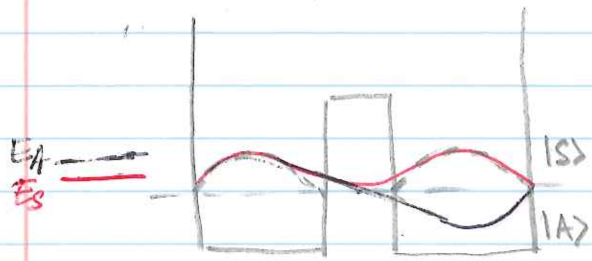
Example: electron motion in a regular solid. What is the effect of such translational symmetry on electron spectrum?

Preliminary "baby" problem: symmetrical double-well

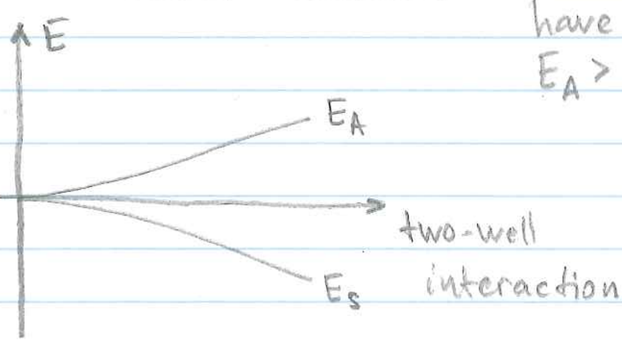


Eigenstates $|R\rangle, |L\rangle$
no parity → no problem,
the states are degenerate

Energy levels in two non-interacting wells are identical



Since $[\hat{\Pi}, \hat{H}] = 0$
the eigenfunctions must have distinct parity
$|S\rangle, |A\rangle$
These two states will have different energy
$E_A > E_S$



$$|S\rangle = \frac{1}{\sqrt{2}}\left(|R\rangle + |L\rangle\right)$$

$$|A\rangle = \frac{1}{\sqrt{2}}\left(|R\rangle - |L\rangle\right)$$

Time-evolution of the localized states at $t=0$ $|R\rangle = \frac{1}{\sqrt{2}}(|S\rangle + |A\rangle)$ $|L\rangle = \frac{1}{\sqrt{2}}(|S\rangle - |A\rangle)$

Time evolution

$$|R(L)\rangle = \frac{1}{\sqrt{2}}\left(e^{-iE_S t/\hbar}|S\rangle \pm e^{-iE_A t/\hbar}|A\rangle\right) =$$

$$= \frac{1}{\sqrt{2}} e^{-iE_S t/\hbar}\left(|S\rangle \pm \underbrace{e^{-i(E_A - E_S)t/\hbar}\;|A\rangle}_{\text{tunneling term}}\right)$$

Let's go back to the periodic potential
Translational symmetry : translation operator

$\tau(\ell)|x\rangle = |x+\ell\rangle$

$\tau(\ell)^{+} = \tau(\ell)^{-1}$

$\hat{x}$: $\tau(\ell)^{+}\hat{x}\,\tau(\ell)|x\rangle = \tau(\ell)^{+}\hat{x}|x+\ell\rangle = \tau(\ell)^{+}(x+\ell)|x+\ell\rangle$
$= (x+\ell)\,\tau(\ell)^{+}|x+\ell\rangle = (x+\ell)|x\rangle$

$$\tau(\ell)^{+}\hat{x}\,\tau(\ell) = (x+\ell)$$

$\hat{p}$: $\tau(\ell)|p\rangle = \tau(\ell)\int \frac{dx}{\sqrt{2\pi\hbar}} e^{ipx/\hbar}|x\rangle = \int \frac{dx}{\sqrt{2\pi\hbar}} e^{ip\overset{x+\ell-\ell}{\downarrow}x/\hbar}|x+\ell\rangle$

$= e^{-ip\ell/\hbar}|p\rangle$

$\tau(\ell) = e^{-ip\ell/\hbar}|p\rangle$; $\tau(\ell)^{+}\hat{p}\,\hat{\tau}(\ell) = \hat{p}$

For a periodic Hamiltonian

$\hat{H} = P^2/2m + V(x)$ such that $V(x+a) = V(x)$

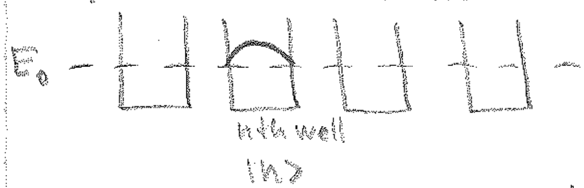
$$\tau^{+}(a)\hat{H}\tau(a) = \frac{P^2}{2m} + \tau^{+}(a)V(x)\tau(a) = \hat{H}$$

$$[\hat{H}, \tau(a)] = 0$$

Must have a set of transversally-invariant eigenstates

Let's first consider a trivial case of infinitely high walls → no tunneling

Then all wells are identical



$$\hat{H}|n\rangle = E_0|n\rangle$$

$$\tau(a)|n\rangle = |n+1\rangle$$

$|n\rangle$ is not the eigenstate of $\hat{\tau}(a)$ (no problem – all the state are degenerate)

What state is the eigenstate of $\hat{H}$ and $\hat{\tau}(a)$?

$$|\theta\rangle = \sum_{n=-\infty}^{+\infty} e^{in\theta}|n\rangle \qquad \hat{H}|\theta\rangle = \sum_{n=-\infty}^{+\infty} e^{in\theta}\hat{H}|n\rangle = E_0|\theta\rangle$$

$$\hat{\tau}(a)|\theta\rangle = \sum_{n=-\infty}^{+\infty} e^{in\theta}\hat{\tau}_a|n\rangle = \sum_{n=-\infty}^{+\infty} e^{in\theta}|n+1\rangle =$$

$$= \sum_{n=-\infty}^{+\infty} e^{i(n-1)\theta}|n\rangle = e^{-i\theta}|\theta\rangle$$

At this moment θ can be any real number $(-\pi < \theta \leq \pi)$, E_0 does not depend on θ

in $\langle n|m\rangle = \delta_{nm}$ $\quad \langle\theta|\theta'\rangle = \sum_{n,m=-\infty}^{+\infty} e^{-in\theta+im\theta'}\underbrace{\langle n|m\rangle}_{\delta_{nm}} =$

all levels are degenerate $\quad = \sum_n e^{in(\theta'-\theta)} = \delta(\theta'-\theta)$

More realistic scenario: tight-binding approximation

The potential walls b/w sights are high, but not infinite
Particles are mostly localized at each site $|n\rangle$, but can tunnel to the nearest neighbours.

$$\langle n'|H|n\rangle = \begin{cases} E_0 & n=n' \\ -\Delta & n-n'=\pm 1 \\ 0 & \text{otherwise} \end{cases}$$

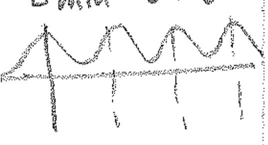
$$\hat{H} = \begin{pmatrix} E_0 & -\Delta & 0 & 0 \\ -\Delta & E_0 & -\Delta & 0 \\ 0 & -\Delta & E_0 & -\Delta \\ 0 & 0 & & \ddots \\ & \ldots & & \end{pmatrix}$$

Since $[\hat{\tau}(a), \hat{H}] = 0$ $\quad |\theta\rangle = \sum e^{in\theta}|n\rangle$
$\tau(a)|\theta\rangle = e^{-i\theta}|\theta\rangle$

$$\hat{H}|\theta\rangle = \sum_{n=-\infty}^{+\infty} e^{in\theta}\hat{H}|n\rangle = \sum_{n,m=-\infty}^{+\infty} e^{in\theta}|m\rangle\langle m|H|n\rangle =$$

$$= \sum_{n,m=-\infty}^{+\infty} e^{in\theta}|m\rangle\left(\delta_{nm}E_0 - \Delta\delta_{nm+1} - \Delta\delta_{nm-1}\right) =$$

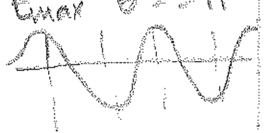
Emin $\theta = 0$



$$= \sum_{n=-\infty}^{+\infty} e^{in\theta}E_0|n\rangle - \Delta\sum_{n=-\infty}^{+\infty} e^{in\theta}\left(|n-1\rangle + |n+1\rangle\right) =$$

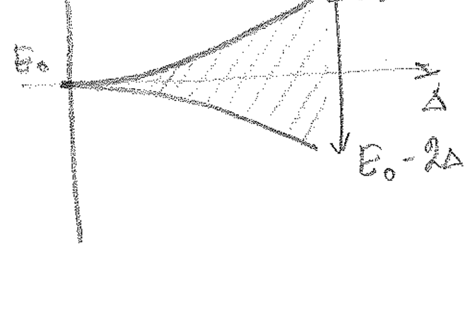
$$= E_0|\theta\rangle - \Delta\sum_{n=-\infty}^{+\infty} e^{i(n-1)\theta}e^{i\theta}|n-1\rangle - \Delta\sum_{n=-\infty}^{+\infty} e^{i(n+1)\theta}e^{-i\theta}|n+1\rangle$$

Emax $\theta = \pm\pi$



$$= (E_0 - 2\Delta\cos\theta)|\theta\rangle$$

So $\hat{H}|\theta\rangle = \underbrace{(E_0 - 2\Delta\cos\theta)}_{E(\theta)}|\theta\rangle$



$E_0 - 2\Delta \le E(\theta) \le E_0 + 2\Delta$

What is the physical meaning of $|\theta\rangle$?

$$\tau(a)\,|p\rangle = e^{-\frac{ipa}{\hbar}}\,|p\rangle$$

and $\tau(a)|\theta\rangle = e^{-i\theta}\,|\theta\rangle$

Does that means that $|\theta\rangle \propto |p\rangle$ $\left(\theta = \frac{pa}{\hbar}\right)$

However for $p \to p + \frac{2\pi\hbar}{a}\cdot n$ $\qquad \frac{2\pi\hbar}{a}$ = Bloch vector

$$\tau(a)\,|p + \frac{2\pi\hbar}{a}\cdot n\rangle = e^{-i\left(p+\frac{2\pi\hbar}{a}n\right)\cdot\frac{a}{\hbar}}\,|p+\frac{2\pi\hbar}{a}\cdot n\rangle =$$

$$= e^{-ipa/\hbar + 2\pi i n}\,|p+\frac{2\pi\hbar}{a}\cdot n\rangle = e^{-ipa/\hbar}\,|p+\frac{2\pi\hbar}{a}n\rangle$$

A better guess

$$|\theta\rangle = \sum_{n=-\infty}^{+\infty} c_n\,|p+\frac{2\pi\hbar}{a}n\rangle \qquad \{c_n\} \text{ depend on } p$$

$$\psi_\theta(x) = \langle x|\theta\rangle = \sum_{n=-\infty}^{+\infty} c_n\,\langle x|p+\frac{2\pi\hbar}{a}n\rangle =$$

$$= \sum_{n=-\infty}^{+\infty} c_n\,\frac{1}{\sqrt{2\pi\hbar}}\,e^{ix(p+2\pi\hbar/(an))/\hbar} =$$

$$= e^{ixp/\hbar}\left[\sum_{n=-\infty}^{+\infty} c_n\,\frac{1}{\sqrt{2\pi\hbar}}\,e^{i\frac{2\pi x}{a}\cdot n}\right] \qquad k = p/\hbar$$

Fourier series of a function of period a

$$u_k(x) = \sum_{n=-\infty}^{+\infty} \frac{c_n}{\sqrt{2\pi\hbar}}\,e^{i\frac{2\pi x}{a}\cdot n}$$

$$\psi_k(x) = u_k(x)\,e^{ikx}$$

[Alternative derivation]

At the moment θ is a random real parameter. Let's determine its physical meaning

Wavefunction $\psi_\theta(x') = \langle x'|\theta\rangle$

For a lattice-translated function

$$\langle x'|\tau(a)|\theta\rangle = \langle x'|\theta\rangle e^{-i\theta}$$

$$\langle x'-a|\theta\rangle = e^{-i\theta}\langle x'|\theta\rangle = e^{-i\overset{\theta}{ka}}\langle x'|\theta\rangle$$

$$\psi(x') = \langle x'|\theta\rangle = e^{ikx}\underbrace{u_k(x)}_{\text{periodic}}$$

$\theta = ka$

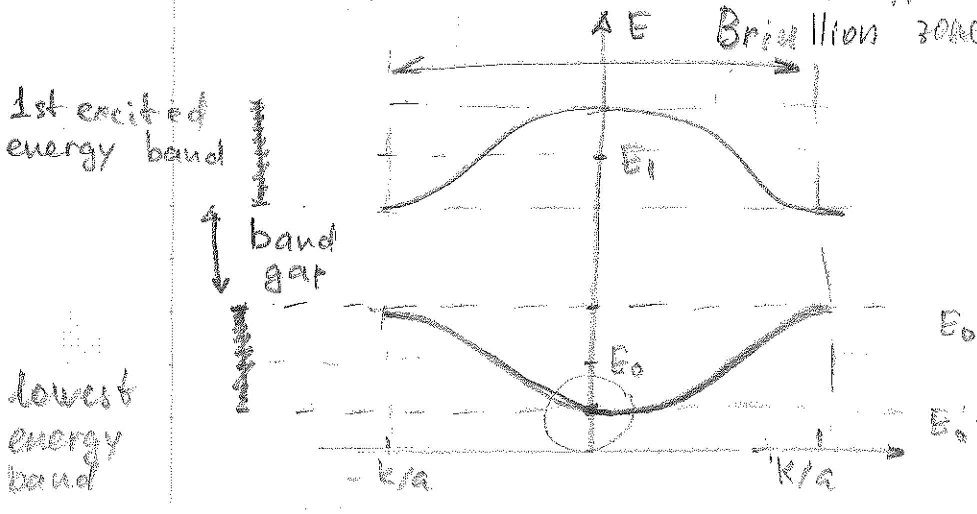
$u_k(x) = u_k(x+a)$

<u>Bloch theorem:</u> the wavefunction that respects the translational symmetry can be written as a plane wave $e^{ikx'}$ times a periodic function with periodicity a.

(The theorem holds beyond tight-binding approximation)

$$\psi_k(x) = e^{ikx}\, u_k(x)$$

$$H|\psi_k\rangle = (E_0 - 2\Delta\cos ka)|\psi_k\rangle$$



near $ka \approx 0$

$$E = (E_0 - 2\Delta) + \Delta(ka)^2 \simeq$$

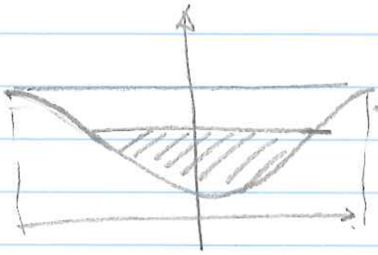
$$\simeq (E_0 - 2\Delta) + \frac{\hbar^2 k^2}{2m^*}$$

effective mass

Band structure + Pauli exclusion principle explain the conductivity in metals and insulators

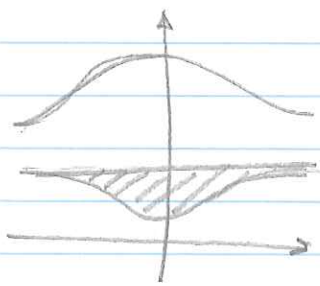
Since all electrons must have different states, we can calculate the density of states in each band. To conduct electricity electrons must be free to move → must have unoccupied k-states to jump to

Metals → partially filled energy band



available states

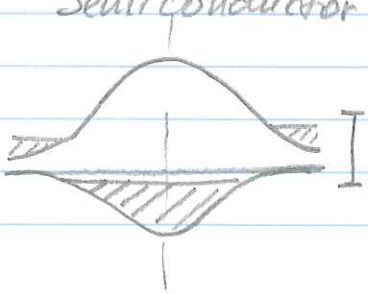
Insulators → filled energy band



no unoccupied states

the only way to produce electric current is to zap the material with enough energy to push electrons to the exited band (ΔE > bandgap)

Semiconductors



bandgap $< k_B T$