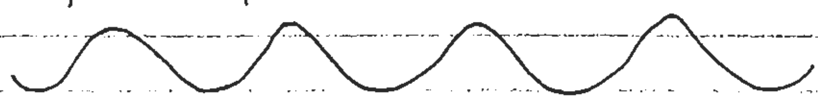
7.4 Lattice translation as a discrete symmetry

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



Ex: motion of an electron in a regular solid.

Want to understand spectrum, symmetry.

Review: translation operators

Define $\tau(l)$ through

$$\tau(l)\,|x\rangle = |x+l\rangle$$

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

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

distinguishes operator

$$= \tau(l)^{+}\,(x+l)\,|x+l\rangle$$

$$= (x+l)\,|x\rangle$$

$$\Rightarrow \quad \tau(l)^{+}\,\hat{x}\,\tau(l) = \hat{x} + l$$

$$\tau(l)\,|p\rangle = \tau(l)\int \frac{dx}{\sqrt{2\pi\hbar}}\, e^{ipx/\hbar}\,|x\rangle$$

$$= \int \frac{dx}{\sqrt{2\pi\hbar}}\, e^{ipx/\hbar}\,|x+l\rangle$$

$$= e^{-ipl/\hbar}\,|p\rangle$$

so $\tau(\ell) = e^{-i\hat{p}\ell/\hbar} = e^{-\ell\frac{\partial}{\partial x}}$

$$\tau^\dagger(\ell)\,\hat{p}\,\tau(\ell) = \hat{p}$$

For general wavefunction

$$\tau(\ell)\,|\psi\rangle = \tau(\ell)\int dx\ \psi(x)\,|x\rangle$$
$$= \int dx\ \psi(x)\,|x+\ell\rangle$$
$$= \int dy\ \psi(y-\ell)\,|y\rangle$$

$\Rightarrow$ when $|\psi'\rangle = \tau(\ell)\,|\psi\rangle$

$$\psi'(x) = \psi(x-\ell) = e^{-\ell\frac{\partial}{\partial x}}\,\psi(x).$$

For a particle in a periodic Hamiltonian $V(x+a) = V(x)$,

$$H = \frac{p^2}{2m} + V(x)$$

$$\tau^\dagger(a)\,H\,\tau(a) = \tau^\dagger(a)\,V(x+a)\,\tau(a) + \frac{p^2}{2m} = H.$$

so $[H, \tau(a)] = 0.$

<u>Group theory</u>:

Discrete translation group $\mathbb{Z}$ is generated by α,

Group elements : $\cdots,\ \alpha^{-1}\circ\alpha^{-1},\ \alpha^{-1},\ 1,\ \alpha,\ \alpha\circ\alpha,\ \alpha\circ\alpha\circ\alpha$

$\cdots\ \alpha^{-2}\ \ \alpha^{-1}\ \ \alpha^{0}\ \ \alpha^{1}\ \ \alpha^{2}\ \cdots$

$\{\alpha^n\}_{n\in\mathbb{Z}}$: $\alpha^n \circ \alpha^m = \alpha^{n+m}$

Group is free group on one element (no relations)

To find representations: diagonalize $\mathcal{D}(\alpha)$
irreps are 1-dimensional, $\mathcal{D}(\alpha) = e^{-i\theta}$ phase.

Since $[H, \tau(a)] = 0$, $\tau(a) = \mathcal{D}(\alpha)$,
can simultaneously diagonalize H, $\tau(a)$. Write $\theta = ka$.

States $|\psi_k\rangle$ satisfy

$$\tau(a)|\psi_k\rangle = e^{-ika}|\psi_k\rangle$$

$$\psi(x-a) = e^{-ika}\psi(x)$$

or $$\psi(x+a) = e^{ika}\psi(x).$$

write $\boxed{\psi(x) = e^{ikx}\tilde{\psi}(x),}$

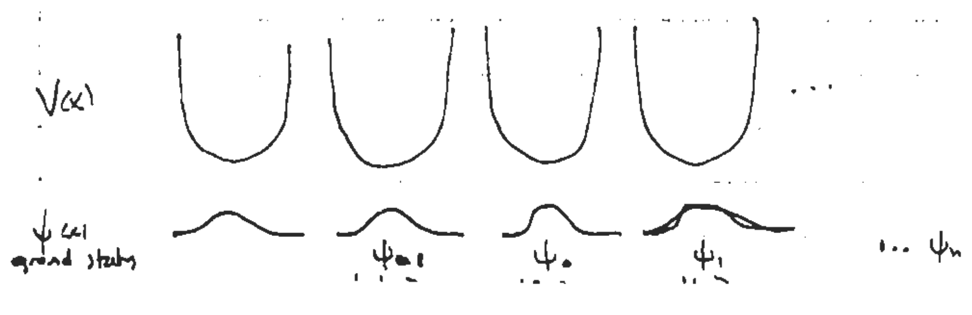
$$e^{ik(x+a)}\tilde{\psi}(x+a) = e^{ik(x+a)}\tilde{\psi}(x)$$

$$\boxed{\tilde{\psi}(x+a) = \tilde{\psi}(x)}$$

So solutions are "quasiperiodic" in $x \to x+a$

[Bloch's theorem]

<u>Example</u>: ∞ potential between sites



∞ potential localizes states in 1 region.

$$H|n_k\rangle = E_k|n_k\rangle$$

n = lattice site #
k = enegy level

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

Denote
$$|\theta_k\rangle = \frac{1}{\sqrt{2\pi}}\sum_{n=-\infty}^{\infty} e^{in\theta}|n_k\rangle$$

$$H|\theta_k\rangle = E_k|\theta_k\rangle$$

$$\tau(a)|\theta_k\rangle = \frac{1}{\sqrt{2\pi}}\sum e^{in\theta}|(n+1)_k\rangle$$
$$= e^{-i\theta}|\theta_k\rangle$$

Normalization: if $\langle n_k|m_\ell\rangle = \delta_{nm}\delta_{k\ell}$

$$\langle\theta_k|\theta'_\ell\rangle = \delta_{k\ell}\,\delta(\theta-\theta')$$

In this example, all <u>levels</u> degenerate (infinitely)

Example: free particle ($V=0$).

Consider eigenstates $|p\rangle$. $H|p\rangle = \frac{p^2}{2m}|p\rangle$.

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

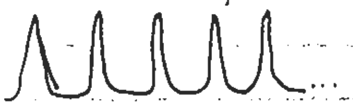
E spectrum continuous, doubly degenerate

<u>General case</u>: part way between free & localized examples.

Tight - binding approximation

A simple model:

- assume potential high, but not ∞, between lattice sites.



- associate state $|n\rangle$ with ground state of each region.

Gives lattice model

$$\langle n | n' \rangle = \delta_{nn'}$$
$$\tau |n\rangle = |n+1\rangle$$

Assume tight - binding approximation

$$\langle n' | H | n \rangle = 0 \quad \text{unless } n' \in \{n-1, n, n+1\}$$

Define $\langle n^{\pm} | H | n \rangle = -\Delta$ (assume $[\tau, H] = 0$)

$$\text{so} \quad H = \begin{pmatrix} E_0 & -\Delta & & & \\ -\Delta & E_0 & -\Delta & & 0 \\ & -\Delta & E_0 & -\Delta & \\ 0 & & -\Delta & E_0 & \ddots \\ & & & \ddots & \ddots \end{pmatrix}$$

[note: many details removed in this simple model]

Define $|\theta\rangle = \sum e^{in\theta} |n\rangle$

$$\tau |\theta\rangle = e^{-i\theta} |\theta\rangle$$

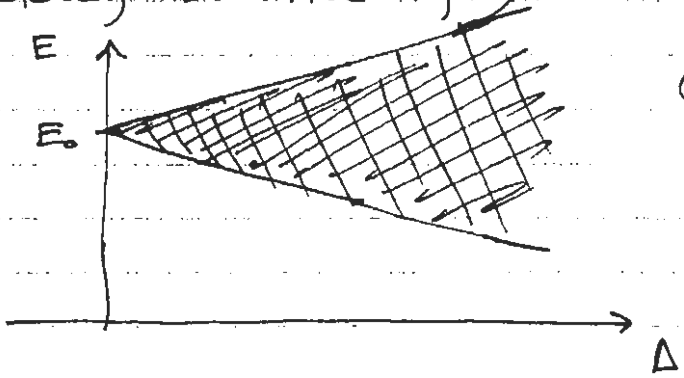
$$H|n\rangle = E_0 |n\rangle - \Delta |n-1\rangle - \Delta |n+1\rangle$$

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

$$= \left[E_0 - \Delta\left(e^{i\theta} + e^{-i\theta}\right)\right]|\theta\rangle$$

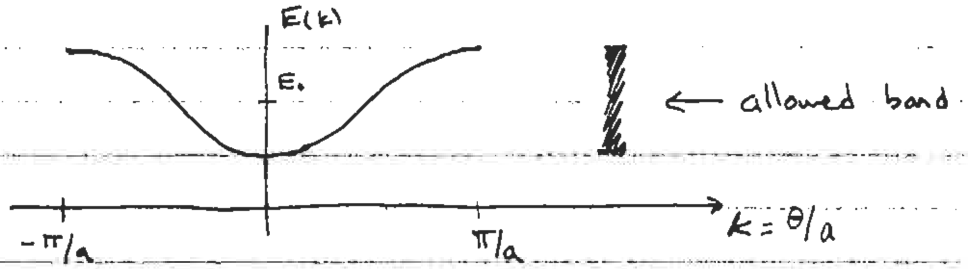
$$= \left(E_0 - 2\Delta\cos\theta\right)|\theta\rangle$$

so degeneracy is lifted by Δ

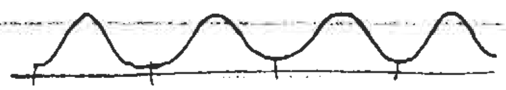


Get continuous band of E in Brillouin zone

$E_0 - 2\Delta \le E \le E_0 + 2\Delta$.

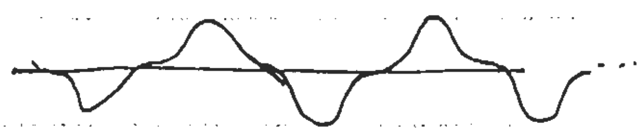


Lowest E state: $|\theta = 0\rangle$



highest E state: $|\theta = \pm\pi\rangle$

$= \sum (-1)^n |n\rangle$



Energy spectrum in general case

Want to solve $\quad H|\psi\rangle = E|\psi\rangle$

$$-\frac{\hbar^2}{2m}\psi''(x) + V(x)\,\psi(x) = E\,\psi(x),$$

$$V(x+a) = V(x).$$

2nd order eq: has 2 linearly independent solutions $\psi_1(x), \psi_2(x)$ for any E.

Periodicity $\Rightarrow$ $\psi_1(x+a)$, $\psi_2(x+a)$ also solutions.

$$\Rightarrow \quad \begin{pmatrix}\psi_1(x+a)\\ \psi_2(x+a)\end{pmatrix} = \begin{pmatrix}A_{11} & A_{12}\\ A_{21} & A_{22}\end{pmatrix}\begin{pmatrix}\psi_1(x)\\ \psi_2(x)\end{pmatrix}$$

$$A = \begin{pmatrix}A_{11} & A_{12}\\ A_{21} & A_{22}\end{pmatrix} \quad : \quad \underline{\text{transfer matrix}}$$

ψ_1, ψ_2 real @ ϕ $\Rightarrow$ A real.

Diagonalize A:

$$\phi_1(x+a) = \lambda_1\,\phi_1(x)$$
$$\phi_2(x+a) = \lambda_2\,\phi_2(x).$$

λ_1, λ_2 eigenvalues of A.

Eq. for λ: $\quad \det(A - \lambda\mathbb{1}) = 0$

$$(A_{11}-\lambda)(A_{22}-\lambda) - A_{12}A_{21} = 0$$

$$\lambda^2 - (A_{11} + A_{22})\lambda + (A_{11}A_{22} - A_{12}A_{21}) = 0$$

$$\lambda^2 - (\mathrm{Tr}\,A)\,\lambda + \det A = 0$$

$$\Rightarrow \quad \lambda = \left[\mathrm{Tr}\,A \pm \sqrt{(\mathrm{Tr}\,A)^2 - 4\det A}\,\right]/2.$$

So either $\boxed{\begin{array}{ll} a) & \lambda_1, \lambda_2 \text{ both real} \\ b) & \lambda_1 = \lambda_2^*. \end{array}}$

Now: $\frac{d}{dx}(\phi_1\phi_2' - \phi_2\phi_1') = \phi_1\phi_2'' - \phi_1''\phi_2 = 0$

so $(\phi_1\phi_2' - \phi_2\phi_1')_{x+a} = (\phi_1\phi_2' - \phi_2\phi_1')_x$

$$= \lambda_1\lambda_2(\phi_1\phi_2' - \phi_2\phi_1')_x$$

so $\boxed{\lambda_1\lambda_2 = 1}$

If λ_1, λ_2 both real, $\lambda_1 = \frac{1}{\lambda_2}$.

Unless (a) and (b), then both ϕ_1, ϕ_2 grow exponentially
— unphysical nonnormalizable solutions.

If $\lambda_1 = \lambda_2^*$, then ϕ_1, ϕ_2 are quasiperiodic.
— physical solutions, normalization like $|p\rangle$ states.

λ's are a function of E, determined through A.

When a), $\lambda + \frac{1}{\lambda} = \mathrm{Tr}\,A \geq 2$

When b), $\lambda_1 + \lambda_2 = \mathrm{Tr}A = e^{i\alpha} + e^{-i\alpha} = 2\cos\alpha \leq 2.$

Thus, allowed energy bands are in regions where

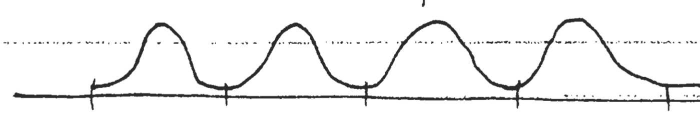
$$\boxed{\mathrm{Tr}\, A \leq 2} \qquad \text{(allowed bands)}$$

Crossover points: $A = \pm \mathbb{1}$, $\phi_i(x+a) = \pm \phi_i(x)$,
exactly periodic or antiperiodic sol'ns

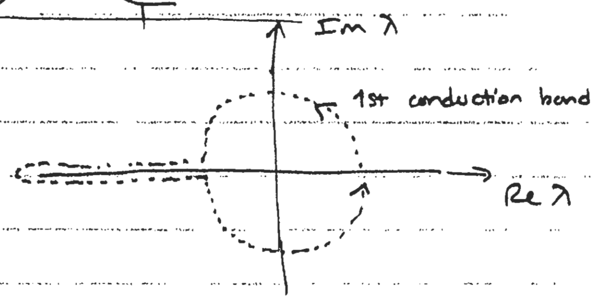
Qualitative description of square well potential

First band:

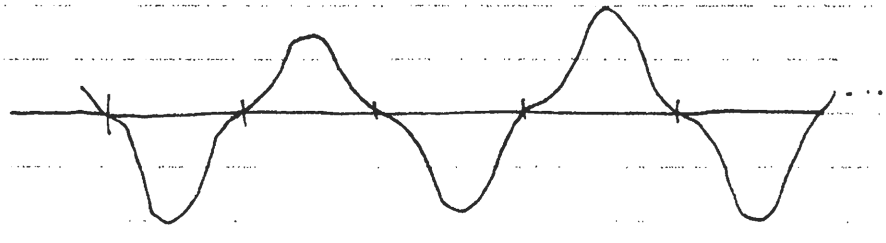
lowest state: $\lambda = 1$ periodic



Follow λ in $\mathbb{C}$

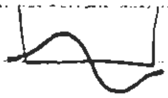


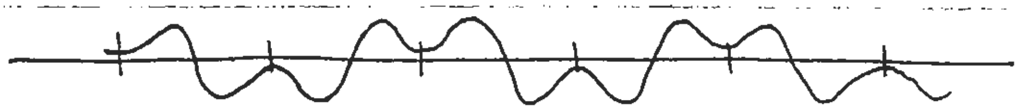
highest state $\lambda = -1$
— flips sign of ground state



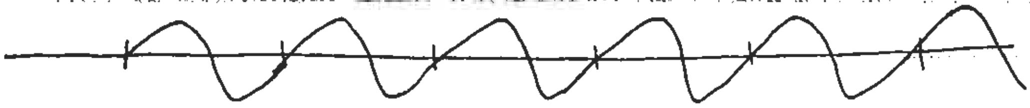
Second band:

lowest state: $\lambda = -1$,

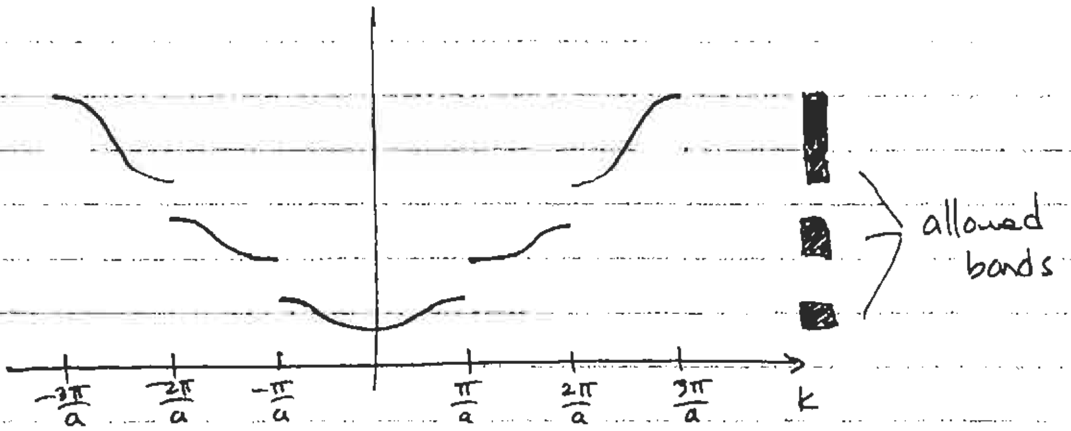
connects  in each well.



highest state: $\lambda = +1$



Spectrum



As height $\to 0$, approaches free spectrum

This is general form of result for any periodic potential
[HW: Kronig - Penney potential]

So far: considered 1 electron. Want to generalize $\longrightarrow$ many electrons.

Allowed band full: insulator: allowed band partly full: conductor