Symmetries in QM (Sakurai Chapter 4)

Classically: Hamiltonian $H(\underbrace{q_1, \dots q_N}_{\text{generalized coordinates}}, \underbrace{p_1, \dots, p_N}_{\text{conjugate momenta}}, t)$

Hamilton's equations: $\frac{\partial H}{\partial p_i} = \dot{q}_i$ and $\frac{\partial H}{\partial q_i} = -\dot{p}_i$.

If H doesn't depend on q_i (has a symmetry under $q_i \to q_i + \delta q_i$), then $\boxed{\dot{p}_i = 0}$. p_i is a conserved quantity.

In QM, symmetries $\leftrightarrow$ unitary operators $\mathcal{U}$.

For symmetries close to the identity (translations, rotations, ...)

$\mathcal{U} = 1 - \frac{i\varepsilon}{\hbar} G$ $\qquad$ G = generator of the symmetry, Hermitian

H is invariant under symmetry $\leftrightarrow$ $\mathcal{U}^\dagger H \mathcal{U} = H$.

This implies $[G, H] = 0$.

In the Heisenberg picture, $\frac{dA^{(H)}}{dt} = \frac{1}{i\hbar}[A^{(H)}, H]$.

So $[G^{(H)}, H] = 0 \Rightarrow \frac{dG^{(H)}}{dt} = 0$

But $G^{(H)} = e^{+iHt/\hbar} G^{(S)} e^{-iHt/\hbar} = G^{(S)}$.

So G is the same in both Schrodinger + Heisenberg pictures, so

$\boxed{\frac{dG}{dt} = 0}$ conserved operator.

Suppose $|\Psi(t_0)\rangle$ is an e-state of G: $\quad G|\Psi(t_0)\rangle = g|\Psi(t_0)\rangle$

At a later time t, $|\Psi(t)\rangle = \underbrace{e^{-iH(t-t_0)/\hbar}}_{U(t,t_0) = \text{time-evolution operator}} |\Psi(t_0)\rangle$

Then $G|\Psi(t)\rangle = U(t,t_0) G |\Psi(t_0)\rangle = U(t,t_0) g |\Psi(t_0)\rangle = g|\Psi(t)\rangle$.

Still an e-state, same e-value.

Suppose $|n\rangle$ is an energy eigenstate: $H|n\rangle = E_n|n\rangle$.

If $\mathcal{U}$ is a symmetry operator, then:

$$H(\mathcal{U}|n\rangle) \underset{[H,\mathcal{U}]=0}{=} \mathcal{U}H|n\rangle = E_n(\mathcal{U}|n\rangle).$$

So, if $|n\rangle$ and $\mathcal{U}|n\rangle$ are different states; then they're degenerate.

Example: Rotations $[\mathcal{D}(R), H] = 0$.

The corresponding generators are $\vec{J}$ (play the role of G above).

So $[J_z, H] = 0$, and $[J^2, H] = 0$, and $[J_z, J^2] = 0$.

States can be labelled by $|n, j, m_j\rangle$.

Since $\mathcal{D}(R)|n, j, m_j\rangle = \sum_{m'} |n, j, m'\rangle \mathcal{D}^{(j)}_{mm'}(R)$ for any rotation R,

all states $|n, j, m_j\rangle$ for different m_j have same energy.

$\Rightarrow$ $(2j+1)$-fold degeneracy.

We saw this repeatedly for H atom:

* Fine structure: $(2j+1)$ degeneracy for $\vec{J} = \vec{L} + \vec{S}$.
* Hyperfine: $(2f+1)$ degeneracy for $\vec{F} = \vec{L} + \vec{S} + \vec{I}$.

To destroy the degeneracy, impose an external special direction ($\vec{B}_{ext}$ or $\vec{E}_{ext}$). Then $[\vec{J}, \vec{H}] \neq 0$, no $2j+1$ degeneracy.

Parity = space inversion = discrete symmetry

Define a parity operator by its action on the basis of position eigenstates:

$$\pi|\vec{r}\rangle = |-\vec{r}\rangle$$

Now consider $\pi \underbrace{\vec{R}}_{\text{operator}} |\vec{r}\rangle = \pi \underbrace{\vec{r}}_{\text{number}} |\vec{r}\rangle = \vec{r}\,\pi|\vec{r}\rangle = \vec{r}\,|-\vec{r}\rangle.$

But also: $= \underbrace{\{\pi,\vec{R}\}}_{\text{anticommutator}}|\vec{r}\rangle - \vec{R}\pi|\vec{r}\rangle = \{\pi,\vec{R}\}|\vec{r}\rangle - \vec{R}|-\vec{r}\rangle = \{\pi,\vec{R}\}|\vec{r}\rangle + \vec{r}|-\vec{r}\rangle$

So $\{\pi,\vec{R}\} = 0$, acting on <u>all</u> states $|\vec{r}\rangle$.

So $\boxed{\vec{R}\pi = -\pi\vec{R}}$ or $\pi^{-1}\vec{R}\pi = -\vec{R}$ or, since π is unitary,

$$\boxed{\pi^{+}\vec{R}\pi = \pi\vec{R}\pi^{+} = -\vec{R}}$$

For a general state $|\Psi\rangle$, parity operation takes $|\Psi\rangle \to \pi|\Psi\rangle$.

So $(\langle\Psi|\pi^{+})\vec{R}(\pi|\Psi\rangle) = \langle\Psi|(\pi^{+}\vec{R}\pi)|\Psi\rangle = -\langle\Psi|\vec{R}|\Psi\rangle$

Parity flips the sign of $\langle\Psi|\vec{R}|\Psi\rangle$.
(Sakurai uses this as his defining property.)

Also $\pi^2|\vec{r}\rangle = \pi|-\vec{r}\rangle = |+\vec{r}\rangle$ for all $\vec{r}$.

So $\pi^2 = 1$. Therefore, $\boxed{\pi^{-1} = \pi^{+} = \pi}$ unitary and Hermitian.

Also, $\boxed{\{\pi,\vec{P}\} = 0 \quad \text{or} \quad \pi^{+}\vec{P}\pi = -\vec{P}}$

(Taking $\vec{r}\to-\vec{r}$ also takes $\vec{\nabla}\to-\vec{\nabla}$. ✓)

Also $\boxed{[\pi,\vec{L}] = 0 \quad \text{or} \quad \pi^{+}\vec{L}\pi = \vec{L}}$

(Follows from $\vec{L} = \vec{R}\times\vec{P}$.)

What about spin? $\vec{S} \neq \vec{R}\times\vec{P}$.

Consider rotations of coordinates:

$$\begin{pmatrix}x\\y\\z\end{pmatrix} \to \begin{pmatrix}x'\\y'\\z'\end{pmatrix} = \underbrace{R^{(rot)}}_{3\times3\text{ matrix}}\begin{pmatrix}x\\y\\z\end{pmatrix}$$

Parity is also represented by a 3x3 matrix on coordinates:

$$\begin{pmatrix} x \\ y \\ z \end{pmatrix} \rightarrow \begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = R^{(par)} \begin{pmatrix} x \\ y \\ z \end{pmatrix} \qquad R^{(par)} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

commutes with all 3x3 matrices

So $R^{(par)} R^{(rot)} = R^{(rot)} R^{(par)}$.

In QM, require operators that represent these symmetries to obey same rule:

$\pi \mathcal{D}(R) = \mathcal{D}(R) \pi$ for any rotation R.

But $\mathcal{D}(R) = 1 - i \vec{J} \cdot \hat{n} \frac{\varepsilon}{\hbar}$ for infinitesimal rotation $\begin{cases} \text{around axis } \hat{n}, \\ \text{angle } \varepsilon \end{cases}$.

$$\Rightarrow \boxed{[\pi, \vec{J}] = 0 \Rightarrow \pi^\dagger \vec{J} \pi = \vec{J}}$$

for total angular momentum $\vec{J} = \vec{L} + \vec{S}$. So $[\pi, \vec{S}] = 0$ also.

Vectors are odd under parity: $\pi \vec{V} \pi = -\vec{V}$.

examples: $\vec{R}, \vec{P}, \vec{E}$ (electric field), $\vec{A}$ (vector potential)

Axial vectors are even under parity. $\pi \vec{P} \pi = +\vec{P}$.

examples: $\vec{L}, \vec{S}, \vec{J}, \vec{B}$ (magnetic field)

a.k.a. "pseudovectors"

What about dot products?

$$\left.\begin{aligned} \pi^\dagger \vec{L} \cdot \vec{S} \, \pi &= +\vec{L} \cdot \vec{S} \\ \pi^\dagger \vec{R} \cdot \vec{P} \, \pi &= +\vec{R} \cdot \vec{P} \\ \pi^\dagger \vec{P} \cdot \vec{P} \, \pi &= +\vec{P} \cdot \vec{P} \end{aligned}\right\} \quad \left.\begin{aligned} &\text{vector} \cdot \text{vector} \\ &(\text{axial vector}) \cdot (\text{axial vector}) \end{aligned}\right\} \quad \begin{aligned} &\text{even under parity} \\ &\underline{\text{scalars}} \end{aligned}$$

$$\text{But:} \quad \left.\begin{aligned} \pi^\dagger \vec{L} \cdot \vec{R} \pi &= -\vec{L} \cdot \vec{R} \\ \pi^\dagger \vec{B} \cdot \vec{E} \pi &= -\vec{B} \cdot \vec{E} \end{aligned}\right\} \quad (\text{vector}) \cdot (\text{axial vector}) \qquad \begin{aligned} &\underline{\text{odd}} \text{ under parity} \\ &\underline{\text{pseudoscalars}}. \end{aligned}$$

What are the eigenvalues of parity?

Suppose $\pi|\lambda\rangle = \lambda|\lambda\rangle$. Then $\pi^2|\lambda\rangle = \pi\lambda|\lambda\rangle = \lambda^2|\lambda\rangle$

But $\pi^2 = 1$. So $\lambda^2 = 1 \Rightarrow \lambda = \pm 1$.

<u>Wave functions under parity</u>

$\langle\vec{r}|\psi\rangle = \psi(\vec{r})$ = position-space wavefunction

$\pi|\psi\rangle$ has wavefunction $\langle\vec{r}|\pi|\psi\rangle = \langle -\vec{r}|\psi\rangle = \psi(-\vec{r})$.

If $|\psi\rangle$ is an eigenstate of parity, then $\pi|\psi\rangle = \pm|\psi\rangle$.

So
$$\begin{array}{c} \langle\vec{r}|\pi|\psi\rangle = \pm\langle\vec{r}|\psi\rangle = \pm\psi(\vec{r}) \\ \| \\ \langle -\vec{r}|\psi\rangle = \psi(-\vec{r}). \end{array}$$

So $\psi(-\vec{r}) = \pm\psi(\vec{r})$ $\begin{cases}\text{even parity state} \\ \text{odd parity state}\end{cases}$ <u>if</u> an eigenstate of parity.

$\vec{P}$ and π <u>don't</u> commute, so plane waves $e^{i\vec{p}\cdot\vec{r}/\hbar}$ <u>aren't</u> parity eigenstates.

$\vec{L}$ and π <u>do</u> commute, so can choose simultaneous e-states.

Consider wavefunctions of such states:

$$\langle\vec{r}|\alpha;\ell,m\rangle = R_\alpha(r)\,Y_{\ell m}(\theta,\phi) = \psi_{\alpha;\ell,m}(\vec{r})$$

α = extra label(s) (= n for H atom)

Parity:
$$\begin{cases} r \to r & \\ \theta \to \pi - \theta & \text{so } \cos\theta \to -\cos\theta \\ \phi \to \phi + \pi & \text{so } e^{im\phi} \to (-1)^m e^{im\phi} \end{cases}$$

Consider $m=0$ states first:

$$Y_{\ell 0}(\theta,\phi) = \underbrace{\sqrt{\frac{2\ell+1}{4\pi}}\;\frac{(-1)^\ell}{2^\ell \ell!}}_{\to \text{ same under parity}}\;\underbrace{\left(\frac{d}{d(\cos\theta)}\right)^\ell}_{\to \left(\frac{d}{d(-\cos\theta)}\right)^\ell = (-1)^\ell \times \text{same}}\;\underbrace{(\sin^2\theta)^\ell}_{= (1-\cos^2\theta)^\ell \to \text{ same}}$$

So, under parity, $\vec{r} \to -\vec{r}$, $\quad Y_{\ell 0}(\theta,\phi) \to (-1)^\ell \, Y_{\ell 0}(\theta,\phi)$.

So $|\alpha; \ell, 0\rangle$ has $\begin{cases} \text{odd parity for } \ell \text{ odd} \\ \text{even " " } \ell \text{ even} \end{cases}$

But states with $m \neq 0$ are obtained by acting with $L_\pm$, and $[L_\pm, \pi] = 0$.

So $\boxed{|\alpha; \ell, m\rangle \text{ has parity } (-1)^\ell}$ (for any α, m).

Does the Hamiltonian of the universe commute with parity?

gravity ✓

EM ✓

strong nuclear force (QCD) ✓

$\underbrace{\text{weak nuclear force}}_{\text{known in early 20th century}}$ (β-decays, neutrino interactions) <u>NO</u>.

found in 1956
Lee & Yang theory
Wu experiment

Left-spin quarks, leptons, neutrinos interact with W bosons
Right-spin " " " don't (at all).

But LH and RH spins are related by parity.

Left-spin anti-quarks, anti-leptons, antineutrinos don't interact with W bosons
Right-spin " " " do.

But, ignoring weak interactions, H_{universe} commutes with π.

However, H for an isolated sub-system may or may not.

Suppose $[H, \pi] = 0$. Then if $|n\rangle$ is a <u>non-degenerate</u> e-state of H, then it is also a parity e-state.

Proof: $H|n\rangle = E_n|n\rangle$. Now consider the two states:

$\frac{1}{2}(1 \pm \pi)|n\rangle$. They are parity eigenstates:

$$\pi \, \tfrac{1}{2}(1 \pm \pi)|n\rangle = \tfrac{1}{2}(\pi \pm \pi^2)|n\rangle = \tfrac{1}{2}(\pi \pm 1)|n\rangle = \pm\left(\tfrac{1}{2}(1 \pm \pi)|n\rangle\right).$$

But also: $H\left(\frac{1}{2}(1\pm\pi)\right)|n\rangle = \frac{1}{2}(1\pm\pi)H|n\rangle = E_n \frac{1}{2}(1\pm\pi)|n\rangle$.

So we have three alleged states; $|n\rangle$, $\frac{1}{2}(1+\pi)|n\rangle$, $\frac{1}{2}(1-\pi)|n\rangle$ all with the same energy E_n.

definitely different; have different parity.

This contradicts the non-degeneracy assumption, unless $|n\rangle$ and one of $\frac{1}{2}(1\pm\pi)|n\rangle$ are actually the <u>same</u> state, and the other of $\frac{1}{2}(1\pm\pi)|n\rangle = 0$ (null ket, not a state).

So $|n\rangle$ has parity $+1$ or -1.

<u>Examples</u> * 1-d harmonic oscillator: $\psi_0(x) \sim e^{-x^2/2x_0^2} \Rightarrow$ parity $+1$.

$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2$ commutes with π.

For excited states $(a^\dagger)^n|0\rangle$, parity is $(-1)^n$, because $a^\dagger$ = linear combination of X, P.

* H atom: ground state is non-degenerate

$\psi(\vec{r}) = \frac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0}$ is parity $+1$ ($\vec{r} \to -\vec{r}$ means $r \to r$).

The (n,l,m) state has parity $(-1)^l$, even though degenerate.

But $c|2,0,0\rangle + c'|2,1,0\rangle$ is not a parity e-state, although it is an energy e-state (neglecting fine structure)

* Momentum eigenstates: $\langle\vec{r}|\vec{p}\rangle = e^{i\vec{p}\cdot\vec{r}/\hbar}$. So $|\vec{p}\rangle$ aren't π e-states.

They are energy eigenstates of $H = \frac{p^2}{2m}$, but degenerate, since $|\vec{p}\rangle$ and $\mathcal{D}(R)|\vec{p}\rangle$ have same energy.

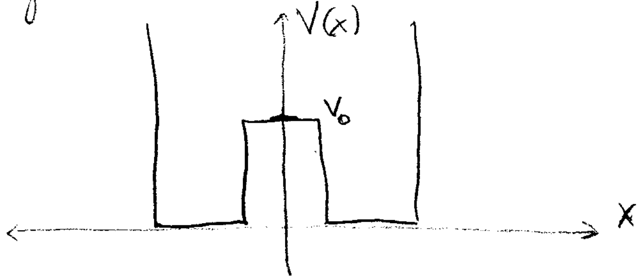
However, $\underbrace{|\vec{p}\rangle + |-\vec{p}\rangle}_{\text{parity } +1}$ and $\underbrace{|\vec{p}\rangle - |-\vec{p}\rangle}_{\text{parity } -1}$ are π-eigenstates

* Symmetric potentials in 1-d (and spherically-symmetric in 3d)

$\Rightarrow H = \frac{p^2}{2m} + V(|x|)$. (or $H = \frac{p^2}{2m} + V(r)$)

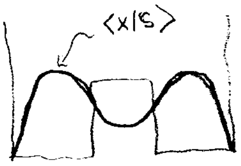
commute with parity.

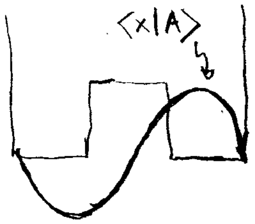
Double well potential:



The ground state $|S\rangle$ is symmetric, 1st excited state $|A\rangle$ antisymmetric

parity +1 — parity −1





$$E_S < E_A$$

Both states have equal probability for particle to be found on the left or right. $\mathcal{P}(x) = |\langle x|S\rangle|^2$ or $|\langle x|A\rangle|^2$

Define $|R\rangle = \frac{1}{\sqrt{2}}(|S\rangle + |A\rangle)$ (peaked for $x > 0$)

$|L\rangle = \frac{1}{\sqrt{2}}(|S\rangle - |A\rangle)$ (peaked for $x < 0$)

$\pi|R\rangle = |L\rangle$ and $\pi|L\rangle = |R\rangle$.

Suppose we prepare a state $|\Psi_{RO}(t)\rangle$ so that $|\Psi_{RO}(0)\rangle = |R\rangle$.

What is this state for later times t?

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

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

$= |R\rangle$ at $t = 0, \frac{2\pi\hbar}{E_A - E_S}, \frac{4\pi\hbar}{E_A - E_S}, \ldots$

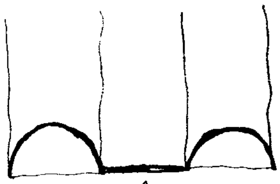
$= |L\rangle$ at $t = \frac{\pi\hbar}{E_A - E_S}, \frac{3\pi\hbar}{E_A - E_S}, \ldots$

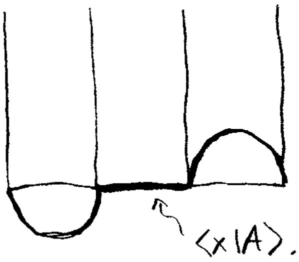
Angular frequency of oscillation $|R\rangle \leftrightarrow |L\rangle$ is:

$$\omega_{RL} = \frac{2\pi\hbar}{E_A - E_S}.$$

What happens if barrier height $V_0 \to \infty$?

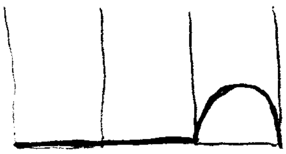
Then $E_A - E_S \to 0$:



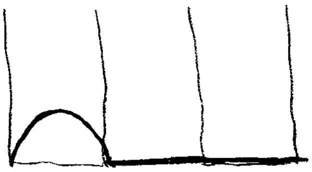


$\omega_{RL} \to 0$, oscillation time $T_{RL} = \frac{2\pi}{\omega_{RL}} \to \infty$

So the degenerate ground states could be taken as $|R\rangle$ and $|L\rangle$



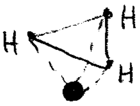
and



Classic example in 3-d: ammonia molecule NH_3:

(like $|R\rangle$)

and



(like $|L\rangle$)

barrier between configurations.

$$\frac{\omega_{flip}}{2\pi} \approx 2{,}4 \times 10^{10} \text{ Hz} \quad = \text{microwave}$$

Many molecules have 2 nearly degenerate parity eigenstates = "optical isomers". (For example, sugar.)

Organisms use superposition with definite handedness (R or L) rather than definite parity.

$1/\omega_{flip} \gg$ years, if barrier is high enough.

Selection Rules

Consider any two states $|\alpha\rangle$, $|\beta\rangle$, each of definite parity.

$\pi|\alpha\rangle = \lambda_\alpha|\alpha\rangle \qquad \pi|\beta\rangle = \lambda_\beta|\beta\rangle$ where $\lambda_\alpha, \lambda_\beta = \pm 1$.

Then: $\langle\beta|\vec{R}|\alpha\rangle \neq 0$ requires $\lambda_\alpha\lambda_\beta = -1$.

Proof: $\langle\beta|\vec{R}|\alpha\rangle = \underbrace{\langle\beta|\pi}_{\lambda_\beta\langle\beta|}\underbrace{\pi\vec{R}\pi}_{-\vec{R}}\underbrace{\pi|\alpha\rangle}_{\lambda_\alpha|\alpha\rangle} = -\lambda_\alpha\lambda_\beta\langle\beta|\vec{R}|\alpha\rangle$.

Alternatively: $\int d^3\vec{r}\ \psi_\beta^*(\vec{r})\,\vec{r}\,\psi_\alpha(\vec{r}) \neq 0$ requires $\lambda_\alpha\lambda_\beta = -1$.

We've seen that in the electric dipole approximation for absorption or emission of light:

$$(\text{rate}) \propto |\langle f|\vec{R}|i\rangle|^2$$

So the transition requires $|i\rangle$ and $|f\rangle$ to have opposite parity.

For eigenstates of L^2, L_z, this requires:

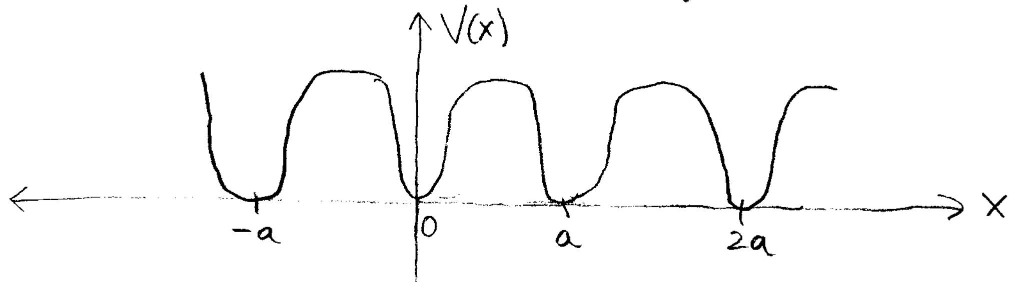
$(-1)^{\ell_i+\ell_f} = -1$, or $\boxed{\ell_i+\ell_f = \text{odd}}$.

For example, on HW4, Problem 1, you will compute the $2p \to 1s$ rate. This is allowed by the parity selection rule.

In contrast, $2s \to 1s$ isn't allowed. (Don't calculate it.)

Lattice Translation (a discrete symmetry)

Consider potentials (in 1-d) satisfying $V(x+a) = V(x)$.



Let $\tau(\ell)$ be the translation operator for $x \to x+\ell$, so:

$$\tau(\ell)|x\rangle = |x+\ell\rangle, \quad \text{and} \quad \tau^\dagger(\ell)X\tau(\ell) = X+\ell,$$

operator

and $\tau^\dagger(\ell) = \tau^{-1}(\ell) = \tau(-\ell)$.

Then $\tau^\dagger(a)V(x)\tau(a) = V(x+a) = V(x)$.

Also $\tau^\dagger(a)\frac{P^2}{2m}\tau(a) = \frac{P^2}{2m}$ (recall $P^2 \Leftrightarrow -\hbar^2\frac{\partial^2}{\partial x^2}$)

So $\tau^\dagger(a)H\tau(a) = H$. Therefore, $H\tau(a) = \tau(a)H$, so

$\boxed{[\tau(a), H] = 0}$ $\Rightarrow$ H and $\tau(a)$ have simultaneous eigenstates.

Since $\tau(a)$ is unitary, has eigenvalues $= e^{i\theta}$.

Proof: if $|\psi\rangle$ is an eigenstate with eigenvalue λ, then

$$\underbrace{\tau^\dagger(a)\tau(a)}_{=1}|\psi\rangle = \tau^\dagger(a)\lambda|\psi\rangle = \lambda\lambda^*|\psi\rangle \quad \Rightarrow \quad |\lambda|^2 = 1.$$

Now consider states $|n\rangle$ that are localized at $x = na$

(the nth site = local minimum of $V(x)$.)

Then $\tau(a)|n\rangle = |n+1\rangle$ (not eigenstates of translation)

Let $\langle n|H|n\rangle = E_0$ But $|n\rangle$ not an eigenstate of H.

Assume also $\langle n\pm1|H|n\rangle = -\Delta$.

This is a coupling between particles in nearest neighbor sites.

Also, assume $\langle n\pm2|H|n\rangle = \langle n\pm3|H|n\rangle = \ldots = 0$.

Non-neighbor sites don't couple. This is the "Tight-binding approximation"

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

To find energy eigenstates, consider:

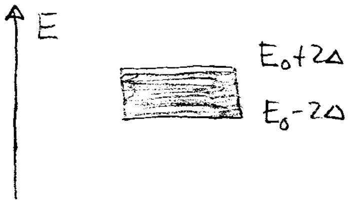
$$|\theta\rangle = \sum_{n=-\infty}^{\infty} e^{in\theta}|n\rangle \qquad \text{for real numbers } \theta.$$

Claim: each $|\theta\rangle$ is a simultaneous eigenstate of $\tau(a)$ and H.

Proof:
$$\tau(a)|\theta\rangle = \sum_{n=-\infty}^{\infty} e^{in\theta}\,\tau(a)|n\rangle = \sum_{n=-\infty}^{\infty} e^{in\theta}|n+1\rangle$$
$$= \sum_{n'=-\infty}^{\infty} e^{i(n'-1)\theta}|n'\rangle = e^{-i\theta}|\theta\rangle \quad \checkmark$$

$$H|\theta\rangle = \sum_{n=-\infty}^{\infty} e^{in\theta} H|n\rangle = \sum_{n=-\infty}^{\infty} e^{in\theta}\left[E_0|n\rangle - \Delta|n+1\rangle - \Delta|n-1\rangle\right]$$
$$= E_0\sum_{n=-\infty}^{\infty} e^{in\theta} - \Delta\sum_{n'=-\infty}^{\infty} e^{i(n'-1)\theta}|n'\rangle - \Delta\sum_{n'=-\infty}^{\infty} e^{i(n'+1)\theta}|n'\rangle$$
$$= \left(E_0 - \Delta e^{-i\theta} - \Delta e^{i\theta}\right)|\theta\rangle$$
$$= \left(E_0 - 2\Delta\cos\theta\right)|\theta\rangle \quad \checkmark$$

So we get continuous energies $E_0 - 2\Delta < E < E_0 + 2\Delta$



Consider the corresponding wavefunctions $\psi_\theta(x) = \langle x|\theta\rangle$.

For the translated state, $\tau(a)|\theta\rangle$, the wavefunction is

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

Solutions: $\psi_\theta(x) = e^{ikx}u_k(x)$ where $\begin{cases} k = \theta/a \\ u_k(x) = u_k(x+a) \quad \text{(periodic)} \end{cases}$

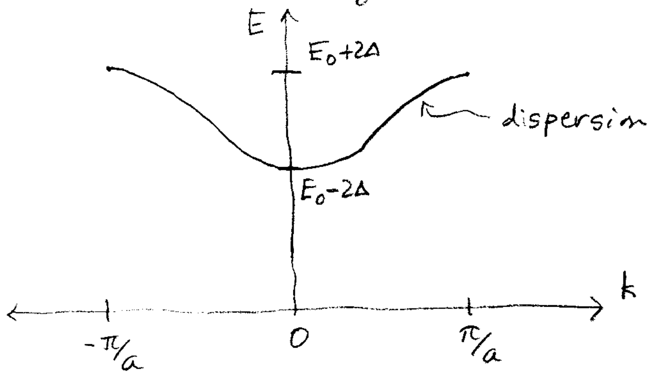
This has $\begin{cases} \text{energy } E = E_0 - 2\Delta\cos(ka). \\ \text{wave-vector } k \text{ (as if plane wave), multiplied by periodic function.} \end{cases}$

$u_k(x)$ still needs to be solved for, on a case-by-case basis.

The solutions $\boxed{\psi_k(x) = e^{ikx} u_k(x)}$ (with $u_k(x) = u_k(x+a)$) are called Bloch waves. This form is valid even if the tight-binding approximation isn't.

Since $\theta \to \theta + 2\pi$ gives the same state, the physical range for k is $\boxed{-\frac{\pi}{a} < k < \pi/a}$.

For the tight-binding model:



Let's do an example: <u>the 1-d Kronig-Penney model</u>. (Baym p. 118; not in Sakurai.)

$$V(x) = \sum_{n=-\infty}^{\infty} V_0\, \delta(x-na)$$

Goal: solve for $u_k(x)$, allowed energies E. (Not a tight-binding model.)

Consider the range $0<x<a$, for which $V=0$, $H = \frac{P^2}{2m}$.

So the solutions there are $\psi_k(x) = Ae^{iqx} + Be^{-iqx}$, where $q = \frac{\sqrt{2mE}}{\hbar}$.

so that $E = \frac{\hbar^2 q^2}{2m}$. Therefore,

$$u_k(x) = Ae^{i(q-k)x} + Be^{-i(q+k)x}.$$

Now require $u_k(x)$ is continuous and periodic

$u_k(0) = A+B$ and $u_k(a) = Ae^{i(q-k)a} + Be^{-i(q+k)a}$ must match.

So $\boxed{A+B = Ae^{i(q-k)a} + Be^{-i(q+k)a}}$

Can now solve for B in terms of A: $B = A\dfrac{[e^{i(q-k)a} - 1]}{[1 - e^{-i(q+k)a}]}$.

The coefficient A is then an arbitrary normalization.

Now look at Schrodinger equation near lattice sites:

$$\left[E + \frac{\hbar^2}{2m}\frac{d^2}{dx^2} - \sum_{n=-\infty}^{\infty} V_0\,\delta(x-na)\right]\psi_k(x) = 0.$$

Integrate both sides from $x=-\epsilon$ to ϵ, (small ϵ):

$$\underbrace{E\int_{-\epsilon}^{\epsilon}\psi_k(x)\,dx}_{\to 0 \text{ as } \epsilon\to 0} + \frac{\hbar^2}{2m}\left[\underbrace{\left.\frac{d\psi_k}{dx}\right|_{x=\epsilon}}_{\to iq(A-B)} - \underbrace{\left.\frac{d\psi_k}{dx}\right|_{x=-\epsilon}}_{=e^{-ika}\left.\frac{d\psi_k}{dx}\right|_{x=a-\epsilon}}\right] - V_0\underbrace{\psi_k(0)}_{=A+B} = 0$$

$$\to e^{-ika}\, iq\left(Ae^{iqx} - Be^{-iqa}\right)$$

So $\frac{\hbar^2}{2m} iq\left(A - B - Ae^{i(q-k)a} + Be^{-i(q+k)a}\right) - V_0(A+B) = 0$

Plug in solution for B, simplify:

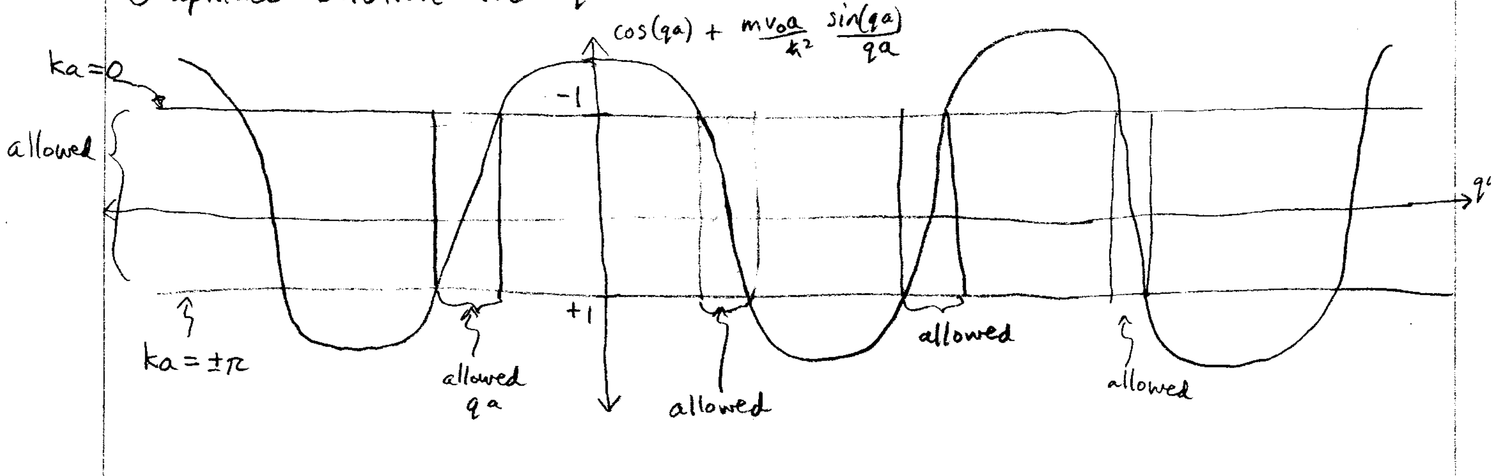
$$\left[\cos(ka) - \cos(qa) - \frac{mV_0}{q\hbar^2}\sin(qa)\right]A = 0$$

So $\boxed{\cos(ka) = \cos(qa) + \frac{mV_0 a}{\hbar^2}\frac{\sin(qa)}{qa}}$

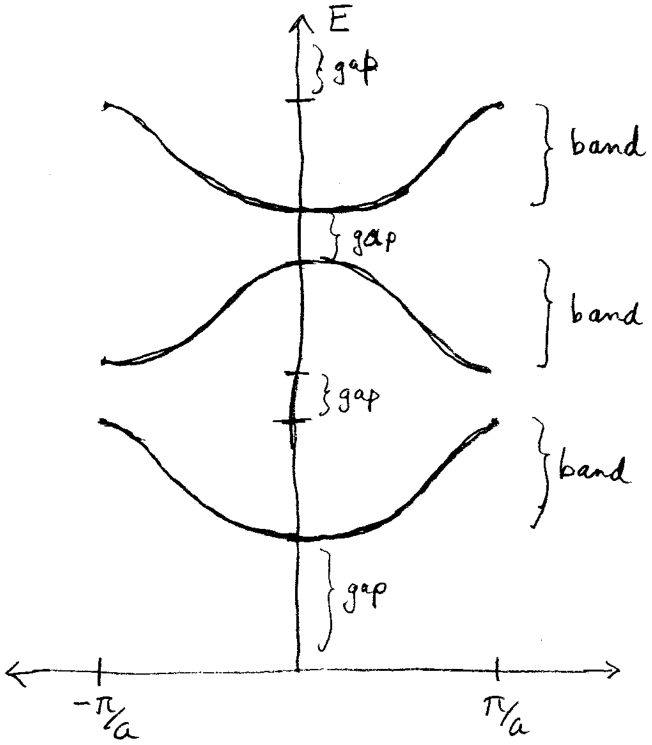
This can be solved (in principle) for q, given k.

Recall $-\frac{\pi}{a} < k < \pi/a$, so $-1 < \cos(ka) < 1$

Graphical solution for qa:



After solving for q in terms of k (numerically), $E = \frac{\hbar^2 q^2}{2m}$



Get bands of allowed energies, with gaps in between.

The lowest band is (qualitatively) like the tight-binding approximation.

This is typical of electron energies in solids with crystal structure.

In 3-d, lattice translations can be much more complicated.
(face-centered cubic, body centered cubic, rectangular but not cubic, tetrahedral, ...)

Bloch waves in 3-d:

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

where $u_{\vec{k}}(\vec{r})$ has the same translation invariances as the lattice potential, $\vec{r} \to \vec{r} + \vec{a}$.

Still get bands and gaps.