Symmetries in QM (Sakurai Chapter 4)

Classically: Hamiltonian \( H(q_1, \ldots, q_N, p_1, \ldots, p_N, t) \)

- generalized coordinates
- conjugate momenta

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 \( q_i \rightarrow q_i + \delta q_i \)),
then \( \dot{p}_i = 0 \). \( p_i \) is a conserved quantity.

In QM, symmetries \( \leftrightarrow \) unitary operators \( \mathcal{U} \).
For symmetries close to the identity (translations, rotations, ...)
\( \mathcal{U} = 1 - i \varepsilon \frac{G}{\hbar} \)

- \( G = \) 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, \( \frac{dA^{(a)}}{dt} = \frac{i}{\hbar} [A^{(a)}, H] \).
So \( [G^{(a)}, H] = 0 \) \( \Rightarrow \frac{dG^{(a)}}{dt} = 0 \)

But \( G^{(a)} = e^{+iHt/\hbar} G G^{-iHt/\hbar} = G^{(c)} \).
So \( G \) is the same in both Schrödinger & Heisenberg pictures, so \( \frac{dG}{dt} = 0 \) conserved operator.

Suppose \( |\psi(t_0)\rangle \) is an e-state of \( G \):
\( G |\psi(t_0)\rangle = g |\psi(t_0)\rangle \)
At a later time \( t \), \( |\psi(t)\rangle = e^{-iH(t-t_0)/\hbar} |\psi(t_0)\rangle \)
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:

$$H(\mathcal{U}|n\rangle) = \mathcal{U}H|n\rangle = E_n (\mathcal{U}|n\rangle).$$

$$[H, \mathcal{U}] = 0$$

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

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

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

So $[J_2, H] = 0$, and $[J_z, H] = 0$, and $[J_2, J_3] = 0$.

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

Since $\mathcal{O}(R)|n, j, m_\ell\rangle = \sum_{m_\ell'} |n, j, m_\ell'\rangle \mathcal{O}^{(j)}_{m_\ell m_\ell'} (R)$ for any rotation $R$,

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

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

We saw this repeatedly for $\text{H}$ 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 ($\vec{B}_{\text{ext}}$ or $\vec{E}_{\text{ext}}$). 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 \( \pi \vec{R} |\vec{r}\rangle = \pi \vec{R} |\vec{r}\rangle = \vec{r} \pi |\vec{r}\rangle = \vec{r} |\vec{r}\rangle \).

But also: \( = \{\pi, \vec{R}\} |\vec{r}\rangle - \vec{R} \{\pi, |\vec{r}\rangle\} - \vec{R} - |\vec{r}\rangle = \{\pi, \vec{R}\} |\vec{r}\rangle + |\vec{r}\rangle \)

\(\delta\) anticommutator

So \( \{\pi, \vec{R}\} = 0\), acting on all states \(|\vec{r}\rangle\).

So \( \vec{R} \pi = -\pi \vec{R} \) and \( \pi^+ \vec{R} \pi = -\vec{R} \), since \( \pi \) is unitary,

\[ \pi^+ \vec{R} \pi = \pi \vec{R} \pi^+ = -\vec{R} \]

For a general state \(|\psi\rangle\), parity operation takes \(|\psi\rangle \rightarrow \pi |\psi\rangle\).

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

Parity flips the sign of \( \langle \psi | \vec{R} |\psi\rangle \).

(Sakurai uses this as his defining property.)

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

So \( \pi^2 = 1\). Therefore, \( \pi^{-1} = \pi^+ = \pi \)

Unitary and Hermitian

Also, \( \{\pi, \vec{P}\} = 0 \) and \( \pi^+ \vec{P}\pi = -\vec{P} \)

(Taking \( \vec{r} \rightarrow -\vec{r}\) also takes \( \vec{V} \rightarrow -\vec{V} \). √)

Also \( [\pi, \vec{L}] = 0 \) and \( \pi^+ \vec{L}\pi = \vec{L} \)

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

What about spin? \( S = \vec{R} \vec{x} \vec{S} \).

Consider rotations of coordinates:

\( \begin{pmatrix} x \\ y \\ z \end{pmatrix} \rightarrow \begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = R^{(\text{rot})} \begin{pmatrix} x \\ y \\ z \end{pmatrix} \)

3x3 matrix.
Parity is also represented by a \(3 \times 3\) matrix on coordinates:
\[
\begin{pmatrix}
  x \\
  y \\
  z 
\end{pmatrix} \rightarrow \begin{pmatrix}
  x' \\
  y' \\
  z' 
\end{pmatrix} = R^{(\text{par})} \begin{pmatrix}
  x \\
  y \\
  z 
\end{pmatrix}
\]

\[
R^{(\text{par})} = \begin{pmatrix}
  -1 & 0 & 0 \\
  0 & -1 & 0 \\
  0 & 0 & -1 
\end{pmatrix}
\]

commutes with all \(3 \times 3\) matrices.

So \(R^{(\text{par})} R^{(\text{rot})} = R^{(\text{rot})} R^{(\text{par})}\).

In QM, require operators that represent these symmetries to obey same rule:
\[
\pi R^{(R)} = R^{(R)} \pi \quad \text{for any rotation } R.
\]

But \(\pi R^{(\text{R})} = 1 - i \hat{\mathbf{j}} \cdot \mathbf{\hat{n}} \mathbf{\hat{e}} \quad \text{for infinitesimal rotation around axis } \mathbf{n}, \text{ angle } \theta\).

\[
\Rightarrow [\pi, \hat{\mathbf{j}}] = 0 \Rightarrow \pi^+ \hat{\mathbf{j}} \pi = \hat{\mathbf{j}}
\]

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

Vectors are odd under parity: \(\pi \mathbf{V} \pi = -\mathbf{V}\).

Examples: \(\mathbf{R}, \mathbf{P}, \mathbf{E}\) (electric field); \(\mathbf{A}\) (vector potential).

Axial vectors are even under parity: \(\pi \mathbf{P} \pi = +\mathbf{P}\).

Examples: \(\mathbf{L}, \mathbf{S}, \mathbf{J}, \mathbf{B}\) (magnetic field).

a.k.a. "pseudovectors."

What about dot products?
\[
\begin{align*}
\pi^+ \mathbf{L} \cdot \mathbf{S} \pi &= + \mathbf{L} \cdot \mathbf{S} \quad \text{vector \cdot vector} \\
\pi^+ \mathbf{R} \cdot \mathbf{P} \pi &= + \mathbf{R} \cdot \mathbf{P} \quad \text{(axial vector) \cdot (axial vector)} \\
\pi^+ \mathbf{P} \cdot \mathbf{P} \pi &= + \mathbf{P} \cdot \mathbf{P}
\end{align*}
\]

Even under parity. Scalars.

But:
\[
\begin{align*}
\pi^+ \mathbf{L} \cdot \mathbf{R} \pi &= - \mathbf{L} \cdot \mathbf{R} \\
\pi^+ \mathbf{B} \cdot \mathbf{E} \pi &= - \mathbf{B} \cdot \mathbf{E}
\end{align*}
\]

Odd under parity. Pseudoscalars.
What are the eigenvalues of parity?

Suppose \( |\lambda\rangle = 2 |\lambda\rangle \). Then \( \pi |\lambda\rangle = \pi |\lambda\rangle = 2 |\lambda\rangle \)

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

Wave functions under parity:

\( \langle \hat{r} | \Psi \rangle = \Psi(r) \) = positon-space wavefunction

\( \pi |\Psi\rangle \) has wavefunction \( \langle \hat{r} | \pi |\Psi\rangle = \langle -\hat{r} | \Psi \rangle = \Psi(-r) \).

If \( |\Psi\rangle \) is an eigenstate of parity, then \( \pi |\Psi\rangle = \pm |\Psi\rangle \).

So \( \langle \hat{r} | \pi |\Psi\rangle = \pm \langle \hat{r} | \Psi \rangle = \pm \Psi(r) \)

\( \langle -\hat{r} | \Psi \rangle = \Psi(-r) \).

So \( \Psi(-r) = \pm \Psi(r) \) \{ even parity state \}

\{ odd parity state \}

So an eigenstate of parity, \( \pi^2 \Psi = \Psi \).

\( \hat{r} \) and \( \pi \) don't commute, so plane waves aren't parity eigenstates.

\( \hat{L} \) and \( \pi \) do commute, so can choose simultaneous \( e \)-states.

Consider wavefunctions of such states:

\( \langle \hat{r} | \alpha; l, m \rangle = R_a(r) Y_{lm} (\theta, \phi) = R_a; l, m (r) \) \( \alpha = \text{extra label(s)} \)

(\( = n \) for \( \text{H atom} \))

Parity:

\[
\begin{align*}
\hat{r} &\rightarrow \hat{r} \\
\theta &\rightarrow \pi - \theta \quad \text{so} \quad \cos \theta &\rightarrow -\cos \theta \\
\phi &\rightarrow \phi + \pi \quad \text{so} \quad e^{i\phi} &\rightarrow (-1)^m e^{i\phi}
\end{align*}
\]

Consider \( m = 0 \) states first:

\[
Y_{l0} (\theta, \phi) = \sqrt{\frac{2l+1}{4\pi}} \frac{(-1)^l}{2^l l!} \frac{d^l}{d(\cos \theta)^l} \left( \frac{\sin \theta}{d(\cos \theta)} \right)^l \rightarrow \text{same under parity}
\]

\[
\rightarrow \frac{d}{d(\cos \theta)} \left( \frac{\sin \theta}{d(\cos \theta)} \right)^l = (-1)^l \text{ same}
\]

\[
= (-1)^l \text{ same}
\]
So, under parity, $\bar{r} \rightarrow -\bar{r}$, $Y_{\ell \sigma}(\theta, \phi) \rightarrow (-1)^\ell Y_{\ell \sigma}(\theta, \phi)$.

So $|\alpha; l, 0\rangle$ has:
odd parity for $l$ odd 

even parity for $l$ even.

But states with $m \neq 0$ are obtained by acting with $L^z$, and $[L^z, \pi] = 0$.

So $|\alpha; l, m\rangle$ has parity $(-1)^l$ (for any $\alpha, m$).

Does the Hamiltonian of the universe commute with parity?

- gravity $\checkmark$
- EM $\checkmark$
- strong nuclear force (QCD) $\checkmark$
- weak nuclear force (β-decay, neutrino interactions) $\overline{\checkmark}$

known in early 20th century

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, universe commutes with $\pi$.
However, $H$ for an isolated sub-system may or may not.

Suppose $[H, \pi] = 0$. Then if $|n\rangle$ is a non-degenerate $e$-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:

$\pi \left( \frac{1}{2} (1 \pm \pi) |n\rangle = \frac{1}{2} (\pi \pm \pi^2) |n\rangle = \frac{1}{2} (\pi \pm 1) |n\rangle = \pm \left( \frac{1}{2} (1 \pm \pi) |n\rangle \right) \right.$.
But also: \[ H(\frac{1}{2}(1+\pi)|n\rangle) = \frac{1}{2}(1+\pi)H|n\rangle = En \frac{1}{2}(1+\pi)|n\rangle. \]

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 \(E_n\).

This contradicts the non-degeneracy assumption, unless

\(|n\rangle\) and one of \(\frac{1}{2}(1+\pi)|n\rangle\) are actually the same state,

and the other of \(\frac{1}{2}(1-\pi)|n\rangle = 0\) (null ket, not a state).

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

Examples

* 1-d harmonic oscillator: \(\psi_0(x) \sim e^{-x^2/2\alpha^2} \Rightarrow \text{parity} +1.\)

\[ H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2x^2 \text{ commutes with } \pi. \]

For excited states \((\alpha^\dagger)^n |0\rangle\), parity is \((-1)^n\),

because \(\alpha^\dagger = \text{linear combination of } X, P.\)

* H atom: ground state is non-degenerate

\[ \psi(r) = \frac{1}{\sqrt{\pi\alpha_0^3}} e^{-r/\alpha_0} \text{ is parity } +1 \quad (r \rightarrow -r \text{ means } r \rightarrow r). \]

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: \(\langle r|\vec{p}\rangle = e^{i\vec{p} \cdot \vec{r}/\hbar}.\) So \(|\vec{p}\rangle\) aren't \(\pi\) e-states.

They are energy eigenstates of \(H = \frac{\vec{p}^2}{2m}\), but degenerate,

since \(|\vec{p}\rangle\) and \(\hat{X}(R)|\vec{p}\rangle\) have same energy.

However, \(|\vec{p}\rangle + |\vec{p}\rangle\) and \(|\vec{p}\rangle - |\vec{p}\rangle\) are \(\pi\)-eigenstates

parity +1 \quad \text{parity} -1
* Symmetric potentials in 1-d (and spherically-symmetric in 3d)

\[ H = \frac{p^2}{2m} + V(x) \quad \text{or} \quad H = \frac{p^2}{2m} + V(r) \]

Commute with parity.

Double well potential:

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

\[ E_S < E_A \]

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

Define

\[ |R\rangle = \frac{1}{\sqrt{2}} (|S\rangle + |A\rangle) \quad \text{(peaked for } x > 0) \]
\[ |L\rangle = \frac{1}{\sqrt{2}} (|S\rangle - |A\rangle) \quad \text{(peaked for } x < 0) \]

\[ \pi |R\rangle = |L\rangle \quad \text{and} \quad \pi |L\rangle = |R\rangle. \]

Suppose we prepare a state \(|\Psi_{R_0}(t)\rangle\) so that \(|\Psi_{R_0}(0)\rangle = |R\rangle\).

What is this state for later times \(t\) ?

\[ |\Psi_{R_0}(t)\rangle = \frac{1}{\sqrt{2}} \left( e^{-iE_s t/\hbar} |S\rangle + e^{-iE_A t/\hbar} |A\rangle \right) \]

\[ = e^{-iE_s t/\hbar} \frac{1}{\sqrt{2}} \left( |S\rangle + e^{-i(E_A - E_s) t/\hbar} |A\rangle \right) \]

\[ = |R\rangle \quad \text{at} \quad t = 0, \quad \frac{2\pi k}{E_A - E_s}, \quad \frac{4\pi k}{E_A - E_s}, \quad \ldots \]

\[ = |L\rangle \quad \text{at} \quad t = \frac{\pi k}{E_A - E_s}, \quad \frac{3\pi k}{E_A - E_s}, \quad \ldots \]
Angular frequency of oscillation $|R\rangle \leftrightarrow |L\rangle$ is:

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

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

Then $E_A - E_S \to 0$:

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

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

Classic example in 3-d: ammonia molecule $\text{NH}_3$:

$\text{NH}_3$

$\text{H}$

$\text{H}$

$\text{H}$

$\text{N}$

(like $|R\rangle$)

(like $|L\rangle$)

 barrier between configurations.

$$\omega_{\text{flip}} \approx 2.4 \times 10^{10} \text{ Hz} = \text{microwave}$$

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.

$1/\omega_{\text{flip}} \gg \text{years}$, if barrier is high enough.
Selection Rules
Consider any two states |α⟩, |β⟩, each of definite parity.
π|α⟩ = λ_α |α⟩  π|β⟩ = λ_β |β⟩ where λ_α, λ_β = ±1.

Then: ⟨β |R|α⟩ ≠ 0 requires λ_α λ_β = -1.

Proof: ⟨β |R|α⟩ = ⟨β |π π R π π|α⟩ = -λ_α λ_β ⟨β |π |α⟩.
     λ_β ⟨β |1 = -R λ_α λ_α |α⟩

Alternatively: \[ \int d^3 \vec{r} \psi_β^*(\vec{r}) \vec{R} \psi_α(\vec{r}) \neq 0 \] requires λ_α λ_β = -1.

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

(rate) ∝ |⟨f |R|i⟩|^2

So the transition requires |i⟩ and |f⟩ to have opposite parity.

For eigenstates of \( L^2, L_z \), this requires:
\(-1)^{l_i + l_f} = -1, \) or \( l_i + l_f = \text{odd} \).

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

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

Lattice Translation (a discrete symmetry)
Consider potentials (in 1-d) satisfying \( V(x+a) = V(x) \).

\[
\begin{array}{c}
V(x) \\
\downarrow \\
V(x+a) \\
\uparrow \\
V(x+2a)
\end{array}
\]
\[
\begin{array}{c}
-a \\
0 \\
a \\
2a \\
x
\end{array}
\]
Let $\tau(l)$ be the translation operator for $x \to x+l$, so:

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

and $\tau^+(l) \tau(l) = \tau(l) \tau^+(l) = \text{1}$. Then $\tau^+(a) V(x) \tau(a) = V(x+a) = V(x)$.

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

So $\tau^+(a) H \tau(a) = H$. Therefore, $H \tau(a) = \tau(a) H$, so $[\tau(a), H] = 0 \implies H$ 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 $\lambda$, then

$$\tau^+(a) \tau(a) |\psi\rangle = \tau^+(a) \lambda |\psi\rangle = \lambda \lambda^* |\psi\rangle \implies |\lambda|^2 = 1.$$ 

Now consider states $|n\rangle$ that are localized at $x = na$ (the $n$th 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 $\langle n+1 | H | n \rangle = -\Delta$.

This is a coupling between particles in nearest neighbor sites.

Also, assume $\langle n+2 | H | n \rangle = \langle n+3 | H | n \rangle = \ldots = 0$.

Non-neighbor sites don't couple. This is the "tight-binding approximation"
So \( H |\theta\rangle = E_0 |\theta\rangle - \Delta |n+1\rangle - \Delta |n-1\rangle \).

To find energy eigenstates, consider:

\[
|\theta\rangle = \sum_{n=-\infty}^{\infty} e^{i\theta} |n\rangle \quad \text{for real numbers } \theta.
\]

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

Proof:

\[
\tau(a) |\theta\rangle = \sum_{n=-\infty}^{\infty} e^{i\theta} \tau(a) |n\rangle = \sum_{n=-\infty}^{\infty} e^{i\theta} |n+1\rangle
\]

\[
= \sum_{n'=\infty}^{\infty} e^{i(n'-1)\theta} |n'\rangle = e^{-i\theta} |\theta\rangle \quad \checkmark
\]

\[
H |\theta\rangle = \sum_{n=-\infty}^{\infty} e^{i\theta} H |n\rangle = \sum_{n=-\infty}^{\infty} e^{i\theta} \left[ E_0 |n\rangle - \Delta |n+1\rangle - \Delta |n-1\rangle \right]
\]

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

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

\[
= (E_0 - 2\Delta \cos \theta) |\theta\rangle \quad \checkmark
\]

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

\[\begin{align*}
\uparrow E \\
E_0 + 2\Delta \\
E_0 - 2\Delta
\end{align*}\]

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

\[
\text{energy } E = E_0 - 2\Delta \cos(ka).
\]

\[
\text{wave-vector } k \quad \text{(as if plane wave), multiplied by periodic function.}
\]

\( U_k(x) \) still needs to be solved for, on a case-by-case basis.
The solutions \( \psi_k(x) = e^{ikx} u_k(x) \) (with \( u_k(x) = u_k(x+\alpha) \)) are called Bloch waves. This form is valid even if the tight-binding approximation isn't.

Since \( \Theta \rightarrow \Theta + 2\pi \) gives the same state, the physical range for \( k \) is \( \frac{-\pi}{\alpha} < k < \frac{\pi}{\alpha} \).

For the tight-binding model:

\[
\text{Energy dispersion relation } \ E(k) = E_0 - 2\Delta \cos(ka) 
\]

Let's do an example: the 1-D Kronig-Penney model. (Baeum 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

\[
u_k(0) = A + B \quad \text{and} \quad u_k(a) = Ae^{i(q-k)a} + Be^{-i(q+k)a} \quad \text{must match.}
\]

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

Can now solve for \( B \) in terms of \( A \):

\[
B = A \frac{e^{i(q-k)a} - 1}{1 - e^{-i(q+k)a}}.
\]
The coefficient $A$ is then an arbitrary normalization.
Now look at Schrödinger 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 $\epsilon$, (small $\epsilon$):
\[
E \int_{-\epsilon}^{\epsilon} \Psi_k(x) \, dx + \frac{\hbar^2}{2m} \left[ \frac{d \Psi_k}{dx} \right]_{x=\epsilon} - \frac{d \Psi_k}{dx} \bigg|_{x=-\epsilon} - V_0 \Psi_k(\epsilon) = 0
\]
\[
\rightarrow 0 \quad \text{as} \quad \epsilon \rightarrow 0
\]
\[
\Rightarrow \quad i \hbar (A-B) = e^{-ika} \left. \frac{d \Psi_k}{dx} \right|_{x=\epsilon-a} = A+B
\]
\[
\rightarrow e^{-ika} \Psi_k (Ae^{i\alpha} - Be^{-i\alpha})
\]
So
\[
\frac{\hbar^2}{2m} i\hbar (A-B - Ae^{i(q-k)a} + Be^{-i(q+k)a}) - V_0 (A+B) = 0
\]
Plug in solution for $B$, simplify:
\[
\left[ \cos(ka) - \cos(qa) - \frac{mV_0}{\hbar^2} \sin(qa) \right] A = 0
\]
So
\[
\cos(ka) = \cos(qa) + \frac{mV_0 a}{\hbar^2} \frac{\sin(qa)}{qa}
\]
This can be solved (in principle) for $q$, given $k$.
Recall $-\frac{\pi}{a} < k < \frac{\pi}{a}$, so $-1 < \cos(ka) < 1$
Graphical solution for $qa$: 
\[
\begin{align*}
ka &= 0 \quad \text{allowed} \\
ka &= \pm \pi \quad \text{allowed}
\end{align*}
\]
After solving for \( q \) in terms of \( k \) (numerically), \( E = \frac{k^2 q^2}{2m} \)

Got 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:
\[
\psi_{k}^{\pm}(\vec{r}) = e^{i\vec{k} \cdot \vec{r}} u_{k}^{\pm}(\vec{r})
\]

where \( u_{k}^{\pm}(\vec{r}) \) has the same translation invariances as the lattice potential, \( \vec{r} \to \vec{r} + \vec{a} \).
Still get bands and gaps.