Lecture 12

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Part I

Symmetry and Degeneracy

Definition: A symmetry of a system is a transformation that leaves the Hamiltonian invariant.

Hamiltonian Symmetry

Using an operator on the state.

$$|\psi(0)\rangle \xrightarrow{\hat{T}} |\psi'(t)\rangle$$

And after using some time evolution operator $U(t)$

$$|\psi(t)\rangle \xleftarrow{\hat{T}} |\psi'(t)\rangle$$

$\hat{T}$ is a symmetry tranformation of the Hamiltonian if

$$|\psi'(t)\rangle = \hat{T}\,|\psi(t)\rangle$$

For all $\psi(0)$ and all t.

$$e^{-i\hat{H}t/\hbar}\,|\psi'(0)\rangle = \hat{T}e^{-i\hat{H}t/\hbar}\,|\psi(0)\rangle$$

The following must be true

$$\left[\hat{T}, e^{-i\hat{H}t/\hbar}\right] = 0$$

Expanding the exponentnial.

$$\left[\hat{T}, e^{-i\hat{H}t/\hbar}\right] = \left[\hat{T}, 1 - \frac{i}{\hbar}\hat{H}t + \frac{1}{2!}\left(-\frac{i}{\hbar}\right)^2 \hat{H}^2 t^2 + \dots\right] = 0$$

$$-\frac{it}{\hbar}\left[\hat{T}, \hat{H}\right] + \frac{1}{2!}\left(-\frac{it}{\hbar}\right)^2 \left[\hat{T}, \hat{H}^2\right] + \cdots = 0$$

To hold for all t,

$$\left[\hat{T}, \hat{H}\right] = 0$$

When $\hat{T}$ is norm preserving (unitary), $\hat{T}^\dagger = \hat{T}^{-1}$.

$$\hat{T}\hat{H} = \hat{H}\hat{T}$$
$$\hat{T}^{-1}\hat{T}\hat{H} = \hat{T}^{-1}\hat{H}\hat{T} = \hat{T}^\dagger\hat{H}\hat{T}$$
$$\hat{H} = \hat{T}^\dagger\hat{H}\hat{T}$$

The easiest way to check if a Hamiltonian has a symmetry is to check if it commutes with some operator $\hat{T}$.

Consequences of Symmetry

1. Some quantities are conserved.

$$\langle T \rangle = \langle \psi(t)| \hat{T} |\psi(t)\rangle$$

does not change in time.

$$\frac{\mathrm{d}}{\mathrm{d}} \langle T \rangle = \left(\underbrace{\frac{\mathrm{d}}{\mathrm{d}t} \langle \psi(t)|}_{-\langle \psi(t)|\hat{H}} \right) \hat{T} |\psi(t)\rangle + \langle \psi(t)| \hat{T} \left(\underbrace{\frac{\mathrm{d}}{\mathrm{d}t} |\psi(t)\rangle}_{\hat{H}|\psi(t)\rangle} \right) = 0$$

$$\langle \psi(t)| \underbrace{\left[\hat{T}, \hat{H}\right]}_{0} |\psi(t)\rangle = 0$$

2. Eigenstates of $\hat{T}$ will remain eigenstates as t changes.

$$\hat{T} |x(t)\rangle = \lambda |x(t)\rangle$$

$$\hat{T} |x(t)\rangle = \hat{T} e^{-i\hat{H}t/\hbar} |x(0)\rangle = e^{-i\hat{H}t/\hbar} \hat{T} |x(0)\rangle = \lambda |x(t)\rangle$$

$|x(t)\rangle$ is and eigenstate of $\hat{T}$ with eigenvalue λ.

3. We can construct a common complete set of eigenstates for $\hat{H}$ and $\hat{T}$. The symmetries of the Hamiltonian implies that the eigenstates of $\hat{T}$ are also eigenstates of $\hat{H}$.

4. Often degenerate energy spectrum.

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

$$\hat{H}\hat{T} |n\rangle = \hat{T}\hat{H} |n\rangle = E_n \hat{T} |n\rangle$$

So $\hat{T} |n\rangle$ is also an energy eigenket with energy E_n. If $\hat{T} |n\rangle \neq |n\rangle$, we have a degeneracy. If there are degeneracy, they are often a consequence of symmetry.

Example: Translational Symmetry

T_a is an operator that transforms $x \to x + a$.

$$T_a |x\rangle = |x + a\rangle$$

Taylor Expansion:

$$\psi(x + a) = \psi(x) + a\psi'(x) + \frac{a^2}{2!}\psi''(x) + \dots$$

Rewriting this as an operator:

$$T_a = 1 + a\frac{\mathrm{d}}{\mathrm{d}x} + \frac{a^2}{2!}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \dots$$

$$\hat{T}\left|x\right\rangle = \left|x+a\right\rangle = \left|x\right\rangle + a\frac{\mathrm{d}}{\mathrm{d}x}\left|x\right\rangle + \frac{a^2}{2!}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\left|x\right\rangle + \dots$$

Using the fact that the taylor expansion is the definition of the exponential function.

$$e^{a\frac{\mathrm{d}}{\mathrm{d}x}} = e^{\frac{ia}{\hbar}\frac{\hbar}{i}\frac{\mathrm{d}}{\mathrm{d}x}}$$

We see that $\hbar/i\frac{\mathrm{d}}{\mathrm{d}x}$ is the momentum operator.

$$T_a = e^{i\frac{a}{\hbar}\hat{p}}$$

Conclusion: Translations are generated by the momentum operator.
If $[T_a, H] = 0$for any a then

$$\left[e^{-i\frac{a}{\hbar}\hat{p}}, \hat{H}\right] = 0$$

$$\left[1, \hat{H}\right] + \frac{ia}{\hbar}\left[\hat{p}, \hat{H}\right] + \frac{1}{2!}\left(\frac{ia}{\hbar}\right)^2\left[\hat{p}, \hat{H}\hat{H}\right], \dots = 0$$

Conclusion: Momentum is conserved and the system is said to be translationally invariant.

Conclusion: $\hat{H}$ is the generator of time-transformation, meaning energy is conserved.

Example: Rotational Symmetry

Rotation around the z-axis done by $\hat{R}_z$.

$$\hat{R}_z(\phi) = e^{-i\frac{\phi}{\hbar}\hat{L}_z} \quad , \quad \hat{L}_z = \frac{\hbar}{i}\frac{\partial}{\partial\phi}$$

Conclusion: If $[\hat{R}_z, H] = 0$ fora ll ϕ, then $[L_z, H] = 0$and so eigenfunctions of L_z are also eigenstates of $\hat{H}$.

Conclusion: If $[R_x, H] = 0 = [R_y, H]$ then $\hat{H}$ is also rotationally symmetric about the x- and y-axes.

Conclusion: Then $R_x\left|E, m\right\rangle$is also an eigenket withe energy E

$$R_x\left|E, m\right\rangle = e^{i\frac{\phi}{\hbar}\hat{L}_x}\left|E, m\right\rangle = \left(1 + \frac{i\phi}{2\hbar}(L_+ + L_-) + \frac{1}{2}\left(\frac{i\phi}{2\hbar}\right)^2(L_+L_z)^2 + \dots\right)$$

$$= \left|E, m\right\rangle + \frac{i\phi}{\hbar}\left(\left|E, m+1\right\rangle + \left|E, m-1\right\rangle\right) + \dots\left|E, m+2\right\rangle, \left|E, m+1\right\rangle$$

$$\neq \left|E, m\right\rangle$$

Conclusion: The rotational symmetry implies the degeneracy of energy levels with different m-values.

Example: Parity (space inversion) Symmetry

Defined for position eigenkets.

$$\hat{\Pi}\left|r\right\rangle = \left|-r\right\rangle$$
$$\hat{\Pi}^2\left|r\right\rangle = \left|r\right\rangle$$

Fact: $\hat{\Pi}$ is Hermitian.

$$\left\langle u\right|\hat{\Pi}^\dagger\left|v\right\rangle = \left\langle v\right|\hat{\Pi}\left|u\right\rangle^* = \left[\int v^*(r)\underbrace{\hat{\Pi}u(r)}_{u(-2)}\ \mathrm{d}r^3\right]^* = \left[\int_{\hat{r}\to-\hat{r}} v^*(-r)u(r)\right]^*$$

$$\int u^*(r)v(-r) = \left\langle u\right|\hat{\Pi}\left|v\right\rangle$$
$$\hat{\Pi}^\dagger = \hat{\Pi}$$
$$\hat{\Pi} = \hat{\Pi}^{-1} = \hat{\Pi}^\dagger$$

This results in eigenvalues being ± 1.

$$\hat{\Pi}\left|\pm\right\rangle = \pm\left|\pm\right\rangle$$

$\left|+\right\rangle$ is an even parity state, while $\left|-\right\rangle$ is an odd parity state.

$$\left\langle r\right|\hat{\Pi}^\dagger\hat{r}\hat{\Pi}\left|r\right\rangle = \left\langle -r\right|\hat{r}\left|-r\right\rangle = -r\left\langle -r|-r\right\rangle$$
$$\hat{\Pi}^\dagger\hat{r}\hat{\Pi} = -\hat{r} \to \hat{r}\hat{\Pi} = -\hat{\Pi}\hat{r}.$$

This also holds for momentum operator. We can check if $\left[\hat{H},\hat{\Pi}\right] = 0$.

$$\hat{H} = \frac{\hat{p}^2}{2m}$$

$$\left[\hat{H},\hat{\Pi}\right] = \frac{1}{2m}\left[\hat{p}^2,\hat{\Pi}\right] = \frac{1}{2m}\left(\hat{p}\hat{p}\hat{\Pi} - \hat{\Pi}\hat{p}\hat{p}\right) = \frac{1}{2m}\left(-\hat{p}\hat{\Pi}\hat{p} + \hat{p}\hat{\Pi}\hat{p}\right) = 0$$

Conclusion: $\hat{\Pi}$is a symmetry and we can construct a common set of eigenkets for each $\hat{H}$ and $\hat{\Pi}$.

Coclusion: The energy eigenkets are

$$e^{i\vec{k}\vec{r}} \quad , \quad E = \frac{\hbar^2k^2}{2m}$$
$$\hat{\Pi}e^{i\vec{k}\vec{r}} = e^{-i\vec{k}\vec{r}}$$

We get that $\cos\vec{k}\vec{r}$and $\sin\vec{k}\vec{r}$ are parity eigenstate as well for + and - respectively.

Conclusion: All non zeros values of $\vec{k}$ gives degeneracy. The only non-degenerate state is the ground state.