Introduction

Symmetry is when a system property where transformation leaves the system unchanged, ex. rotation or translation.

There are translation operators:

$$T(a)\,\psi(x) = \psi(x-a)$$

There are parity operators:

$$\Pi\,\psi(x,y,z) = \psi(-x,-y,-z)$$

There are rotation operators:

$$R_z(\varphi)\,\psi(r,\theta,\phi) = \psi(r,\theta,\phi-\varphi)$$

A symmetry is discrete or continuous.

Translation Operators

The translation operator as defined by its effect on ψ may be Taylor expanded:

$$T(a) = \sum\nolimits_n \frac{(-a)^n}{n!}\frac{d^n}{dx^n} = \exp\left(-\frac{iap}{\hbar}\right)$$

Note that the translation operator is both hermitian and unitary:

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

Shifting the wave function is an active transformation; shifting the coordinate system is a passive transformation.

Operators may be translated as:

$$\langle T\psi|Q|T\psi\rangle = \langle\psi|Q'|\psi\rangle \Rightarrow Q' = T^\dagger Q T$$

Find for translated operators that:

$$Q'(x,p) = Q(x+a,p)$$

A system is translationally invariant iff:

$$T^\dagger H T = H \iff [H,T] = 0$$

For $H = E_k + E_p$, with translational symmetry with respect to $T(a)$:

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

Thm: if two operators commute, they have a complete set of simultaneous eigenstates.

$$H\psi = E\psi; \quad T\psi = \lambda\psi \Rightarrow \lambda = e^{ika}$$

Then reformulate as Bloch's theorem:

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

Note that $\hbar k$ is the crystal momentum.

For continuous symmetries, it is useful to consider infinitesimal translations:

$$T(\varepsilon) = \exp(-i\varepsilon p/\hbar) \approx 1 - \frac{i\varepsilon}{\hbar}p$$

Observe the commutation relation:

$$[H,T] = [H, 1 - i\varepsilon p/\hbar] = 0 \Longrightarrow [H,p] = 0$$

Momentum conservation follows from the generalized Ehrenfest theorem:

$$\frac{d\langle p\rangle}{dt} = \frac{i}{\hbar}\langle[H,p]\rangle = 0$$

Conservation Laws

Conservation of a quantity within QM means that $\langle Q\rangle$ is independent of time.

If Q does not vary with time, then:

$$[H,Q] = 0$$

Thence, the probability $P(n) = |c_n|^2$ is time independent, and thus conserved.

Parity

The parity operator is both hermitian and unitary:

$$\Pi = \Pi^\dagger = \Pi^{-1}$$

Operators may be transformed as:

$$\langle\Pi\psi|Q|\Pi\psi\rangle = \langle\psi|Q'|\psi\rangle \Rightarrow Q' = \Pi^\dagger Q \Pi$$

Observe that under spatial inversion:

$$\Pi^\dagger x\,\Pi = -x; \qquad \Pi^\dagger p\,\Pi = -p$$

A system has inversion symmetry iff:

$$\Pi^\dagger H\,\Pi = H \iff [H,\Pi] = 0$$

For a system with inversion symmetry:

$$V(x) = V(-x)$$

These stationary states of H are also eigenstates of Π, whose eigenvalues are ± 1, so the eigenstates are even or odd.

Parity conservation for even-V follows from the general Ehrenfest theorem:

$$\frac{d\langle\Pi\rangle}{dt} = \frac{i}{\hbar}\langle[H,\Pi]\rangle = 0$$

"Selection rules tell you when a matrix element is zero based on symmetry."

Laporte's selection rule: "electronic transitions that conserve parity wrt an inversion center are forbidden."

Rotational Symmetry

The rotation operator is expressed as:

$$R_z(\varphi) = \exp\left(-\frac{i\varphi}{\hbar}L_z\right)$$

For continuous symmetries, it is useful to consider infinitesimal translations:

$$R_z(\varepsilon) = \exp(-i\varepsilon L_z/\hbar) \approx 1 - \frac{i\varepsilon}{\hbar}L_z$$

The position operators transform:

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \begin{pmatrix} \cos(\varphi) & -\sin(\varphi) & 0 \\ \sin(\varphi) & \cos(\varphi) & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

The commutation relation generally is:

$$[L_i, Q_j] = i\hbar\epsilon_{ijk}Q_k$$

If $V = V(r)$, then $[H,L] = 0$, and thus angular momentum conservation follows from the Ehrenfest theorem.

Class	Parity	Rotations
true vector	$\{\Pi,Q\} = 0$	$[L,Q] = ...$
pseudovector	$[\Pi,Q] = 0$	$[L,Q] = ...$
true scalar	$[\Pi,Q] = 0$	$[L,Q] = 0$
pseudoscalar	$\{\Pi,Q\} = 0$	$[L,Q] = 0$

Degeneracy

"Symmetry is the source of most of the degeneracy in quantum mechanics."

If $[H,Q] = 0$, then $Q|\psi\rangle$ may be a new state with the same energy as $|\psi\rangle$.

Also, "the presence of non-commuting symmetry operators guarantees some degeneracy of the energy spectrum."

Rotation Selection Rules

Rotational selection rules are entirely given by the Wigner-Eckart Theorem.

For scalar operators, and a constant c:

$$\langle n'l'm'|Q|nlm\rangle = c\,\delta_{ll'}\delta_{mm'}\langle n'l|Q|nl\rangle$$

For vector operators with constants times by Clebsch-Gordan coefficients:

$$\langle n'l'm'|V_+|nlm\rangle = c_+\,\langle nl'|V|nl\rangle$$

$$\langle n'l'm'|V_-|nlm\rangle = c_-\,\langle nl'|V|nl\rangle$$

$$\langle n'l'm'|V_z|nlm\rangle = c_z\,\langle nl'|V|nl\rangle$$

Which is the selection rule that:

$$\Delta l = \{-1,0,1\}; \quad \Delta m = \{-1,0,1\}$$

This is useful for atomic transitions.

Translations in Time

A time translation operator is given as:

$$U(t)\,\Psi(x,0) = \Psi(x,t)$$

The time translation operator may be defined by its effect on Ψ, as may be Taylor expanded around 0:

$$U(t) = \sum\nolimits_n \frac{t^n}{n!}\frac{\partial^n}{\partial t^n} = \exp\left(-\frac{it}{\hbar}H\right)$$

Operators may be transformed as:

$$Q_H(t) = U^\dagger Q\,U$$

This inspires three pictures of QM, based upon what evolves in time:

Schrödinger picture	$\psi(t)$	Q
Heisenberg picture	ψ	$Q(t)$
Interaction picture	$\psi(t)$	$Q(t)$

Time translation invariance holds when $\partial_t H = 0$, and by Ehrenfest theorem, energy is conserved. Noting the thm:

$$\frac{d}{dt}\langle Q\rangle = \frac{i}{\hbar}\langle[H,Q]\rangle + \left\langle\frac{\partial Q}{\partial t}\right\rangle$$