Symmetries in Quantum Mechanics

Symmetries are some ‘operation(s)’ that can be performed on a system under which the system ‘remains the same’ or invariant

Symmetries can be continuous (rotation of a circle continuously) or discrete (rotation of an equilateral triangle about its center by integral multiples of 120 degrees)

For continuous symmetries, the symmetry operation can be performed infinitesimally close to the identity (i.e, no symmetry transformation on system)

In physics we are more concerned with dynamical symmetries of the Lagrangian (or action), rather than static symmetries of shape/form etc.

In classical mechanics, a physical theory defined by a Hamiltonian $H = H(x^i, p^i)$ is said to possess a symmetry if it is invariant under the corresponding transformations

Consider infinitesimal canonical transformations (which preserves the fundamental Poisson brackets)

$$x^i \to x'^i = x^i + \epsilon \frac{\partial g}{\partial p_i} = x^i + \delta x^i$$

$$p^i \to p'^i = p^i - \epsilon \frac{\partial g}{\partial x^i} = p^i + \delta p^i$$

ϵ is an infinitesimal parameter of the transformation and $g = g(x^i, p^i)$ is called the generator of the infinitesimal transformation

Under this transformation the Hamiltonian changes as

$$\delta H(x^i, p^i) = \sum_i \left(\frac{\partial H}{\partial x^i}\, \delta x^i + \frac{\partial H}{\partial p^i}\, \delta p^i \right)$$

$$= \sum_i \left(\frac{\partial H}{\partial x^i} \epsilon \frac{\partial g}{\partial p_i} + \frac{\partial H}{\partial p^i} \left(-\epsilon \frac{\partial g}{\partial x^i} \right) \right)$$

$$= \epsilon \sum_i \left(\frac{\partial H}{\partial x^i} \frac{\partial g}{\partial p_i} - \frac{\partial H}{\partial p^i} \frac{\partial g}{\partial x^i} \right)$$

$$= \epsilon \{H, g\}$$

where $\{A, B\}$ is the classical Poisson bracket of A and B

If H is invariant under the above transformation , then $\delta H(x^i, p^i) = 0$ or

$$\{H, g\} = 0$$

By Hamilton's eqn. $\frac{dg}{dt} = \{g, H\} = 0$

Hence $g(x^i, p^i)$ is a constant of motion. Conversely every conserved quantity generates a continuous symmetry of the Hamiltonian

Any dynamical variable $\omega(x^i, p^i)$ transforms under the canonical coordinate and momenta transformations as

$$\delta\omega(x^i, p^i) = \sum_i \left(\frac{\partial \omega}{\partial x^i}\, \delta x^i + \frac{\partial \omega}{\partial p^i}\, \delta p^i \right)$$

$$= \epsilon \sum_i \left(\frac{\partial \omega}{\partial x^i} \frac{\partial g}{\partial p_i} - \frac{\partial \omega}{\partial p^i} \frac{\partial g}{\partial x^i} \right)$$

$$= \epsilon\{\omega, g\}$$

This is why g is known as the generator of the symmetry transformation

Choosing $\omega(x^i, p^i) = x^i$, we get $\delta x^i = \epsilon\{x^i, g\} = \epsilon \frac{\partial g}{\partial p^i}$ and similarly choosing $\omega(x^i, p^i) = p^i$ we get $\delta p^i = \epsilon\{p^i, g\} = -\epsilon \frac{\partial g}{\partial x^i}$

These are the same as the canonical transformations for x^i and p^i considered earlier

<u>Example</u>: Consider a 1-dim. system with Hamiltonian $H(x, p)$. Choose $g(x, p) = p$. Then $\delta x = \epsilon\{x, g\} = \epsilon\{x, p\} = \epsilon \ \Rightarrow x \to x' = x + \epsilon$

$$\delta p = \epsilon\{p, g\} = \epsilon\{p, p\} = 0 \ \Rightarrow p \to p' = p$$

Thus momentum is the generator of infinitesimal translations

<u>Exercise</u>: Choose $g(x, p) = H(x, p)$. Show that $x'(t) = x(t + \epsilon)$ and $p'(t) = p(t + \epsilon)$. Thus this transformation corresponds to translation of time

Theorem: If the Hamiltonian of a system is invariant under some transformation $(x, p) \to (x', p')$, which is not necessary infinitesimal, then if $\big(x(t), p(t)\big)$ is a solution of Hamilton's equations of motion, then $\big(x'(t), p'(t)\big)$ is also a solution

<u>Symmetries in QM</u>

In QM x and p are not well defined because of the uncertainty principle. To implement symmetries in QM, we have to use expectation values of observables, since these correspond to classical variables (Ehrenfest's theorem) So the generalization of the coordinate shift would be

$$\langle X\rangle \to \langle X\rangle + \epsilon, \qquad \langle P\rangle \to \langle P\rangle$$

Under the 'active transformation' point of view, the <u>states</u> change under the transformation as

$$|\psi\rangle \to |\psi_\epsilon\rangle = |\psi'\rangle = T(\epsilon)|\psi\rangle$$

where $T(\epsilon)$ is the operator which implements an infinitesimal translation on Hilbert space of states (i.e., on the kets)

Hence $$\langle\psi|X|\psi\rangle \to \langle\psi'|X|\psi'\rangle = \langle\psi|X|\psi\rangle + \epsilon$$, i.e,

$$\langle\psi\big|T^\dagger(\epsilon)XT(\epsilon)\big|\psi\rangle = \langle\psi|X|\psi\rangle + \epsilon$$

$$\langle\psi|P|\psi\rangle \to \langle\psi'|P|\psi'\rangle = \langle\psi\big|T^\dagger(\epsilon)PT(\epsilon)\big|\psi\rangle = \langle\psi|P|\psi\rangle$$

The 'passive transformation' point of view is that the <u>operators</u> change, but states remain unchanged. From the above eqns. the operators change as

$$X \to T^\dagger(\epsilon)XT(\epsilon) = X + \epsilon\mathbf{1}, \qquad P \to T^\dagger(\epsilon)PT(\epsilon) = P$$

Consider again the active point of view. To understand how arbitrary state transform under translations, first consider how x-basis vectors transform:

$$T(\epsilon)|x\rangle = |x+\epsilon\rangle \quad \text{and} \quad \langle x|T^\dagger(\epsilon) = \langle x+\epsilon|$$

Then consider the $x'x$ matrix element (the inner product) of $T^\dagger T$:

$$\langle x'\left|T^\dagger T\right|x\rangle = \langle x'+\epsilon|x+\epsilon\rangle = \delta(x'-x) = \langle x'|x\rangle$$

Since the states are normalized it follows that $T(\epsilon)^\dagger T(\epsilon) = \mathbf{1}$, i.e. $T(\epsilon)^\dagger = T^{-1}(\epsilon)$. In QM translations are represented by a <u>Unitary</u> operator

Now states (kets) transform as

$$|\psi'\rangle = T(\epsilon)|\psi\rangle = T(\epsilon)\int dx\, |x\rangle\langle x|\psi\rangle = T(\epsilon)\int dx\, |x\rangle\psi(x)$$

$$= \int dx\ |x+\epsilon\rangle\psi(x)$$

Now change variables to $x' \to x + \epsilon$, so that

$$|\psi'\rangle = \int dx' \;\; |x'\rangle \psi(x' - \epsilon)$$

Or taking inner product on both sides with $\langle x|$,

$$\langle x|\psi'\rangle = \psi'(x) = \int dx' \;\; \delta(x - x')\psi(x' - \epsilon) = \psi(x - \epsilon)$$

Similarly $\langle \psi'|P|\psi'\rangle = \int dx \;\; \psi'^{*}(x)\left(-i\,\hbar\frac{d}{dx}\right)\psi'(x)$

$$= \int dx \;\; \psi^{*}(x - \epsilon)\left(-i\,\hbar\frac{d}{dx}\right)\psi(x - \epsilon)$$

$$= \int dx'\,\psi^{*}(x')\left(-i\,\hbar\frac{d}{dx'}\right)\psi(x') = \langle \psi|P|\psi\rangle$$

Define the <u>generator</u> of infinitesimal translations G as

$$T(\epsilon) = \mathbf{1} - \frac{i\epsilon}{\hbar}\, G$$

The i is introduced so that G would be Hermitian, i.e,

$$T^{\dagger}(\epsilon)T(\epsilon) = \left(\mathbf{1} + \frac{i\epsilon}{\hbar}\, G^{\dagger}\right)\left(\mathbf{1} - \frac{i\epsilon}{\hbar}\, G\right)$$

$$= \mathbf{1} + \frac{i\epsilon}{\hbar}\left(G^{\dagger} - G\right) + \mathcal{O}(\epsilon^2) = \mathbf{1}$$

Thus $G^{\dagger} = G$ and thus G is Hermitian. To determine G note that

$$\langle x|T(\epsilon)|\psi\rangle = \psi(x-\epsilon)$$

$$\langle x|\left(\mathbf{1} - \frac{i\epsilon}{\hbar}\, G\right)|\psi\rangle = \psi(x) - \epsilon\frac{d\psi(x)}{dx} + \mathcal{O}(\epsilon^2)$$

The LHS is $\psi(x) - \frac{i\epsilon}{\hbar}\langle x|G|\psi\rangle = \psi(x) - \epsilon\frac{d\psi(x)}{dx}$, or,

$$\frac{i}{\hbar}\langle x|G|\psi\rangle = \frac{d\psi(x)}{dx}$$

This determines $G = -i\hbar\frac{d}{dx} = P$

So momentum is the generator of infinitesimal translations in QM as well and

$$T(\epsilon) = 1 - \frac{i\epsilon}{\hbar}G = 1 - \frac{i\epsilon}{\hbar}P$$

A QM theory would be invariant under translations if

$$\langle\psi'|H|\psi'\rangle = \langle\psi|H|\psi\rangle \text{ or}$$

$$\langle\psi\left|T^{\dagger}(\epsilon)H\,T(\epsilon)\right|\psi\rangle = \langle\psi|H|\psi\rangle,$$

$$\langle\psi\left|\left(1 + \frac{i\epsilon}{\hbar}P\right)H\left(1 - \frac{i\epsilon}{\hbar}P\right)\right|\psi\rangle = \langle\psi|H|\psi\rangle$$

The LHS simplifies to $\frac{i\epsilon}{\hbar}\langle\psi|[P,H]|\psi\rangle = 0$, i.e $\langle\psi|[P,H]|\psi\rangle = 0$

Since this is true for an arbitrary state it holds that $[P,H] = 0$

By Ehrenfest's theorem $\frac{d}{dt}\langle P\rangle = 0$

Translations in the Passive Picture

In the passive picture, the states do not change with the action of the symmetry operation. Rather, the operators change as

$$T^{\dagger}(\epsilon)XT(\epsilon) = X + \epsilon\mathbf{1}$$
$$P \rightarrow T^{\dagger}(\epsilon)PT(\epsilon) = P$$

We can determine the form of the generator G independently from the above conditions as well

Substituting $T(\epsilon) = 1 - \frac{i\epsilon}{\hbar}\, G$ in the eqn. for X gives

$$\left(\mathbf{1} + \frac{i\epsilon}{\hbar}\, G\right) X \left(\mathbf{1} - \frac{i\epsilon}{\hbar}\, G\right) = X + \epsilon\mathbf{1}$$

(Since $G^\dagger = G$) Expanding to order ϵ and comparing terms gives

$$\frac{i\epsilon}{\hbar}[G, X] = \epsilon\mathbf{1}$$

or $[G, X] = -i\hbar$, i.e., $[X, G] = i\hbar$

The general solution of the commutator for G is $G = P + f(X)$

(Since X commutes with any function of itself, i.e., $[X, f(X)] = 0$

How do we determine $f(X)$?

Use the 2nd relation for the P operator under translation: $T^\dagger(\epsilon) P T(\epsilon) = P$

Substituting $G = P + f(X)$ in this relation and expanding and comparing terms of order ϵ gives

$$\frac{i\epsilon}{\hbar}[G, P] = 0$$

$$\text{i.e.}, [P + f(X), P] = 0$$

Since X has a non-zero commutation relation with P, this can only be satisfied for arbitrary $f(X)$ only if $f(X) = \text{constant}$. This constant can simply be chosen to be zero, without any loss of generality.

Choose $f(X) = 0$. Thus, $G = P$ and the form of the infinitesimal translation operator is

$$T(\epsilon) = \mathbf{1} - \frac{i\epsilon}{\hbar}G = \mathbf{1} - \frac{i\epsilon}{\hbar}P$$

Invariance of the Hamiltonian of the system under translations implies that

$$T^\dagger(\epsilon) H T(\epsilon) = H \quad \text{i.e.,} \qquad [P, H] = 0$$

In the passive picture, the infinitesimal change in the operators X and P are

$$\delta X = T^\dagger(\epsilon) X T(\epsilon) - X = \frac{i\epsilon}{\hbar}[P, X] = \epsilon \mathbf{1}$$

$$\delta P = T^\dagger(\epsilon) P T(\epsilon) - P = \frac{i\epsilon}{\hbar}[P, P] = 0$$

In general if $\Omega(X, P)$ is any observable (operator), then one can show that under an infinitesimal symmetry operation it transforms as

$$\Omega(X, P) \longrightarrow T^\dagger(\epsilon)\, \Omega(X, P)\, T(\epsilon)$$

Or the infinitesimal change in the operator is

$$\delta\Omega(X, P) = T^\dagger(\epsilon)\, \Omega(X, P)\, T(\epsilon) - \Omega(X, P) = \frac{i\epsilon}{\hbar}[G, \Omega(X, P)]$$

Finite translations

The form of the translation operator for finite transformations is easy to figure out from the form of the infinitesimal operator

Any finite translation can be though about as a series of successive infinitesimal translations

If a is a finite translation, then define $\epsilon = a/N$ as the parameter of an infinitesimal translation, where N is large

I.e, a finite translation is achieved by N successive translation, each by an amount ϵ. Hence,

$$T(a) = \lim_{N\to\infty} \left(T(\epsilon)\right)^N = \lim_{N\to\infty} \left(\mathbf{1} - \frac{i\epsilon}{\hbar} P\right)^N$$

$$= \lim_{N\to\infty} \left(\mathbf{1} - \frac{ia}{\hbar N} P\right)^N = e^{-\frac{i}{\hbar}aP}$$

Physically, a translation by an amount a followed by a translation by an amount b is equivalent to a translation by an amount $a + b$

In terms of the finite translation operator this implies that,

$$T(a)T(b) = T(a+b)$$

$$\text{i.e.}, e^{-\frac{i}{\hbar}aP} e^{-\frac{i}{\hbar}bP} = e^{-\frac{i}{\hbar}(a+b)P}$$

Which shows that $[P, P] = 0$, as it should

This is true even in 3-dimensions for translations by the vector $\mathbf{a}, \mathbf{b}$ etc:

$$e^{-\frac{i}{\hbar}\mathbf{a}\cdot\mathbf{P}} e^{-\frac{i}{\hbar}\mathbf{b}\cdot\mathbf{P}} = e^{-\frac{i}{\hbar}(\mathbf{a}+\mathbf{b})\cdot\mathbf{P}}$$

Which confirms that $[P_i, P_j] = 0$, as expected

It is generally true that for continuous transformations, the commutation relations of the generators determine how two transformations combine