Symmetry

Noether's theorem
To every differentiable (continuous) symmetry generated by local actions, there corresponds a conserved current.
A symmetry refers to a physical property that is invariant under a continuous transformation
We consider three different transformations:

- Translation $\rightarrow$ momentum
- "Time-translation" $\rightarrow$ energy
- Rotation $\rightarrow$ angular momentum

Also, for example Lorentz transformations belong to above group
Conserved current $\mathbf{j} = \rho\mathbf{v}$ fullfills a conservation law,
e.g. conservation of charge,

$$\frac{\partial\rho}{\partial t} + \nabla\cdot\mathbf{j} = 0$$

in which ρ is the charge density.
Inverting the statement, "charge" can be considered as a generator of a continuous symmetry
For example, electric charge is a generator for $U(1)$ ($=e^{i\phi}$) symmetry in electrodynamics and the corresponding conserved current is the electric current.
In classical mechanics, Noether's theorem expresses a relationship between pairs of conjugate variables such that
if the action is invariant under a shift in one of the two physical variables, then the equations of motion resulting from holding the action stationary, conserve the value of the other of the pair of variables
Classical mechanics can be re-formulated in two ways

Lagrangian formalism
System is described with generalized coordinates q_i and generalized velocities $\dot{q}_i$
The trajectory of a classical object is found by minimizing the action

$$S[q(t)] = \int_{t_1}^{t_2} \mathcal{L}\Bigg(q_i(t), \dot{q}_i(t)\Bigg)dt$$

in which the Lagrangian $\mathcal{L}$ (in classical mechanics) is the sum of kinetic and potential energy

$$\begin{aligned}\mathcal{L}\Bigg(q_i(t), \dot{q}_i(t)\Bigg) &= \mathcal{L}\Bigg(x_i(t), \dot{x}_i(t)\Bigg) = T - V \\ (&= \frac{1}{2}m\dot{x}^2 - V(x))\end{aligned}$$

Notice! In field theories the Lagrangian density is often called Lagrangian. No problem as long as we know what we are doing. Here we stick with the definition given before.
Looking at the Lagrange equation of motion

$$\frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \dot{q}_i}\right) - \frac{\partial \mathcal{L}}{\partial q_i} = 0$$

of classical mechanics one can see that if the Lagrangian $\mathcal{L}(q_i, \dot{q}_i)$ is invariant under translations, i.e.

$$\mathcal{L}(q_i, \dot{q}_i) \longrightarrow \mathcal{L}(q_i + \delta q_i, \dot{q}_i) = \mathcal{L}(q_i, \dot{q}_i),$$

the momentum

$$p_i = \frac{\partial \mathcal{L}}{\partial \dot{q}_i}$$

is a conserved quantity, i.e.

$$\frac{dp_i}{dt} = \frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \dot{q}_i}\right) = 0.$$

Hamiltonian formalism
Formulating classical mechanics using the Hamiltonian function $\mathcal{H}(q_i, p_i)$ the equations of motion take the forms

$$\begin{aligned} \dot{p}_i &= -\frac{\partial \mathcal{H}}{\partial q_i} \\ \dot{q}_i &= \frac{\partial \mathcal{H}}{\partial p_i}. \end{aligned}$$

Also looking at these one can see that if $\mathcal{H}$ is symmetric under the operation

$$q_i \longrightarrow q_i + \delta q_i$$

there exists a conserved quantity:

$$\dot{p}_i = 0.$$

The Hamiltonian is a Legendre transform of the Lagrangian, whose symmetry properties are of the uppermost importance in QM

$$\mathcal{H}(q_j, p_j, t) = \sum_i \dot{q}_i p_i - \mathcal{L}(q_j, \dot{q}_j, t)$$

Symmetries and constants of motion in QM
In quantum mechanics continuous operations (translations, rotations, ...) are associated with a unitary *symmetry operator*.

Let $\mathcal{S}$ be an arbitrary symmetry operator. We say that the Hamiltonian H is *symmetric*, if

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

or due to the unitarity of the operator $\mathcal{S}$ equivalently

$$\mathcal{S}^\dagger H \mathcal{S} = H.$$

The matrix elements of the Hamiltonian are then invariant under that operation.
In the case of a continuum symmetry we can look at infinitesimal operations

$$\mathcal{S} = 1 - \frac{i\epsilon}{\hbar} G,$$

where the Hermitean operator G is the *generator* of that symmetry. From the condition

$$\mathcal{S}^\dagger H \mathcal{S} = H$$

it follows now

$$[G, H] = 0,$$

so according to the Heisenberg equation of motion

$$\frac{dA}{dt} = \frac{1}{i\hbar}[A, H]$$

we have

$$\frac{dG}{dt} = 0.$$

In the Heisenberg formalism the observable G is thus a constant of motion.
If H is invariant under

- translations then the momentum is constant of motion.
- rotations then the angular momentum is a constant motion.

Let us suppose now that the Hamiltonian is symmetric under the operations $\mathcal{S}$ generated by G:

$$\begin{aligned} \mathcal{S}^\dagger H \mathcal{S} &= H \\ [\mathcal{S}, H] &= 0 \\ [G, H] &= 0. \end{aligned}$$

Let $|g'\rangle$ be the eigenstates of G, i.e.

$$G|g'\rangle = g'|g'\rangle$$

and let the system at the moment t_0 be in the eigenstate $|g'\rangle$ of G. Since the time evolution operator is a functional of the Hamiltonian only,

$$U = U[H],$$

so

$$[G, U] = 0.$$

At the moment t we then have

$$\begin{aligned} G|g', t_0; t\rangle &= GU(t_0, t)|g'\rangle = U(t_0, t)G|g'\rangle \\ &= g'|g', t_0; t\rangle, \end{aligned}$$

or an eigenstate associated with a particular eigenvalue of G remains always an eigenstate belonging to the same eigenvalue.

Degeneracy revisited

Let us consider now the energy eigenstates $|n\rangle$, i.e.

$$H|n\rangle = E_n|n\rangle.$$

When the Hamiltonian is symmetric under the operations $\mathcal{S}$ we have

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

If now

$$|n\rangle \neq \mathcal{S}|n\rangle,$$

then the energy states E_n are degenerate. Thus a symmetry is also usually associated with a degeneracy.

Let us suppose now that the symmetry operation $\mathcal{S}$ can be parametrized with a continuous quantity, say λ:

$$\mathcal{S} = \mathcal{S}(\lambda).$$

When the Hamiltonian is symmetric under these operations all states $\mathcal{S}(\lambda)|n\rangle$ have the same energy.

Example Rotations $\mathcal{D}(R)$.

If

$$[\mathcal{D}(R), H] = 0,$$

then

$$[\boldsymbol{J}, H] = 0, \quad [\boldsymbol{J}^2, H] = 0.$$

So there exist simultaneous eigenvectors $|n; jm\rangle$ of the operators H, $\boldsymbol{J}^2$ ja J_z. Now all rotated states

$$\mathcal{D}(R)|n; jm\rangle$$

belong to the same energy eigenvalue. We know that

$$\mathcal{D}(R)|n; jm\rangle = \sum_{m'} |n; jm'\rangle \mathcal{D}^{(j)}_{m'm}(R),$$

that is, every rotated state is a superposition of $(2j+1)$ linearly independent states. The degeneracy is thus $(2j+1)$-fold.

Example Atomic electron.

The potential acting on an electron is of form

$$U = V(r) + V_{LS}\boldsymbol{L}\cdot\boldsymbol{S}.$$

Now

$$[\boldsymbol{J}, H] = 0, \quad [\boldsymbol{J}^2, H] = 0,$$

where

$$\boldsymbol{J} = \boldsymbol{L} + \boldsymbol{S}.$$

The energy levels are thus $(2j+1)$-foldly degenerated.
Let's set the atom in magnetic field parallel to the z-axis. The Hamiltonian is then appended by the term

$$Z = cS_z.$$

Now

$$[\boldsymbol{J}^2, S_z] \neq 0,$$

so the rotation symmetry is broken and the $(2j+1)$-fold degeneracy lifted (different m states have different energy).

Parity

The parity or space inversion operation converts a right handed coordinate system to left handed:

$$x \longrightarrow -x, y \longrightarrow -y, z \longrightarrow -z.$$

This is a case of a *non continuous* operation, i.e. the operation cannot be composed of infinitesimal operations. Thus the non continuous operations have no generator.
We consider the parity operation, i.e. we let the parity operator π to act on vectors of a Hilbert space and keep the coordinate system fixed:

$$|\alpha\rangle \longrightarrow \pi|\alpha\rangle.$$

Like in all symmetry operations we require that π is unitary, i.e.

$$\pi^\dagger\pi = 1.$$

Furthermore we require:

$$\langle\alpha|\pi^\dagger\boldsymbol{x}\pi|\alpha\rangle = -\langle\alpha|\boldsymbol{x}|\alpha\rangle \;\forall|\alpha\rangle.$$

So we must have

$$\pi^\dagger\boldsymbol{x}\pi = -\boldsymbol{x},$$

or

$$\pi\boldsymbol{x} = -\boldsymbol{x}\pi.$$

The operators $\boldsymbol{x}$ ja π *anti*commute.

Let $|\boldsymbol{x}'\rangle$ be a position eigenstate, i.e.

$$\boldsymbol{x}|\boldsymbol{x}'\rangle = \boldsymbol{x}'|\boldsymbol{x}'\rangle.$$

Then

$$\boldsymbol{x}\pi|\boldsymbol{x}'\rangle = -\pi\boldsymbol{x}|\boldsymbol{x}'\rangle = (-\boldsymbol{x}')\pi|\boldsymbol{x}'\rangle,$$

and we must have

$$\pi|\boldsymbol{x}'\rangle = e^{i\varphi}|-\boldsymbol{x}'\rangle.$$

The phase is usually taken to be $\varphi = 0$, so

$$\pi|\boldsymbol{x}'\rangle = |-\boldsymbol{x}'\rangle.$$

Applying the parity operator again we get

$$\pi^2|\boldsymbol{x}'\rangle = |\boldsymbol{x}'\rangle$$

or

$$\pi^2 = 1.$$

We see that

- the eigenvalues of the operator π can be only ± 1,
- $\pi^{-1} = \pi^\dagger = \pi$.

Momentum and parity
We require that operations

- translation followed by space inversion
- space inversion followed by translation to the opposite direction

are equivalent:

$$\pi\mathcal{T}(d\boldsymbol{x}') = \mathcal{T}(-d\boldsymbol{x}')\pi.$$

Substituting

$$\mathcal{T}(d\boldsymbol{x}') = 1 - \frac{i}{\hbar}d\boldsymbol{x}' \cdot \boldsymbol{p},$$

we get the condition

$$\{\pi, \boldsymbol{p}\} = 0 \text{ or } \pi^\dagger\boldsymbol{p}\pi = -\boldsymbol{p},$$

or the momentum changes its sign under the parity operation.

Angular momentum and parity
In the case of the orbital angular momentum

$$\boldsymbol{L} = \boldsymbol{x} \times \boldsymbol{p}$$

one can easily evaluate

$$\begin{aligned}\pi^\dagger L \pi &= \pi^\dagger \boldsymbol{x} \times \boldsymbol{p} \pi = \pi^\dagger \boldsymbol{x} \pi \times \pi^\dagger \boldsymbol{p} \pi = (-\boldsymbol{x}) \times (-\boldsymbol{p}) \\ &= \boldsymbol{L},\end{aligned}$$

so the parity and the angular momentum commute:

$$[\pi, \boldsymbol{L}] = 0.$$

In $\mathcal{R}^3$ the parity operator is the matrix

$$P = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix},$$

so quite obviously

$$PR = RP, \ \forall R \in \mathrm{O}(3).$$

We require that the corresponding operators of the Hilbert space satisfy the same condition, i.e.

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

Looking at the infinitesimal rotation

$$\mathcal{D}(\epsilon \hat{\boldsymbol{n}}) = 1 - i \boldsymbol{J} \cdot \hat{\boldsymbol{n}} \epsilon / \hbar,$$

we see that

$$[\pi, \boldsymbol{J}] = 0 \text{ or } \pi^\dagger \boldsymbol{J} \pi = \boldsymbol{J},$$

which is equivalent to the transformation of the orbital angular momentum. We see that under

- rotations $\boldsymbol{x}$ and $\boldsymbol{J}$ transform similarly, that is, like vectors or tensors of rank 1.
- space inversions $\boldsymbol{x}$ is odd and $\boldsymbol{J}$ even.

We say that under the parity operation

- odd vectors are *polar*,
- even vectors are *axial* or *pseudo*vectors.

Let us consider such scalar products as $\boldsymbol{p} \cdot \boldsymbol{x}$ and $\boldsymbol{S} \cdot \boldsymbol{x}$. One can easily see that under rotation these are invariant, scalars. Under the parity operation they transform like

$$\begin{aligned}\pi^\dagger \boldsymbol{p} \cdot \boldsymbol{x} \pi &= (-\boldsymbol{p}) \cdot (-\boldsymbol{x}) = \boldsymbol{p} \cdot \boldsymbol{x} \\ \pi^\dagger \boldsymbol{S} \cdot \boldsymbol{x} \pi &= \boldsymbol{S} \cdot (-\boldsymbol{x}) = -\boldsymbol{S} \cdot \boldsymbol{x}.\end{aligned}$$

We say that quantities behaving under rotations like scalars, spherical tensors of rank 0, which under the parity operation are

- even, are (ordinary) *scalars*,
- odd, are *pseudoscalars*.

Wave functions and parity
Let ψ be the wave function of a spinless particle in the state $|\alpha\rangle$, i.e.

$$\psi(\boldsymbol{x}') = \langle \boldsymbol{x}' | \alpha \rangle.$$

Since the position eigenstates satisfy

$$\pi | \boldsymbol{x}' \rangle = | - \boldsymbol{x}' \rangle,$$

the wave function of the space inverted state is

$$\langle \boldsymbol{x}' | \pi | \alpha \rangle = \langle -\boldsymbol{x}' | \alpha \rangle = \psi(-\boldsymbol{x}').$$

Suppose that $|\alpha\rangle$ is a parity eigenstate, i.e.

$$\pi | \alpha \rangle = \pm | \alpha \rangle.$$

The corresponding wave function obeys the the relation

$$\psi(-\boldsymbol{x}') = \langle \boldsymbol{x}' | \pi | \alpha \rangle = \pm \langle \boldsymbol{x}' | \alpha \rangle = \pm \psi(\boldsymbol{x}'),$$

i.e. it is an even or odd function of its argument.
Note Not all physically relevant wave function have parity. For example,

$$[\boldsymbol{p}, \pi] \neq 0,$$

so a momentum eigenstate is not an eigenstate of the parity. The wave function corresponding to an eigenstate of the momentum is the plane wave

$$\psi_{\boldsymbol{p}'}(\boldsymbol{x}') = e^{i\boldsymbol{p}' \cdot \boldsymbol{x}' / \hbar},$$

which is neither even nor odd.
Because

$$[\pi, \boldsymbol{L}] = 0,$$

the eigenstate $|\alpha, lm\rangle$ of the orbital angular momentum $(\boldsymbol{L}^2, L_z)$ is also an eigenstate of the parity. Now

$$R_\alpha(r) Y_l^m(\theta, \phi) = \langle \boldsymbol{x}' | \alpha, lm \rangle.$$

In spherical coordinates the transformation $\boldsymbol{x}' \longrightarrow -\boldsymbol{x}'$ maps to

$$\begin{array}{lcll} r & \longrightarrow & r & \\ \theta & \longrightarrow & \pi - \theta & (\cos\theta \longrightarrow -\cos\theta) \\ \phi & \longrightarrow & \phi + \pi & (e^{im\phi} \longrightarrow (-1)^m e^{im\phi}). \end{array}$$

The explicit expression for spherical functions is

$$Y_l^m(\theta,\phi) = (-1)^m \sqrt{\frac{(2l+1)(l-m)!}{4\pi(l+m)!}} P_l^m(\theta) e^{im\phi},$$

from which as a special case, $m=0$, we obtain

$$Y_l^0(\theta,\phi) = \sqrt{\frac{2l+1}{4\pi}} P_l(\cos\theta).$$

Depending on the degree l of the Legendre polynomial it is either even or odd:

$$P_l(-z) = (-1)^l P_l(z).$$

We see that

$$\langle \boldsymbol{x}'|\pi|\alpha, l0\rangle = (-1)^l \langle \boldsymbol{x}'|\alpha, l0\rangle,$$

so the state vectors obey

$$\pi|\alpha, l0\rangle = (-1)^l |\alpha, l0\rangle.$$

Now

$$[\pi, L_\pm] = 0$$

and

$$L_\pm^r |\alpha, l0\rangle \propto |\alpha, l, \pm r\rangle,$$

so the orbital angular momentum states satisfy the relation

$$\pi|\alpha, lm\rangle = (-1)^l |\alpha, lm\rangle.$$

Theorem 1 *If*

$$[H, \pi] = 0,$$

and $|n\rangle$ is an eigenstate of the Hamiltonian H belonging to the nondegenerate eigenvalue E_n, i.e.

$$H|n\rangle = E_n|n\rangle,$$

then $|n\rangle$ is also an eigenstate of the parity.
Proof: Using the property $\pi^2 = 1$ one can easily see that the state

$$\frac{1}{2}(1 \pm \pi)|n\rangle$$

is a parity eigenstate belonging to the eigenvalue ± 1. On the other hand, this is also an eigenstate of the Hamiltonian H with the energy E_n:

$$H(\frac{1}{2}(1 \pm \pi)|n\rangle) = E_n \frac{1}{2}(1 \pm \pi)|n\rangle.$$

Since we supposed the state $|n\rangle$ to be non degenerate the states $|n\rangle$ and $\frac{1}{2}(1 \pm \pi)|n\rangle$ must be the same excluding a phase factor,

$$\frac{1}{2}(1 \pm \pi)|n\rangle = e^{i\varphi}|n\rangle,$$

so the state $|n\rangle$ is a parity eigen state belonging to the eigenvalue ± 1 ■
Example The energy states of a one dimensional harmonic oscillator are non degenerate and the Hamiltonian even, so the wave functions are either even or odd.

$$H = \frac{p^2}{2m} + \frac{mw^2x^2}{2} \quad ; \quad H|n\rangle = (n + \frac{1}{2})\hbar w|n\rangle$$

Ground state being gaussian is even under parity, while

$$|1\rangle = a^\dagger|0\rangle \quad ; \quad a^\dagger = \sqrt{\frac{mw}{2h}}\left(x - \frac{ip}{mw}\right)$$

is odd.
Note The nondegeneracy condition is essential. For example, the Hamiltonian of a free particle, $H = \frac{p^2}{2m}$, is even but the energy states

$$H|\boldsymbol{p}'\rangle = \frac{p'^2}{2m}|\boldsymbol{p}'\rangle$$

are not eigenstates of the parity because

$$\pi|\boldsymbol{p}'\rangle = |-\boldsymbol{p}'\rangle.$$

The condition of the theorem is not valid because the states $|\boldsymbol{p}'\rangle$ and $|-\boldsymbol{p}'\rangle$ are degenerate. We can form parity eigenstates

$$1/\sqrt{2}(|\boldsymbol{p}'\rangle \pm |-\boldsymbol{p}'\rangle),$$

which are also degenerate energy (but not momentum) eigenstates. The corresponding wave functions

$$\psi_{\pm\boldsymbol{p}'}(\boldsymbol{x}') = \langle\boldsymbol{x}'|\pm\boldsymbol{p}'\rangle = e^{\pm i\boldsymbol{p}'\cdot\boldsymbol{x}'/\hbar}$$

are neither even nor odd, whereas

$$\begin{aligned} \langle\boldsymbol{x}'|(|\boldsymbol{p}'\rangle + |-\boldsymbol{p}'\rangle) &\propto \cos\boldsymbol{p}'\cdot\boldsymbol{x}'/\hbar \\ \langle\boldsymbol{x}'|(|\boldsymbol{p}'\rangle - |-\boldsymbol{p}'\rangle) &\propto \sin\boldsymbol{p}'\cdot\boldsymbol{x}'/\hbar \end{aligned}$$

are.

Example One dimensional symmetric double well

The ground state is the symmetric state $|S\rangle$ and the first excited state the antisymmetric state $|A\rangle$:

$$\begin{aligned} H|S\rangle &= E_S|S\rangle \\ \pi|S\rangle &= |S\rangle \\ H|A\rangle &= E_A|S\rangle \\ \pi|A\rangle &= -|A\rangle, \end{aligned}$$

where $E_S < E_A$. When the potential barrier V between the wells increases the energy difference between the states decreases:

$$\lim_{V\to\infty}(E_A - E_S) \to 0.$$

We form the superpositions

$$\begin{aligned} |L\rangle &= \frac{1}{\sqrt{2}}(|S\rangle + |A\rangle) \\ |R\rangle &= \frac{1}{\sqrt{2}}(|S\rangle - |A\rangle), \end{aligned}$$

which are neither energy nor parity eigenstates.
Let us suppose that at the moment $t_0 = 0$ the state of the system is $|L\rangle$. At a later moment, t, the system is descibed by the state vector

$$\begin{aligned} &|L, t_0 = 0; t\rangle \\ &\quad = \frac{1}{\sqrt{2}}(e^{-iE_St/\hbar}|S\rangle + e^{-iE_At/\hbar}|A\rangle) \\ &\quad = \frac{1}{\sqrt{2}}e^{-iE_St/\hbar}(|S\rangle + e^{-i(E_A-E_S)t/\hbar}|A\rangle), \end{aligned}$$

because now the time evolution operator is simply

$$\mathcal{U}(t, t_0 = 0) = e^{-iHt/\hbar}.$$

At the moment $t = T/2 = 2\pi\hbar/2(E_A - E_S)$ the system is in the pure $|R\rangle$ state and at the moment $t = T$ again in its pure initial state $|L\rangle$. The system oscillates (tunnels through the barrier) between the states $|L\rangle$ and $|R\rangle$ at the angular frequency

$$\omega = \frac{E_A - E_S}{\hbar}.$$

When $V \to \infty$, then $E_A \to E_S$. Then the states $|L\rangle$ and $|R\rangle$ are degenerate energy eigenstates but not parity eigenstates. A particle which is localized in one of the wells will remain there forever. Its wave function does not, however, obey the same symmetry as the Hamiltonian:
we are dealing with a *broken symmetry.*
As an example one may consider a ferromagnet. The basic Hamiltonian for iron atoms is rotationally invariant while the magnet itself is obviously not since all the spins are aligned to some definitive direction.

Selection rules
Suppose that the states $|\alpha\rangle$ and $|\beta\rangle$ are parity eigenstates:

$$\begin{aligned}\pi|\alpha\rangle &= \epsilon_\alpha|\alpha\rangle \\ \pi|\beta\rangle &= \epsilon_\beta|\beta\rangle,\end{aligned}$$

where ϵ_α and ϵ_β are the parities (± 1) of the states. Now

$$\langle\beta|\boldsymbol{x}|\alpha\rangle = \langle\beta|\pi^\dagger\pi\boldsymbol{x}\pi^\dagger\pi|\alpha\rangle = -\epsilon_\alpha\epsilon_\beta\langle\beta|\boldsymbol{x}|\alpha\rangle,$$

so

$$\langle\beta|\boldsymbol{x}|\alpha\rangle = 0 \text{ unless } \epsilon_\alpha = -\epsilon_\beta.$$

Example The intensity of the dipole transition is proportional to the matrix element of the operator $\boldsymbol{x}$ between the initial and final states. Dipole transitions are thus possible between states which have opposite parity.
Example Dipole moment.
If

$$[H, \pi] = 0,$$

then no non degenerate state has dipole moment:

$$\langle n|\boldsymbol{x}|n\rangle = 0.$$

(but in the case of degeneracy it is possible to have permanent dipole moment)
Generally, operators that are odd under parity ($\mathbf{p}$, $\mathbf{S} \cdot \mathbf{x}$) have non-vanishing matrix elements between states of opposite parity
and operators that are even in parity connect the states with the same parity