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 spinles 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

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

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 Hamiltonia 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.

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

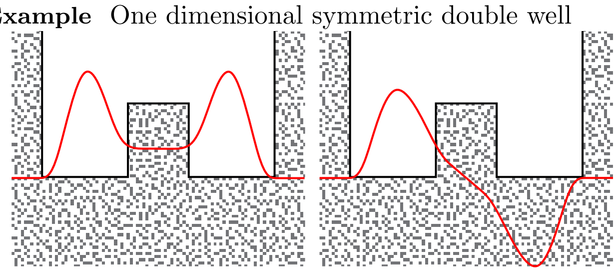
$$\psi_{\pm\boldsymbol{p}'}(\boldsymbol{x}') = \langle\boldsymbol{x}'|\pm\boldsymbol{p}'\rangle = e^{\pm i\boldsymbol{p}'\cdot\boldsymbol{x}'/\hbar}$$

are neither even nor odd, whereas

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

are.

Example One dimensional symmetric double well



Symmetric ($\mathcal{S}$) Antisymmetric ($\mathcal{A}$)

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

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

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

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

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 between the states $|L\rangle$ and $|R\rangle$ at the angular velocity

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

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.*

Selection rules

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

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

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:

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

The same holds for any quantity if the corresponding operator o is odd:

$$\pi^\dagger o\pi = -o.$$