Chapter 4 Symmetry in Quantum Mechanics

4.1 Symmetries, Conservation laws and Degeneracies

Symmetries in Classical Physics

• If the Lagrangian $\mathcal{L}(q_i, \dot{q}_i)$ is invariant under displacement, the canonical moment conjugate to q_i is conserved.

$\Rightarrow$ If $q_i \to q_i + \delta q_i$, then we must have $\dfrac{\partial \mathcal{L}}{\partial q_i} = 0.$

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

$$\therefore \quad \frac{dp_i}{dt} = 0$$

• If $\mathcal{H}(p_i, q_i)$ has a symmetry under $q_i \to q_i + \delta q_i$, the canonical moment is conserved.

$$\begin{cases} \dfrac{dp_i}{dt} = -\dfrac{\partial \mathcal{H}}{\partial q_i} = 0 \quad \text{whenever } \dfrac{\partial \mathcal{H}}{\partial q_i} = 0 \\ \quad \dfrac{dq_i}{dt} = \dfrac{\partial \mathcal{H}}{\partial p_i} \end{cases}$$

- **Symmetry in quantum mechanics**

A symmetry is a physical operation that leaves the physics unchanged.

As an example, we consider a free particles, $\mathbf{H} = \dfrac{p^2}{2m}$.

(1) Under the translation $x \to x + a$,

$\mathbf{H}$ is unchanged and $\left[x + a, p\right] = i\hbar$.

$\rightarrow$ Translation is a symmetry of the free-particle system.

(2) Under inversion (or parity) $x \to -x$, $p \to -p$

$\left[-x, -p\right] = i\hbar$ and $\mathbf{H}$ is preserved.

(3) Under time reversal $t \to -t$,

$\mathbf{H}$ is invariant.

• **Continuous symmetries and conservation laws**

Given a symmetry operation is described by a unitary operator U,

this is a symmetry of the Hamiltonian if H is unchanged by the action of U.

Namely, $\mathscr{S}^{+}\mathbf{H}\mathscr{S} = \mathbf{H} \Leftrightarrow \left[\mathbf{H}, U\right] = 0.$

• Continuous symmetry if the symmetry transformation can be continuously built up as a series of infinitesimal transformations starting from the identity operator.

e.g. translation and rotation

• Discrete symmetries if symmetries cannot be built up in this way

e.g. parity

Infinitesimal unitary (symmetry) operation can be written as

$$\mathscr{S} = 1 - \frac{i\varepsilon}{\hbar}\mathbf{G},$$

then the statment $\mathscr{S}^{\dagger}\mathscr{S} = 1$ implies $\mathbf{G}^{+}\mathbf{G} = 1$ $\left(\mathbf{G} = \text{Hermitian operator}\right)$.

(i) For an infinitesimal translation by a displacement dx' in the x-direction,

$$\mathbf{G} \to p_x, \quad \varepsilon \to dx'$$

(ii) For an infinitesimal time evolution with time displacement dt,

$$\mathbf{G} \to \mathbf{H}, \quad \varepsilon \to dt$$

(iii) For an infinitesimal rotation around the kth axis by angle $d\phi$,

$$\mathbf{G} \to J_k, \quad \varepsilon \to d\phi$$

- Suppose that $\mathbf{H}$ is invariant under $\mathscr{S}$, then we have

$$\mathscr{S}^{+}\mathbf{H}\mathscr{S} = \mathbf{H}.$$

$$\left(1+\frac{i\varepsilon}{\hbar}\mathbf{G}\right)\mathbf{H}\left(1-\frac{i\varepsilon}{\hbar}\mathbf{G}\right)=\mathbf{H} \quad \Leftrightarrow \quad \left[G,\mathbf{H}\right]=\frac{dG}{dt}=0;$$

G is a constant of motion.

Noether's theorem For every continuous symmetry of the Hamiltonian in quantum mechanics, there is a corresponding conserved quantity. Conversely, if some observable G is conserved, then $\left[G,\mathbf{H}\right]$=0, and we can define unitary operators

$$U(\theta) = e^{i\theta G/\hbar},$$

which will satisfy $U^{+}(\theta)\mathbf{H}\,U(\theta)$=H, showing that $U(\theta)$ is a continuous symmetry of the Hamiltonian.

For example) If $\mathbf{H}$ is invariant under translation, p is a constant of the motion.

When $[G,\mathcal{H}]=0$, $[G,U]=0$.
A ket $|g'\rangle$ is an G eigenket.
Suppose at t_0 the system is in an eigenstate of G, then the ket at a later time

$$|g',t_0;t\rangle = U(t,t_0)|g'\rangle$$

is also an eigenket of G with the same eigenvalue g'.

$$G\left[U(t,t_0)|g'\rangle\right] = U(t,t_0)G|g'\rangle = g'\left[U(t,t_0)|g'\rangle\right]$$

Once a ket is a G eigenket, it is always a G eigenket with the same value.

- **Degeneracies**

Suppose that $[\mathcal{H},\mathscr{S}]=0$ and $|n\rangle$ is an energy eigenket with eigenvalue E_n.
Then $\mathscr{S}|n\rangle$ is also an energy eigenket with the same energy,

$$\because \quad \mathcal{H}\left(\mathscr{S}|n\rangle\right) = \mathscr{S}\mathcal{H}|n\rangle = E_n\left(\mathscr{S}|n\rangle\right).$$

Suppose $|n\rangle$ and $\mathscr{S}|n\rangle$ represent different states, two states are degenerate.
Notation ! $\mathscr{S}(\lambda)|n\rangle$ with continuous parameters λ have the same energy.

• Exampe) Suppose the Hamiltonian is rotationally invariant, so

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

$$\Rightarrow \left[\mathbf{J}, \mathcal{H}\right] = 0, \text{ and } \left[\mathbf{J}^2, \mathcal{H}\right] = 0$$

$\left|n; j, m\right\rangle =$ simultaneous eigenkets of $\mathcal{H}, \mathbf{J}^2$, and $\mathbf{J}_z$

$\mathscr{D}(R)\left|n; j, m\right\rangle = \sum_m \left|n; j, m'\right\rangle \mathscr{D}_{m'm}(R)$ has the same energy.

$\rightarrow$ $(2j+1)$-fold degeneracy= the number of possible m-values

• An atomic electron having potential $V(r) + V_{LS}(r)\mathbf{L}\cdot\mathbf{S}$ has a $(2j+1)$-fold degeneracy for each atomic level because r and $\mathbf{L}\cdot\mathbf{S}$ are both rotationally invariant.

Applying an external electric or magnetic field leads to a breaking of the rotational symmetry; as a result, the $(2j+1)-$fold degeneracy is lifted.

4.2 Discrete symmetries, parity, or space inversion

• The parity operation (space inversion), applied to transformtion on the coordinate system, changes a right-handed system into a left-handed system.

• Given $|\alpha\rangle$, a space-inverted state is obtained by applying a parity operator π:

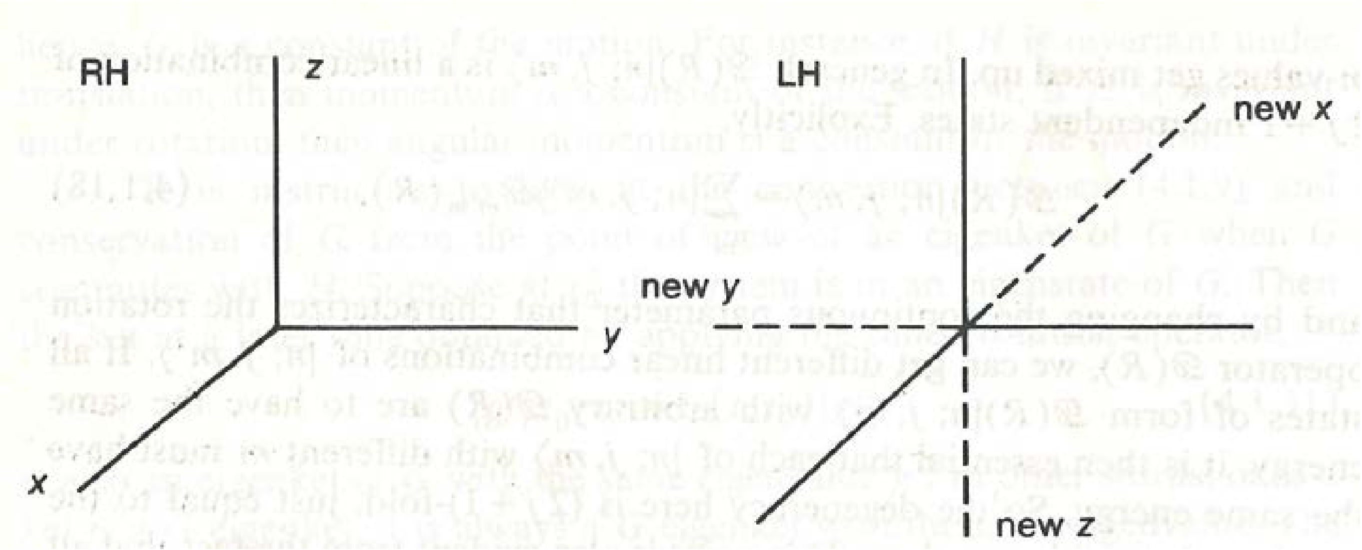
$$|\alpha\rangle \;\to\; \boldsymbol{\pi}|\alpha\rangle$$

• The expectation value of **x** with respect to the spaced-inverted state is opposite in sign

$$\langle\alpha|\boldsymbol{\pi}^{+}\mathbf{x}\boldsymbol{\pi}|\alpha\rangle = -\langle\alpha|\mathbf{x}|\alpha\rangle$$

$$\therefore\;\; \boldsymbol{\pi}^{+}\mathbf{x}\boldsymbol{\pi} = -\mathbf{x}$$

$$\text{or}\quad \mathbf{x}\boldsymbol{\pi} = -\boldsymbol{\pi}\mathbf{x} \quad \{\mathbf{x}, \boldsymbol{\pi}\} = 0.$$



- How does an eigenstate of the position operator transform under parity ?

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

Proof) $\mathbf{x}\boldsymbol{\pi}|\mathbf{x}'\rangle = -\boldsymbol{\pi}\mathbf{x}|\mathbf{x}'\rangle = (-\mathbf{x}')\boldsymbol{\pi}|\mathbf{x}'\rangle.$

$\boldsymbol{\pi}|\mathbf{x}'\rangle$ is an eigenket of $\mathbf{x}$ with eigenvalue -x'. So it must be the same as a position eigenket $|\mathbf{-x}'\rangle$ up to a phase factor.

- Taking $e^{i\delta} = 1$ by convention,

$$\boldsymbol{\pi}^2|\mathbf{x}'\rangle = |\mathbf{x}'\rangle;\ \text{hence}\ \boldsymbol{\pi}^2 = 1.$$

$\boldsymbol{\pi}$ is not only unitary but also Hermitian; $\boldsymbol{\pi}^{-1} = \boldsymbol{\pi}^{+} = \boldsymbol{\pi}$ with eigenvalue ± 1.

- What about the momentum operator ?

Intuitively, $\mathbf{p} = m\dfrac{d\mathbf{x}}{dt}$ is expected to be odd under parity.

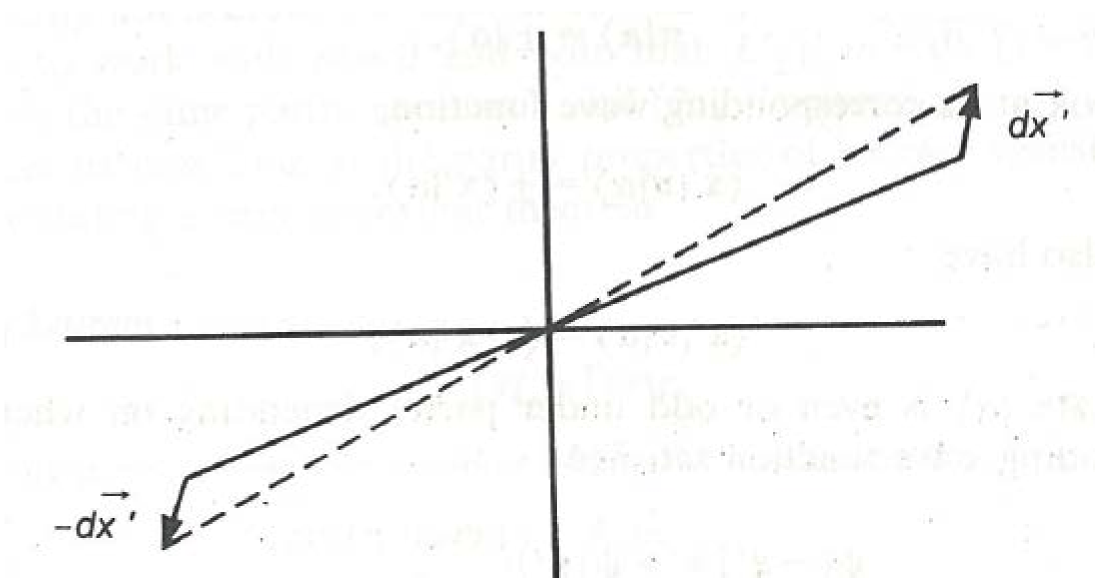
More sophicated argument: Translation followed by parity is equivalent to parity followed by translation in the opposite direction.

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

$$\boldsymbol{\pi}\left(1 - \frac{i\mathbf{p}\cdot d\mathbf{x}'}{\hbar}\right)\boldsymbol{\pi}^{+} = 1 + \frac{i\mathbf{p}\cdot d\mathbf{x}'}{\hbar}$$

$$\Rightarrow \quad \left\{\boldsymbol{\pi}, \mathbf{p}\right\} = 0 \qquad \text{or} \qquad \boldsymbol{\pi}^{+}\mathbf{p}\boldsymbol{\pi} = -\mathbf{p}$$

- Translation followed by parity vs parity followed by translation



- The behavior of $\mathbf{J}$ under parity

  For orbital angular momentum, $[\boldsymbol{\pi}, \mathbf{L}] = 0$

because $\mathbf{L} = \mathbf{x} \times \mathbf{p}$ and both $\mathbf{x}$ and $\mathbf{p}$ are odd under parity.

- For 3×3 orthogonal matrices, we have

$$\mathrm{R}^{(\mathrm{parity})}\mathrm{R}^{(\mathrm{rotation})} = \mathrm{R}^{(\mathrm{rotation})}\mathrm{R}^{(\mathrm{parity})}$$

where $$\mathrm{R}^{(\mathrm{parity})} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

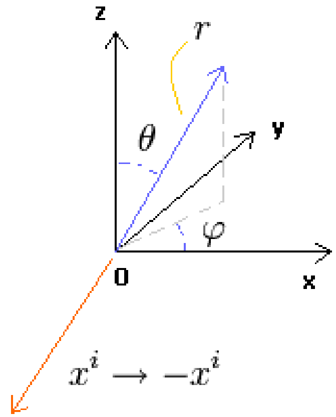
- In quantum mechanics,

$$\boldsymbol{\pi}\mathcal{D}(R) = \mathcal{D}(R)\boldsymbol{\pi} \quad \text{where} \quad \mathcal{D}(R) = 1 - \frac{i\mathbf{J}\cdot\hat{\mathbf{n}}\varepsilon}{\hbar}.$$

$$[\boldsymbol{\pi}, \mathbf{J}] = 0 \quad \text{or} \quad \boldsymbol{\pi}^{+}\mathbf{J}\boldsymbol{\pi} = \mathbf{J}.$$

→ The spin operator $\mathbf{S}$ given by $\mathbf{J} = \mathbf{L} + \mathbf{S}$ must be even under parity, transforming in the same way as $\mathbf{L}$.

$$\begin{cases} \mathbf{x} \to -\mathbf{x} \\ \mathbf{p} \to -\mathbf{p} \\ \mathbf{L} \to \mathbf{L} \end{cases}$$



$$P : x^i \to -x^i$$

$$= \quad r \to r, \quad \theta \to \pi - \theta, \quad \varphi \to \varphi + \pi$$

- $\boldsymbol{\pi}\mathbf{p}\,\psi(\mathbf{r}) = \boldsymbol{\pi}\left\{-i\hbar\dfrac{\partial\psi(\mathbf{r})}{\partial\mathbf{r}}\right\} = -\,i\hbar\dfrac{\partial\psi(-\mathbf{r})}{\partial(-\mathbf{r})} = i\hbar\dfrac{\partial\psi(-\mathbf{r})}{\partial\mathbf{r}}$

  $\mathbf{p}\boldsymbol{\pi}\psi(\mathbf{r}) = -i\hbar\dfrac{\partial\psi(-\mathbf{r})}{\partial\mathbf{r}}$

$\therefore \quad \boldsymbol{\pi}\mathbf{p} = -\mathbf{p}\boldsymbol{\pi}$

- $\boldsymbol{\pi}^{-1}\mathbf{exp}\left(\dfrac{-i\mathbf{p}\cdot\mathbf{d}}{\hbar}\right)\boldsymbol{\pi} = \mathbf{exp}\left(\dfrac{-i\boldsymbol{\pi}^{-1}\mathbf{p}\boldsymbol{\pi}\cdot\mathbf{d}}{\hbar}\right) = \mathbf{exp}\left(\dfrac{i\mathbf{p}\cdot\mathbf{d}}{\hbar}\right)$ where d is a displacement vector.

  $\left[\boldsymbol{\pi}, \mathcal{T}_{\mathbf{d}}\right] \neq 0$

- $\boldsymbol{\pi}^{-1}\mathbf{exp}\left(\dfrac{-i\mathbf{J}\cdot\widehat{\mathbf{n}}\phi}{\hbar}\right)\boldsymbol{\pi} = \mathbf{xp}\left(\dfrac{-i\boldsymbol{\pi}^{-1}\mathbf{J}\boldsymbol{\pi}\cdot\widehat{\mathbf{n}}\phi}{\hbar}\right) = \mathbf{exp}\left(\dfrac{-i\mathbf{J}\cdot\widehat{\mathbf{n}}\phi}{\hbar}\right)$

  $\left[\boldsymbol{\pi}, \mathcal{D}(\widehat{\mathbf{n}}, \phi)\right] = 0$

- Scalar that is invariant under rotations and even under parity such as $\mathbf{p}^2$ and $\mathbf{x}^2$
- Pseudoscalar that is invariant under rotations, but odd under parity

For example, $\mathbf{L}\cdot\mathbf{S}$ or $\mathbf{x}\cdot\mathbf{p}$ are ordinary scalars because under space inversion we have

$$\boldsymbol{\pi}^{+}\mathbf{L}\cdot\mathbf{S}\boldsymbol{\pi} = \mathbf{L}\cdot\mathbf{S}.$$

- $\mathbf{S}\cdot\mathbf{x}$ is a pseudoscalar because $\mathbf{S}\cdot\mathbf{x}$ transforms like ordinary scalars under rotations

but $\boldsymbol{\pi}^{+}\mathbf{S}\cdot\mathbf{x}\boldsymbol{\pi} = -\mathbf{S}\cdot\mathbf{x}$ is under space inversion.

- Vectors that are odd under parity are called polar vectors.

For example) $\mathbf{p}$ and $\mathbf{x}$

- Vectors that are even under parity are called axial vectors.

For example) $\mathbf{L}, \mathbf{S}, \mathbf{J}$

- **Wave functions under parity**

$\psi(\mathbf{x}') = \langle \mathbf{x}' | \alpha \rangle$ and $|\alpha\rangle$=an eigenket of parity

The wave function of the space-inverted state is

$$\begin{aligned} \langle \mathbf{x}' | \boldsymbol{\pi} | \alpha \rangle &= \langle -\mathbf{x}' | \alpha \rangle = \psi(-\mathbf{x}'). \\ &= \pm \langle \mathbf{x}' | \alpha \rangle \quad \because \ \boldsymbol{\pi} | \alpha \rangle = \pm | \alpha \rangle \end{aligned}$$

The state $|\alpha\rangle$ is even or odd under parity depending on whether the corresponding wave function satisfies

$$\psi(-\mathbf{x}') = \pm\psi(\mathbf{x}') \begin{cases} \text{even parity,} \\ \text{odd parity} \end{cases}$$

$\rightarrow$ $\pm\psi(\mathbf{x}')$ are symmetry and antisymmetric under $\mathbf{x} \rightarrow -\mathbf{x}$.

$\rightarrow$ Not all wave functions have definite parities.

Momentum

The momentum eigenket is not a parity eigenket since $\{\boldsymbol{\pi}, \boldsymbol{p}\} = 0$.

As an example, consider the free particle $\mathbf{H} = \dfrac{p^2}{2m}$.

The plane wave is the wave function for a momentum eigenket:

$$\frac{1}{\sqrt{2\pi\hbar}} e^{i\boldsymbol{p}\cdot\mathbf{x}/\hbar}$$

is not parity eigenstates since $\psi(-\mathbf{x}') = e^{-i\boldsymbol{p}\cdot\mathbf{x}'/\hbar} \neq \pm\psi(\mathbf{x}')$.

However, $[\boldsymbol{\pi}, \mathbf{H}] = 0$, which means that we can choose energy eigenstates that are also parity eigenstates in this case. We can choose energy and parity eigenstates, but are not momentum eigenstates as

$$\frac{1}{\sqrt{2}}\left(\frac{1}{\sqrt{2\pi\hbar}} e^{i\boldsymbol{p}\cdot\mathbf{x}/\hbar} \pm \frac{1}{\sqrt{2\pi\hbar}} e^{-i\boldsymbol{p}\cdot\mathbf{x}/\hbar}\right).$$

$\boxed{\text{An eigenstate of orbital angular momentum is a parity eigenstate since } \left[\boldsymbol{L},\boldsymbol{\pi}\right]=0.}$

Let's examine the properties of L^2 and L_z wave function under the space inversion,

in a rectangular coordinate: $x \to -x, \quad y \to -y, \quad z \to -z$

in a spherical polar coordinate: $\left(r,\theta,\phi\right) \quad \to \quad \left(r,\pi-\theta,\phi+\pi\right).$

$$\sin\theta \;\to\; \sin(\pi-\theta) = \sin\theta$$

$$\cos\theta \;\to\; \cos(\pi-\theta) = -\cos\theta$$

and $\quad e^{im\phi} \;\to\; e^{im(\phi+\pi)} = e^{im\phi}(\cos m\pi + i\sin m\pi) = (-1)^m e^{im\phi}.$

$$\left\langle \mathbf{x}' \middle| \alpha, lm \right\rangle = R_\alpha(r) Y_l^m(\theta,\phi)$$

Using the explicit form of

$$Y_l^m(\theta,\phi) = \frac{(-1)^l}{2^l l!}\sqrt{\frac{(2l+1)!(l+m)!}{4\pi(l-m)!}}\; e^{im\phi}\frac{1}{\sin^m\theta}\frac{d^{l-m}}{d(\cos\theta)^{l-m}}\sin^{2l}\theta \quad \text{for a positive } m$$

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

$$= (-1)^m \times (-1)^{l-m}\frac{(-1)^l}{2^l l!}\sqrt{\frac{(2l+1)!(l+m)!}{4\pi(l-m)!}}\; e^{im\phi}\frac{1}{\sin^m\theta}\frac{d^{l-m}}{d(\cos\theta)^{l-m}}\sin^{2l}\theta$$

$$= (-1)^l Y_l^m(\theta,\phi)$$

$$\therefore \quad \boldsymbol{\pi}\left|\alpha, lm\right\rangle = (-1)^l \left|\alpha, lm\right\rangle$$

even parity for l=0, 2, 4,...

odd parity for l=1, 3, 5,...

Example

l=0 $Y_0^0(\theta,\phi)$ is constant, meaning that $\boldsymbol{\pi}\left|\alpha, l=0, m=0\right\rangle = \left|\alpha, l=0, m=0\right\rangle$.

l=1 $\quad Y_1^1(\theta,\phi) = \sqrt{\dfrac{3}{8\pi}}\ \sin\theta e^{i\phi} \rightarrow \sqrt{\dfrac{3}{8\pi}}\ \sin(\pi\text{-}\theta)e^{i(\pi+\phi)} = -\sqrt{\dfrac{3}{8\pi}}\sin\theta e^{i\phi}$

$\rightarrow$ $Y_1^1(\theta,\phi)$ transforms like x+iy. Because vectors are odd under parity,

$\boldsymbol{\pi}\left|\alpha, l=1, m=1\right\rangle = -\left|\alpha, l=1, m=1\right\rangle$.

l=2 $\quad Y_2^2(\theta,\phi) = \sqrt{\dfrac{15}{32\pi}}\ \sin^2\theta e^{2i\phi} \rightarrow \sqrt{\dfrac{3}{8\pi}}\ \sin^2(\pi\text{-}\theta)e^{2i(\pi+\phi)} = \sqrt{\dfrac{15}{32\pi}}\ \sin^2\theta e^{2i\phi}$

Theorem Suppose $\left[\mathcal{H}, \boldsymbol{\pi}\right] = 0$
and $\left|n\right\rangle$ is a nondegenerate eigenket of $\mathcal{H}$ with eigenvalue E_n:

$$\mathcal{H}\left|n\right\rangle = E_n\left|n\right\rangle; \quad \text{then} \quad \left|n\right\rangle \text{ is also a parity eigenket.}$$

Proof) $\frac{1}{2}\left(1 \pm \boldsymbol{\pi}\right)\left|n\right\rangle$ is a parity eigenket with eigenvalues ± 1.

$$\because \quad \boldsymbol{\pi}\left\{\frac{1}{2}\left(1 \pm \boldsymbol{\pi}\right)\left|n\right\rangle\right\} = \frac{1}{2}\left(\boldsymbol{\pi} \pm 1\right)\left|n\right\rangle = \pm\left|n\right\rangle$$

$\frac{1}{2}\left(1 \pm \boldsymbol{\pi}\right)\left|n\right\rangle$ is also an energy eigenket with eigenvalue E_n.

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

Thus, $\left|n\right\rangle$ and $\frac{1}{2}\left(1 \pm \boldsymbol{\pi}\right)\left|n\right\rangle$ must represent the same state, otherwise there would be two states with the same energy - a contradiction of the nondegenerate assumption.
Therefore, $\left|n\right\rangle$ is a parity eigenket with parity ± 1.

Comment) $\left[\mathcal{H}, \boldsymbol{\pi}\right] = 0$ if V(**r**, **p**, **J**)=V(-**r**, -**p**, **J**).

Example 1) The Hamiltonian of the simple harmonic oscillator is

$$\mathcal{H} = \frac{\mathbf{p}^2}{2m} + \frac{m\omega^2\mathbf{x}^2}{2}.$$

$\left[\mathcal{H}, \boldsymbol{\pi}\right]=0$ and thus $\left|n\right\rangle$ is a parity eigenket.

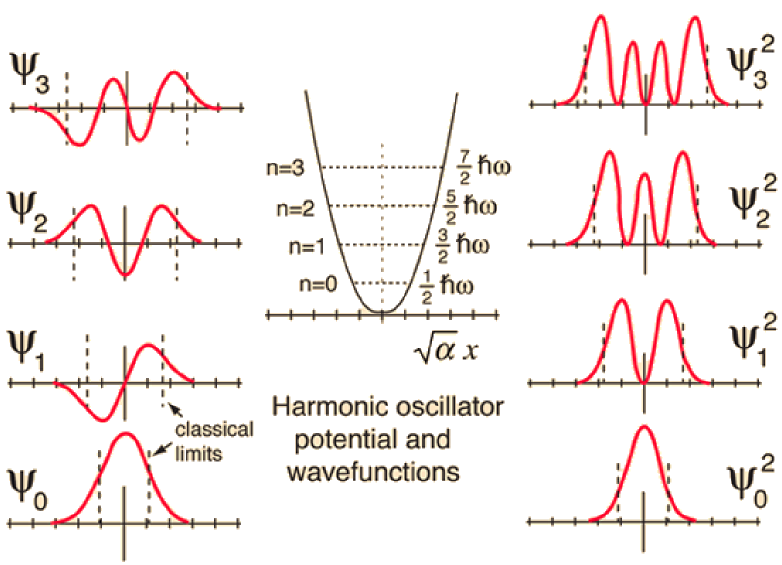
The ground state $\psi_0(x')$ has even parity because $\psi_0(x') = \frac{1}{\pi^{1/4} x_0^{1/2}} \exp\left(-\frac{1}{2}\left(\frac{x'}{x_0}\right)^2\right)$

is Gaussian. The first excited state,

$$\left|1\right\rangle = \mathbf{a}^\dagger\left|0\right\rangle = \sqrt{\frac{m\omega}{2\hbar}}\left(\mathbf{x} - \frac{i\mathbf{p}}{m\omega}\right)\left|0\right\rangle = \sqrt[4]{\frac{4}{\pi x_0^6}}\, x \exp\left(-\frac{1}{2}\left(\frac{x'}{x_0}\right)^2\right)$$

has an odd parity because both **x** and **p are odd.**

In general, the parity of the SHO is given by $(-1)^n$.



Example 2) Consider the hydrogen atom in nonrelativistic quantum mechanics. As the energy depends only on the prinicipal quantum number n and $2p$ and $2s$ states are degenerate.

The Coulomb potential $\mathrm{V}(r)=-\dfrac{Ze^2}{r}$ is invariant under parity as $r \rightarrow r$ under space inversion. However,

$$c_p\left|2p\right\rangle + c_s\left|2s\right\rangle = c_p R_{20}(r) Y_0^m(\theta,\phi) + c_s R_{20}(r) Y_1^m(\theta,\phi)$$

$\rightarrow$ $(-1)^0 c_p R_{20}(r) Y_0^m(\theta,\phi) + (-1)^1 c_s R_{20}(r) Y_1^m(\theta,\phi)$ is not a parity eigenket.
This illustrates the significance of the nondegenrate assumption.

Example 3) Consider a momentum eigenket. Even if $\left[\mathcal{H},\boldsymbol{\pi}\right]=0$ for a free particle Hamiltonian $\mathcal{H}$, the momentum eigenket is not a parity eigenket since $\left\{\mathbf{p},\boldsymbol{\pi}\right\}=0$. However, since $\left|\mathbf{p'}\right\rangle$ and $\left|\mathbf{-p'}\right\rangle$ are degenerate, the theorem remains intact. In fact, we can easily construct

$$\frac{1}{\sqrt{2}}\left\{\left|\mathbf{p'}\right\rangle \pm \left|\mathbf{-p'}\right\rangle\right\},$$ which are parity eigenkets with eigenvalues ± 1.

$e^{-i\mathbf{p'}\cdot\mathbf{x'}/\hbar}$ does not have a definite parity, but $\cos\left(\mathbf{p'}\cdot\mathbf{x'}/\hbar\right)$ and $\sin\left(\mathbf{p'}\cdot\mathbf{x'}/\hbar\right)$ do.

• Schroedinger equation $\mathcal{H}\psi(r) = -\frac{\hbar^2}{2m}\nabla^2\psi(r) + V(r)\psi(r) = E\psi(r)$

Changing $r \to -r$,

$$\mathcal{H}\psi(-r) = -\frac{\hbar^2}{2m}\nabla^2\psi(-r) + V(-r)\psi(-r) = E\psi(-r).$$

If $V(r) = V(-r)$, $\psi(r)$ and $\psi(-r)$ are the eigenfunctions of $\mathcal{H}$ with the same energy E.

(i) If the eigenvalues of $\mathcal{H}$ are nondegenerate, $\psi(r) = \alpha\psi(-r)$.

Changing $r \to -r$, we have $\psi(-r) = \alpha\psi(r)$.

$$\psi(-r) = \alpha\psi(r) = \alpha^2\psi(-r)$$

$$\therefore \quad \alpha = \pm 1$$

Namely, the eigenfunctions of $\mathcal{H}$ have either an even or an odd parity.

(ii) If the eigenvalues of $\mathcal{H}$ are degenerate, $\psi(r)$ and $\psi(-r)$ have the same eigenvalue but should be an independent function. Thus,

$$\mathcal{H}\psi(r) = -\frac{\hbar^2}{2m}\nabla^2\psi(r) + V(r)\psi(r) = E\psi(r)$$

$$\mathcal{H}\psi(-r) = -\frac{\hbar^2}{2m}\nabla^2\psi(-r) + V(-r)\psi(-r) = E\psi(-r)$$

$$\rightarrow \qquad \mathcal{H}\left\{\psi(r) \pm \psi(-r)\right\} = E\left\{\psi(r) \pm \psi(-r)\right\}$$

$$\psi_{\text{even}}(r) = \psi(r) + \psi(-r) \;\; \text{or} \;\; \psi_{\text{odd}}(r) = \psi(r) - \psi(-r).$$

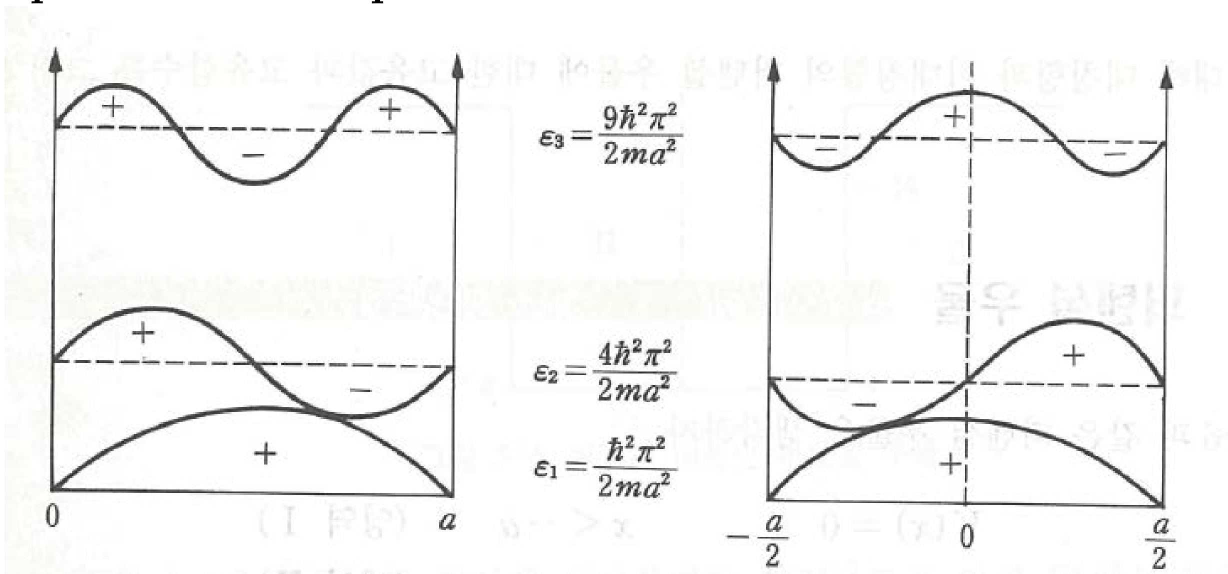
• If the solutions of $\mathcal{H}$ are chosen to have an even parity,

$$\boldsymbol{\pi}\mathcal{H}\psi(r) = \mathcal{H}\psi(-r) = \mathcal{H}\boldsymbol{\pi}\psi(r) = E\psi(-r).$$

$$\left[\mathcal{H}, \boldsymbol{\pi}\right] = \frac{d}{dt}\left\langle \boldsymbol{\pi} \right\rangle = 0 \text{ for a symmetric potential.}$$

$\rightarrow$ The parity violation occurs for β-decay in weak interaction.

Example : Infinite well potential



$$V(x) = \begin{cases} 0 & 0 \le x \le a \\ \infty & x < 0,\ x > a \end{cases} \quad \xrightarrow{x \to x + \frac{a}{2}} \quad V(x) = \begin{cases} 0 & -\frac{a}{2} \le x \le \frac{a}{2} \\ \infty & x < -\frac{a}{2},\ x > \frac{a}{2} \end{cases}$$

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a} x\right)$$

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\frac{n\pi}{a}\left(x + \tfrac{a}{2}\right) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a} x + \frac{n\pi}{2}\right)$$

$$= \begin{cases} \sqrt{\frac{2}{a}} \cos\frac{n\pi x}{a} & n = 1, 3, 5, \ldots \\ \sqrt{\frac{2}{a}} \sin\frac{n\pi x}{a} & n = 2, 4, 6, \ldots \end{cases}$$

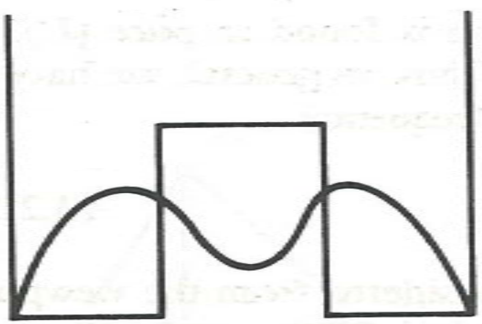
$$E_n = \frac{n^2\hbar^2\pi^2}{2ma^2}$$

- **Symmetrical double - well potential**

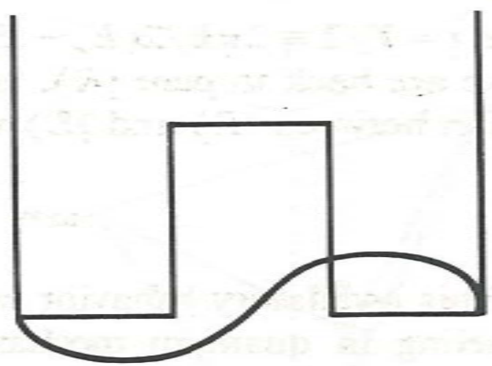
The Hamiltonian is invariant under parity. The two lowest lying states are called the symmetrical state $|S\rangle$ and the antisymmetric state $|A\rangle$. They are simultaneous eigenkets of $\mathcal{H}$ and π.

$$|R\rangle = \frac{1}{\sqrt{2}}\left(|S\rangle + |A\rangle\right) \qquad \text{and} \qquad |L\rangle = \frac{1}{\sqrt{2}}\left(|S\rangle - |A\rangle\right)$$

$|R\rangle$ and $|L\rangle$ are not parity eigenstates because $|R\rangle$ and $|L\rangle$ are interchanged under parity. They are not energy eigenstate either (nonstationary states).



Symmetric IS>



Anti-symmetric IA>

The system is represented by $\left|R\right\rangle$ at t=0. At a later time,

$$\left|R, t_0 = 0; t\right\rangle = \frac{1}{\sqrt{2}}\left(e^{-iE_S t}\left|S\right\rangle + e^{-iE_A t}\left|A\right\rangle\right)$$
$$= \frac{1}{\sqrt{2}} e^{-iE_S t}\left(\left|S\right\rangle + e^{-i(E_A - E_S)t}\left|A\right\rangle\right).$$

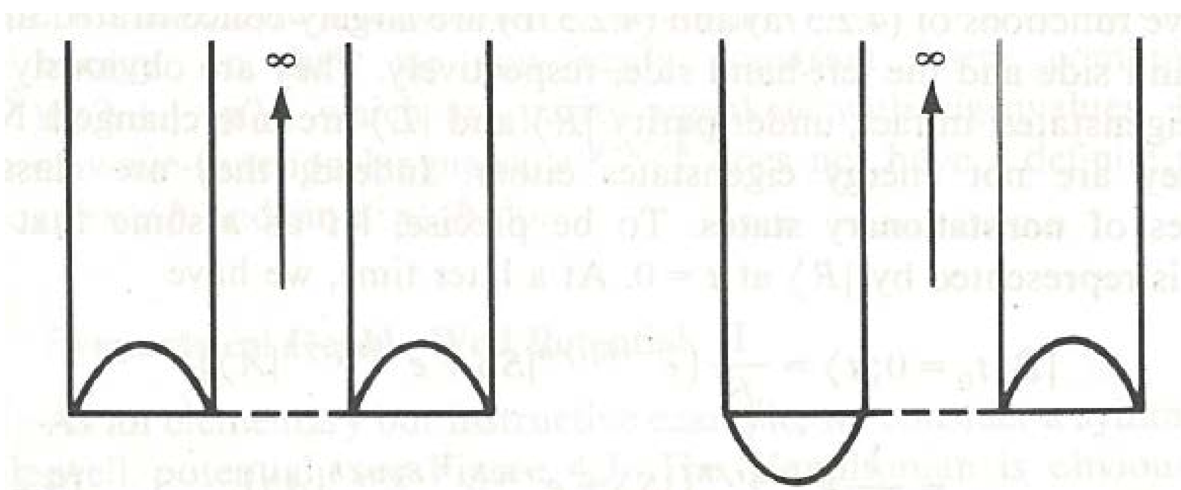
At time $t = T/2 \equiv 2\pi\hbar/2(E_A - E_S)$, the system is found in pure $\left|L\right\rangle$.

At time $t = T$, the system is back to pure $\left|R\right\rangle$.

An oscillation between $\left|R\right\rangle$ and $\left|L\right\rangle$ with angular frequency $\omega = \dfrac{(E_A - E_S)}{\hbar}$.

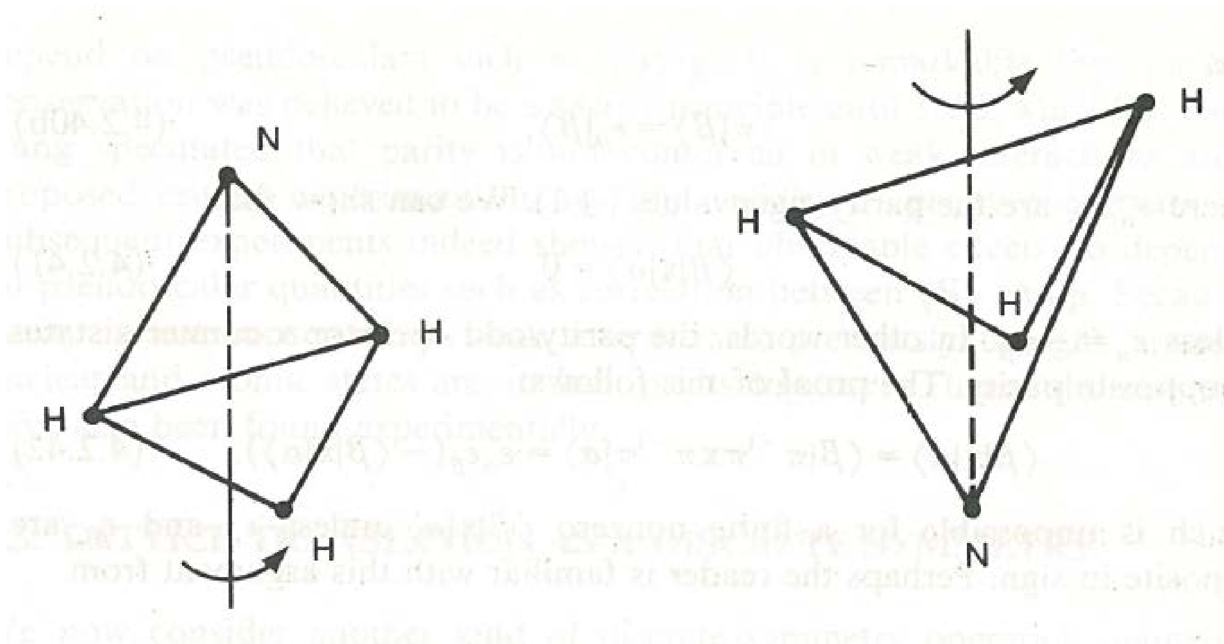
Let the middle barrier become high enough. The $\left|S\right\rangle$ and $\left|A\right\rangle$ states are now degenerate. $\left|R\right\rangle$ and $\left|L\right\rangle$ are energy eigenkets even though they are not parity eigenkets.

A ground state is asymmetrical despite the fact that the Hamiltonian itself is symmetrical under space inversion. This is an example of broken symmetry and degeneracy.



The example of the symmetrical double well is an ammonia molecule, NH_3.
The up and down positions for the N atom are analogous to R and L.
The parity and energy eigenstates are superpositions of the up and down positions.
The energy difference between the simultaneous eigenstates of energy and parity correspond to an oscillation frequency of 24,000 MHz ($\lambda \sim 1$ cm).

Optical isomers (sugar or amino acids) are of the R-type (or L-type) only.
In many cases, the oscillation time is an order of 10^4-10^6 years. The R-type molecules remain right-handed for all practical purposed.



- **Parity - Selection rule**

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

$$\pi|\alpha\rangle = \varepsilon_\alpha|\alpha\rangle \quad \text{and} \quad \pi|\beta\rangle = \varepsilon_\beta|\beta\rangle,$$

where ε_α, ε_β are the parity eigenvalues (± 1).

$$\boxed{\langle\beta|\mathbf{x}|\alpha\rangle = 0 \ \text{ unless } \ \varepsilon_\alpha = -\varepsilon_\beta.}$$

Proof) $\langle\beta|\mathbf{x}|\alpha\rangle = \langle\beta|\pi^{-1}\pi\mathbf{x}\pi^{-1}\pi|\alpha\rangle = \varepsilon_\alpha\varepsilon_\beta\left(-\langle\beta|\mathbf{x}|\alpha\rangle\right)$,

which is impossible for a finite nonzero $\langle\beta|\mathbf{x}|\alpha\rangle$ unless ε_α and ε_β are opposite in sign.

If ψ_α and ψ_β have the same parity,

$$\int \psi_\beta^* \mathbf{x} \psi_\alpha d\tau = 0.$$

Radiative transitions take place between states of opposite parity as a consequence of multipole expansion (Laporte's rule).

- **Parity Nonconservation**

The Hamiltonian for the weak interaction is not invariant under parity.

Because parity is not conserved in weak interactions, "pure" nuclear and atomic states are parity mixtures.