Chapter 26 Parity operator
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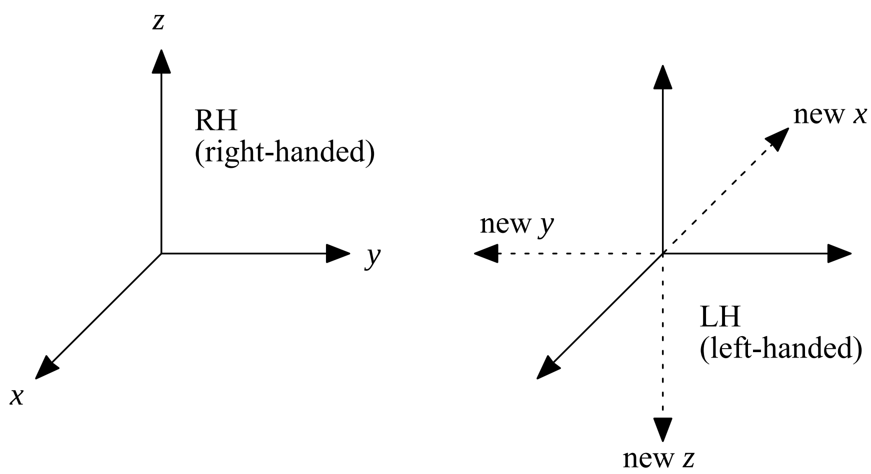
26.1 Property of parity operator



$\hat{\pi}$: parity operator (unitary operator)

$$|\psi'\rangle = \hat{\pi}|\psi\rangle$$

or

$$\langle\psi'| = \langle\psi|\hat{\pi}^{+}$$

Definition: the average of $\hat{x}$ in the new state $|\psi'\rangle$ is opposite to that in the old state $|\psi\rangle$

$$\langle\psi'|\hat{x}|\psi'\rangle = -\langle\psi|\hat{x}|\psi\rangle$$

or

$$\langle\psi|\hat{\pi}^{+}\hat{x}\hat{\pi}|\psi\rangle = -\langle\psi|\hat{x}|\psi\rangle$$

or

$$\hat{\pi}^{+}\hat{x}\hat{\pi} = -\hat{x} \qquad (1)$$

The position vector is called a polar vector.

Normalization:

$$\langle \psi' | \psi' \rangle = \langle \psi | \hat{\pi}^{+} \hat{\pi} | \psi \rangle = \langle \psi | \psi \rangle = 1$$

or

$$\hat{\pi}^{+} \hat{\pi} = \hat{1} \qquad (2)$$

Thus the parity operator is an unitary operator. From Eqs.(1) and (2),

$$\hat{x}\hat{\pi} + \hat{\pi}\hat{x} = 0$$

or

$$\hat{x}\hat{\pi} | x \rangle = -\hat{\pi}\hat{x} | x \rangle = -x\hat{\pi} | x \rangle$$

Thus

$\hat{\pi} | x \rangle$ is the eigenket of $\hat{x}$ with the eigenvalue ($-x$).

or

$$\hat{\pi} | x \rangle = | -x \rangle$$

$$\hat{\pi}\hat{\pi} | x \rangle = \hat{\pi} | -x \rangle = | x \rangle$$

or

$$\hat{\pi}^{2} = \hat{1}$$

Since $\hat{\pi}^{+} \hat{\pi} = \hat{1}$ and $\hat{\pi}^{2} = \hat{1}$,

$$\hat{\pi}^{+} \hat{\pi}\hat{\pi} = \hat{\pi}$$

or

$$\hat{\pi}^{+} = \hat{\pi}$$

So the parity operator is a Hermite operator.

$$\hat{\pi}|p\rangle = \hat{\pi}\int_{-\infty}^{\infty} dx'|x'\rangle\langle x'|p\rangle = \int_{-\infty}^{\infty} dx'\,\hat{\pi}|x'\rangle\langle x'|p\rangle = \int_{-\infty}^{\infty} dx'|-x'\rangle\langle x'|p\rangle$$
$$= \int_{-\infty}^{\infty} dx'|-x'\rangle \frac{1}{\sqrt{2\pi\hbar}}\exp(\frac{ipx'}{\hbar}) = \int_{-\infty}^{\infty} dx|x\rangle \frac{1}{\sqrt{2\pi\hbar}}\exp(-\frac{ipx}{\hbar}) = \int_{-\infty}^{\infty} dx|x\rangle\langle x|-p\rangle$$
$$=|-p\rangle$$

Note that $x' = -x$ and $dx' = -dx$.

$$\hat{\pi}|p\rangle = |-p\rangle$$

$$\hat{p}|p\rangle = p|p\rangle$$

$$\hat{\pi}\hat{p}|p\rangle = p\hat{\pi}|p\rangle = p|-p\rangle$$

$$\hat{p}\hat{\pi}|p\rangle = \hat{p}|-p\rangle = -p|-p\rangle$$

Thus we have

$$\hat{\pi}\hat{p} + \hat{p}\hat{\pi} = 0$$

Thus the linear momentum is called a polar vector.

26.2 Eigenvalue problem for the parity operator

We consider the eigenvalue problem for the parity operator.

$$\hat{\pi}|\psi_\alpha\rangle = \alpha|\psi_\alpha\rangle$$

$$\hat{\pi}^2|\psi_\alpha\rangle = \alpha\hat{\pi}|\psi_\alpha\rangle = \alpha\hat{\pi}|\psi_\alpha\rangle = \alpha^2|\psi_\alpha\rangle = |\psi_\alpha\rangle$$

Thus we have

$$\alpha^2 = 1 \qquad \text{or} \qquad \alpha = \pm 1.$$

We define $|\psi_+\rangle$ and $|\psi_-\rangle$ such that

$$\hat{\pi}|\psi_\pm\rangle = \pm|\psi_\pm\rangle$$

Note that

$$\hat{\pi}|x\rangle = |-x\rangle$$

or

$$\langle x|\hat{\pi}^{+} = \langle x|\hat{\pi} = \langle -x|$$

$$\langle x|\hat{\pi}|\psi_{\pm}\rangle = \pm\langle x|\psi_{\pm}\rangle$$

or

$$\langle -x|\psi_{\pm}\rangle = \pm\langle x|\psi_{\pm}\rangle$$

or

$$\psi_{\pm}(-x) = \pm\psi_{\pm}(x)$$

$\psi_{+}(x)$ is an even function with respect to *x*. $\psi_{-}(x)$ is an odd function with respect to *x*.

26.3 Commutation relation between the Hamiltonian and parity operator

$V(-\hat{x}) = V(\hat{x})$: symmetric potential

$$\hat{H} = \frac{1}{2m}\hat{p}^2 + V(\hat{x})$$

$$\hat{\pi}^{+}V(\hat{x})\hat{\pi} = V(-\hat{x}) = V(\hat{x})$$

$$\hat{\pi}^{+}\hat{p}^2\hat{\pi} = (-\hat{p})^2 = \hat{p}^2$$

Thus we have

$$\hat{\pi}^{+}\hat{H}\hat{\pi} = \hat{H}$$

or

$$[\hat{\pi}, \hat{H}] = 0$$

The Hamiltonian $\hat{H}$ is invariant under parity. $|\psi_{\alpha}\rangle$ is the simultaneous eigenket of $\hat{H}$ and $\hat{\pi}$.

$$\hat{H}|\psi_{\alpha}\rangle = E_{\alpha}|\psi_{\alpha}\rangle$$

and

$$\hat{\pi}|\psi_\alpha\rangle = \alpha|\psi_\alpha\rangle$$

with $\alpha = \pm 1$. For $\alpha = 1$, symmetric state. For $\alpha = -1$, antisymmetric state.

26.4 Projection Operartor

Any function $\psi(x)$ can be expressed by an addition of even function $\psi_+(x)$ and odd function $\psi_-(x)$.

$$\psi(x) = \psi_+(x) + \psi_-(x)$$

with

$$\psi_+(x) = \frac{\psi(x) + \psi(-x)}{2}$$

$$\psi_-(x) = \frac{\psi(x) - \psi(-x)}{2}$$

Since

$$\hat{\pi}|x\rangle = |-x\rangle$$

or

$$\langle x|\hat{\pi}^+ = \langle x|\hat{\pi} = \langle -x|$$

$$\hat{\pi}|x\rangle = |-x\rangle$$

$$\psi_+(x) = \frac{\psi(x) + \psi(-x)}{2}$$

or

$$\begin{aligned}\langle x|\psi_+\rangle &= \frac{1}{2}[\langle x|\psi\rangle + \langle -x|\psi\rangle] \\ &= \frac{1}{2}[\langle x|\psi\rangle + \langle x|\hat{\pi}^+|\psi\rangle] \\ &= \frac{1}{2}[\langle x|\psi\rangle + \langle x|\hat{\pi}|\psi\rangle]\end{aligned}$$

or

$$|\psi_+\rangle = \frac{1}{2}(\hat{1} + \hat{\pi})|\psi\rangle = \hat{P}_+|\psi\rangle$$

$$\langle x|\psi_-\rangle = \frac{1}{2}[\langle x|\psi\rangle - \langle -x|\psi\rangle]$$
$$= \frac{1}{2}[\langle x|\psi\rangle - \langle x|\hat{\pi}|\psi\rangle$$

$$|\psi_-\rangle = \frac{1}{2}(\hat{1} - \hat{\pi})|\psi\rangle = \hat{P}_-|\psi\rangle$$

We define the following operators (projection operators)

$$\hat{P}_+ = \frac{1}{2}(\hat{1} + \hat{\pi})$$

$$\hat{P}_- = \frac{1}{2}(\hat{1} - \hat{\pi})$$

We have

$$\hat{\pi}|\psi_+\rangle = \frac{1}{2}\hat{\pi}(\hat{1} + \hat{\pi})|\psi\rangle = \frac{1}{2}(\hat{1} + \hat{\pi})|\psi\rangle = \hat{P}_+|\psi\rangle = |\psi_+\rangle$$

Thus $|\psi_+\rangle$ is the eigenket of $\hat{\pi}$ with the eigenvalue +1. We also have

$$\hat{\pi}|\psi_-\rangle = \frac{1}{2}\hat{\pi}(\hat{1} - \hat{\pi})|\psi\rangle = -\frac{1}{2}(\hat{1} - \hat{\pi})|\psi\rangle = -\hat{P}_-|\psi\rangle = -|\psi_-\rangle$$

Thus $|\psi_-\rangle$ is the eigenket of $\hat{\pi}$ with the eigenvalue -1. In summary, the projection operators satisfy the following properties.

1. $\hat{P}_+ + \hat{P}_- = \hat{1}$

2. $[\hat{P}_+, \hat{P}_-] = \hat{0}$

3. $\hat{P}_\pm^{\ 2} = \hat{P}_\pm$

4. $\hat{P}_+\hat{P}_- = \hat{0}$, $\hat{P}_-\hat{P}_+ = \hat{0}$

5. $\hat{\pi}\hat{P}_+ = \hat{P}_+$, $\hat{\pi}\hat{P}_- = -\hat{P}_-$

((**Proof**))
2.

$$\hat{P}_+\hat{P}_- = \frac{1}{4}(\hat{1}+\hat{\pi})(\hat{1}-\hat{\pi}) = \hat{0}$$

$$\hat{P}_-\hat{P}_+ = \frac{1}{4}(\hat{1}-\hat{\pi})(\hat{1}+\hat{\pi}) = \hat{0}$$

$$[\hat{P}_+, \hat{P}_-] = \hat{0}$$

26.5 Parity Selection Rule (Even and Odd parity Operators)

We define a new operator as

$$\hat{\pi}^+\hat{A}_+\hat{\pi} = \hat{A}_+$$

for operator with even parity

$$\hat{\pi}^+\hat{A}_-\hat{\pi} = -\hat{A}_-$$

and for operator with odd parity.

((**Example**))

$$\hat{\pi}^+\hat{J}_x\hat{\pi} = \hat{J}_x \text{ (even parity).}$$

$$\hat{\pi}^+\hat{x}\hat{\pi} = -\hat{x} \text{ (odd parity)}$$

$$\hat{\pi}^+\hat{p}\hat{\pi} = -\hat{p} \text{ (odd parity)}$$

Suppose that $|\varphi_\alpha\rangle$ and $|\varphi_\beta\rangle$ (parity eigenstate, $\alpha = \pm 1$, $\beta = \pm 1$)

$$\hat{\pi}|\varphi_\alpha\rangle = \alpha|\varphi_\alpha\rangle, \ \hat{\pi}|\varphi_\beta\rangle = \beta|\varphi_\beta\rangle$$

with $\alpha = \pm 1$ and $\beta = \pm 1$.

$$\langle\varphi_\beta|\hat{\pi}^+\hat{A}_+\hat{\pi}|\varphi_\alpha\rangle = \alpha\beta\langle\varphi_\beta|\hat{A}_+|\varphi_\alpha\rangle = \langle\varphi_\beta|\hat{A}_+|\varphi_\alpha\rangle$$

When α = -β (different parity) the matrix element $\langle\varphi_\beta|\hat{A}_-|\varphi_\alpha\rangle$ is equal to zero.

$$\langle \varphi_\beta | \hat{\pi}^+ \hat{A}_- \hat{\pi} | \varphi_\alpha \rangle = \alpha\beta \langle \varphi_\beta | \hat{A}_- | \varphi_\alpha \rangle = -\langle \varphi_\beta | \hat{A}_- | \varphi_\alpha \rangle$$

When $\alpha = \beta$ (the same parity), the matrix element $\langle \varphi_\beta | \hat{A}_- | \varphi_\alpha \rangle$ is equal to zero.

((**Example**))

Simple harmonics

$$\hat{\pi}|n\rangle = (-1)^n |n\rangle, \qquad \langle n|\hat{\pi}^+ = (-1)^n \langle n|$$

$$\langle n|\hat{\pi}^+ \hat{x} \hat{\pi}|m\rangle = -\langle n|\hat{x}|m\rangle = (-1)^{n+m} \langle n|\hat{x}|m\rangle$$

or

$$\langle n|\hat{x}|m\rangle = (-1)^{n+m+1} \langle n|\hat{x}|m\rangle$$

26.6 Applications to the Simple Harmonics

Suppose that $[\hat{H}, \hat{\pi}] = \hat{0}$. The Hamiltonian $\hat{H}$ and $\hat{\pi}$ are commutable and $|n\rangle$ is nondegererate eigenket of $\hat{H}$ with the energy E_n.

$$\hat{H}|n\rangle = E_n |n\rangle.$$

Then $|n\rangle$ is also a parity eigenket.

((**Proof**))

$\hat{P}_+|n\rangle$ (even parity) and $\hat{P}_+|n\rangle$ (odd parity) are the eigenkets of $\hat{\pi}$ with eigenvalues ±1.

Since $[\hat{H}, \hat{\pi}] = \hat{0}$,

$$\hat{H}\hat{P}_\pm |n\rangle = \hat{P}_\pm \hat{H}|n\rangle = E_n \hat{P}_\pm |n\rangle$$

$\hat{P}_\pm|n\rangle$ is the eigenket of $\hat{H}$ with the eigenvalue E_n. $|n\rangle$ and $\hat{P}_\pm|n\rangle$ must represent the same energy. Otherwise there could be two states with the same energy-contradiction of our nondegenerate assumption.

$\hat{P}_\pm|n\rangle$ should be proportional to $|n\rangle$.

or

$$\hat{P}_{\pm}\left|n\right\rangle = a_{\pm}\left|n\right\rangle$$

$$\hat{\pi}\hat{P}_{\pm}\left|n\right\rangle = \pm\hat{P}_{\pm}\left|n\right\rangle = a_{\pm}\hat{\pi}\left|n\right\rangle$$

or

$$\pm a_{\pm}\left|n\right\rangle = a_{\pm}\hat{\pi}\left|n\right\rangle$$

or

$$\hat{\pi}\left|n\right\rangle = \pm\left|n\right\rangle$$

$\left|n\right\rangle$ must be a parity eigenket with the parity ±1.

26.6 ((Example)) Simple harmonic oscillator (nondegenerate)

Since

$$\left\langle x\right|\hat{\pi}\left|0\right\rangle = \left\langle x|0\right\rangle = \left\langle -x|0\right\rangle \text{ (even function),}$$

$$\hat{\pi}\left|0\right\rangle = \left|0\right\rangle$$

$$\hat{\pi}\left|1\right\rangle = \hat{\pi}\hat{a}^{+}\left|0\right\rangle = \frac{\beta}{\sqrt{2}}\hat{\pi}(\hat{x} - \frac{i\hat{p}}{m\omega_0})\left|0\right\rangle = -\hat{a}^{+}\hat{\pi}\left|0\right\rangle = -\hat{a}^{+}\left|0\right\rangle = -\left|1\right\rangle$$

Then $\left|1\right\rangle$ must have an odd parity. Similarly $\left|n\right\rangle$ has a $(-1)^n$ parity.

26.7 Parity of spherical harmonics

$$[\hat{\pi}, \hat{J}_x] = [\hat{\pi}, \hat{J}_y] = [\hat{\pi}, \hat{J}_z] = \hat{0}$$

$$[\hat{\pi}, \hat{J}_x^{\ 2}] = [\hat{\pi}, \hat{J}_y^{\ 2}] = [\hat{\pi}, \hat{J}_z^{\ 2}] = \hat{0}$$

((**Proof**))

Note that

$$\hat{\pi}^{+}\hat{J}_x\hat{\pi} = \hat{J}_x \text{ or } [\hat{\pi}, \hat{J}_x] = \hat{0}$$

$$[\hat{\pi}, \hat{J}_x{}^2] = \hat{\pi}\hat{J}_x\hat{J}_x - \hat{J}_x\hat{J}_x\hat{\pi} = [\hat{\pi}, \hat{J}_x]\hat{J}_x = \hat{0}$$

We now use the following relations:

$$[\hat{\pi}, \hat{J}_z] = \hat{0}, \qquad [\hat{\pi}, \hat{J}^2] = \hat{0}$$

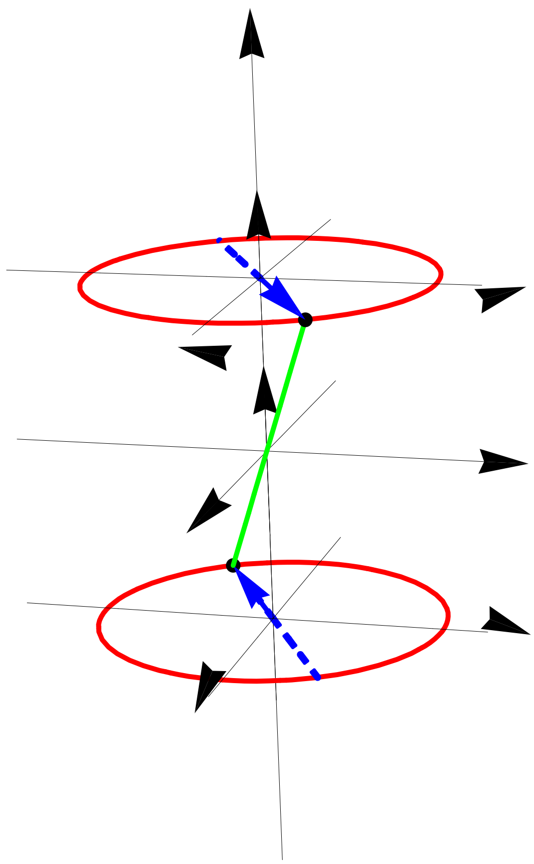
$\left| lm \right\rangle$ is an eigenket of $\hat{\pi}$:

$$\hat{\pi}\left| lm \right\rangle = (-1)^l \left| lm \right\rangle$$

From the definition of the spherical harmonics

$$\left\langle \mathbf{n} \middle| \ell m \right\rangle = Y_\ell^m(\theta,\phi)$$

$$\left\langle \mathbf{n} \right| \hat{\pi} = \left\langle \theta,\phi \right| \hat{\pi} = \left\langle \pi - \theta, \phi + \pi \right|$$



(Note that $\langle \mathbf{r} | \hat{\pi} = \langle -\mathbf{r} |$)

$$\langle \mathbf{n} | \hat{\pi} | lm \rangle = \langle \pi - \theta, \phi + \pi | lm \rangle = Y_l^m(\pi - \theta, \phi + \pi)$$

Here

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

for $m \geq 0$.

and

$$Y_l^{-m}(\theta,\phi) = (-1)^m [Y_l^m(\theta,\phi)]^*$$

Note that

for $\theta \to \pi - \theta$, $\cos\theta \to -\cos\theta$

for $\phi \to \phi + \pi$, $e^{im\phi} \to (-1)^m e^{im\phi}$

$$\begin{aligned}\langle \pi - \theta, \phi + \pi | lm \rangle &= Y_l^m(\pi - \theta, \phi + \pi) \\ &= (-1)^m (-1)^{l-m} Y_l^m(\theta,\phi) \\ &= (-1)^l Y_l^m(\theta,\phi)\end{aligned}$$

Therefore

$$\langle \mathbf{n} | \hat{\pi} | lm \rangle = (-1)^l \langle \mathbf{n} | lm \rangle$$

or

$$\hat{\pi} | lm \rangle = (-1)^\ell | lm \rangle$$