Parity operator
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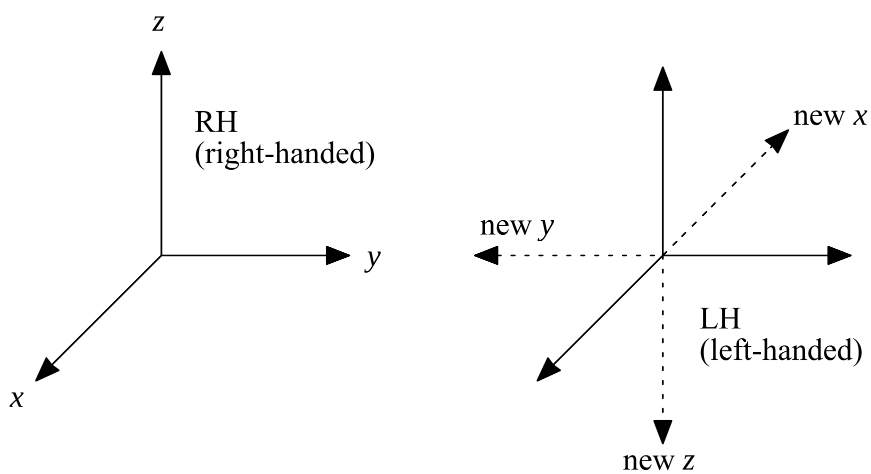
(Date: November 24, 2015)

We consider the inversion transformation, which consists in simultaneously changing the sign of all the coordinates, i.e., a reversal of the direction of each coordinate axis; a right-handed coordinate system then becomes left-handed, and vice versa. The invariance of the Hamiltonian under this transformation expresses the symmetry of space under mirror reflections. In classical mechanics, the invariance of Hamiltonian's function with respect to inversion does not lead to a conservation law, but the situation is different in quantum mechanics.
((Landau and Lifshits, Quantum Mechanics, Pergamon Press).

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**.

From the normalization condition

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

we have

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

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

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

We apply the ket vector $|x\rangle$ on this operator,

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

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

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

Since

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

we have

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

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

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

or

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

which means that $\hat{\pi}$ is the Hermite operator.

2. The linear momentum $\hat{p}$

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

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

or

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

or

$$\hat{\pi}^{+}\hat{p}\hat{\pi} = -\hat{p}\,.$$

or

$$\hat{p}\hat{\pi} = -\hat{\pi}\hat{p}\,.$$

Thus the linear momentum is called a polar vector.

Now we apply the ket vector $|p\rangle$ on this from the right side

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

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

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

This relation can be also derived as follows.

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

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

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

3. Polar vectors and pseudovectors

The vectors that are odd under parity, are called *polar vectors*. The vectors that are even under parity, are called axial vectors, or pseudovectors.

(a) Position vector $\hat{\boldsymbol{r}}$ (polar vector)

$$\hat{\pi}\hat{\boldsymbol{r}}\hat{\pi} = -\hat{\boldsymbol{r}}$$

(b) Linear momentum $\hat{\boldsymbol{p}}$ (polar vector)

$$\hat{\pi}\hat{\boldsymbol{p}}\hat{\pi} = -\hat{\boldsymbol{p}}$$

(c) Orbital angular momentum $\hat{\boldsymbol{L}} = \hat{\boldsymbol{r}} \times \hat{\boldsymbol{p}}$ *(axial vectors, or pseudovectors)*

$$\begin{aligned}
\hat{\pi}\hat{L}_z\hat{\pi} &= \hat{\pi}(\hat{x}\hat{p}_y - \hat{y}\hat{p}_x)\hat{\pi} \\
&= \hat{\pi}\hat{x}\hat{\pi}\hat{\pi}\hat{p}_y\hat{\pi} - \hat{\pi}\hat{y}\hat{p}_x\hat{\pi}\hat{\pi}x\hat{\pi} \\
&= (-\hat{x})(-\hat{p}_y) - (-\hat{p}_y)(-\hat{x}) \\
&= \hat{x}\hat{p}_y - \hat{y}\hat{p}_x
\end{aligned}$$

or

$$\hat{\pi}\hat{L}_z\hat{\pi} = \hat{L}_z$$

Similarly we have

$$\hat{\pi}\hat{L}_y\hat{\pi} = \hat{L}_y, \quad \text{and} \quad \hat{\pi}\hat{L}_x\hat{\pi} = \hat{L}_x.$$

(d) Infinitesimal translation operator: $\hat{T}(\delta x) = \hat{1} - \frac{i}{\hbar}\hat{p}_x\delta x$

We have the relation for the infinitesimal translation operator as

$$\hat{\pi}\hat{T}(-\delta x)\hat{\pi} = \hat{T}(\delta x)$$

since

$$\hat{\pi}\hat{T}(\delta x)\hat{\pi} = \hat{\pi}(\hat{1} - \frac{i}{\hbar}\hat{p}_x\delta x)\hat{\pi}$$

$$= \hat{1} - \frac{i}{\hbar}\hat{\pi}\hat{p}_x\hat{\pi}\delta x$$

$$= \hat{1} + \frac{i}{\hbar}\hat{p}_x\delta x$$

(e) Translation operator $\hat{T}(a)$

We have the relation for the translation operator as

$$\hat{\pi}\hat{T}(-a)\hat{\pi} = \hat{T}(a)$$

since

$$\hat{\pi}\hat{T}(a)|x\rangle = \hat{\pi}|x + a\rangle = |-(x + a)\rangle$$

$$\hat{T}(-a)\hat{\pi}|x\rangle = \hat{T}(-a)|-x\rangle = |-(x + a)\rangle$$

(f) Rotation operator $\hat{R}$ and the angular momentum $\hat{\boldsymbol{J}}$

We start with the relation

$$\hat{R}|\boldsymbol{r}\rangle = |\Re\boldsymbol{r}\rangle$$

Then we get

$$\hat{\pi}\hat{R}|\boldsymbol{r}\rangle = \hat{\pi}|\Re\boldsymbol{r}\rangle = |-\Re\boldsymbol{r}\rangle$$

and

$$\hat{R}\hat{\pi}|\boldsymbol{r}\rangle = \hat{R}|-\boldsymbol{r}\rangle = |\Re(-\boldsymbol{r})\rangle$$

Since

$$\Re(-\boldsymbol{r}) = -\Re\boldsymbol{r}$$

we have

$$\hat{\pi}\hat{R} = \hat{R}\hat{\pi}$$

or

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

We now consider the infinitesimal rotation operator around the *i* axis (i = x, y, and z),

$$\hat{R}_i=\hat{1}-\frac{i}{\hbar}\hat{J}_i\delta\theta_i \qquad (i = x, y, \text{and } z)$$

Using the above commutation relation we have

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

Then the angular momentum $\hat{\boldsymbol{J}}$ is even under parity (*axial vector*, or *pseudovector*). We note that $\hat{\boldsymbol{J}}$ is an general angular momentum operator including the spin angular momentum $\hat{\boldsymbol{S}}$ and the orbital angular momentum $\hat{\boldsymbol{L}}$.

((**Note**))

$$\Re(-\boldsymbol{r})=-\Re\boldsymbol{r}$$

$$\Re\boldsymbol{r}=\begin{pmatrix}\Re_{11} & \Re_{12} & \Re_{13}\\ \Re_{21} & \Re_{22} & \Re_{23}\\ \Re_{31} & \Re_{32} & \Re_{33}\end{pmatrix}\begin{pmatrix}x\\ y\\ z_3\end{pmatrix}$$

where for example,

$$\Re_z(\phi)=\begin{pmatrix}\cos\phi & -\sin\phi & 0\\ \sin\phi & \cos\phi & 0\\ 0 & 0 & 1\end{pmatrix}$$

around the *z* axis by a rotation angle ϕ.
Then we get

$$\Re(-\boldsymbol{r})=\begin{pmatrix}\Re_{11} & \Re_{12} & \Re_{13}\\ \Re_{21} & \Re_{22} & \Re_{23}\\ \Re_{31} & \Re_{32} & \Re_{33}\end{pmatrix}\begin{pmatrix}-x\\ -y\\ -z\end{pmatrix}=-\begin{pmatrix}\Re_{11} & \Re_{12} & \Re_{13}\\ \Re_{21} & \Re_{22} & \Re_{23}\\ \Re_{31} & \Re_{32} & \Re_{33}\end{pmatrix}\begin{pmatrix}x\\ y\\ z\end{pmatrix}=-\Re\boldsymbol{r}.$$

(g) Spin vector $\hat{\boldsymbol{S}}$: axial vector

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

(h) The scalar $\hat{S}\cdot\hat{r}$: pseudoscalar

$$\hat{\pi}(\hat{\boldsymbol{S}}\cdot\hat{\boldsymbol{r}})\hat{\pi} = \hat{\pi}\hat{\mathbf{S}}\hat{\pi}\cdot\hat{\pi}\hat{\boldsymbol{r}}\hat{\pi} = -\hat{\boldsymbol{S}}\cdot\hat{\boldsymbol{r}} .$$

(i) The spin-orbit interaction $\hat{L}\cdot\hat{S}$: an ordinary scalar

$$\hat{\pi}(\hat{\boldsymbol{L}}\cdot\hat{\boldsymbol{S}})\hat{\pi} = \hat{\pi}\hat{\mathbf{L}}\hat{\pi}\cdot\hat{\pi}\hat{\mathbf{S}}\hat{\pi} = \hat{\boldsymbol{L}}\cdot\hat{\boldsymbol{S}} .$$

4. 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*.

5. Commutation relation between the Hamiltonian and parity operator

Suppose that the potential energy is $V(x)$ is an even function such that

$V(-x) = V(x)$: symmetric potential

We consider the Hamiltonian given by

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

Note that

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

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

Thus we have

$$\hat{\pi}^+ \hat{H}\hat{\pi} = \hat{H}\ , \qquad \text{or} \qquad \hat{\pi}\hat{H}\hat{\pi} = \hat{H}$$

In other words, we have the commutation relation.

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

This means that the average of $\hat{H}$ is invariant under the parity operation,

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

The Hamiltonian $\hat{H}$ is invariant under parity. Since $[\hat{\pi}, \hat{H}] = 0$, $|\psi_\alpha\rangle$ 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 $\alpha = \pm 1$: $\alpha = 1$, symmetric state (even parity) and $\alpha = -1$, antisymmetric state (odd parity).

6. 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

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

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

Then we get

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

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.

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

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

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

7. 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

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

8. 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

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

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

or

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

or

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

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

9. ((Example)) Simple harmonic oscillator (nondegenerate)

Since

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

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

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

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

10. 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

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

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

We now use the following relations:

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

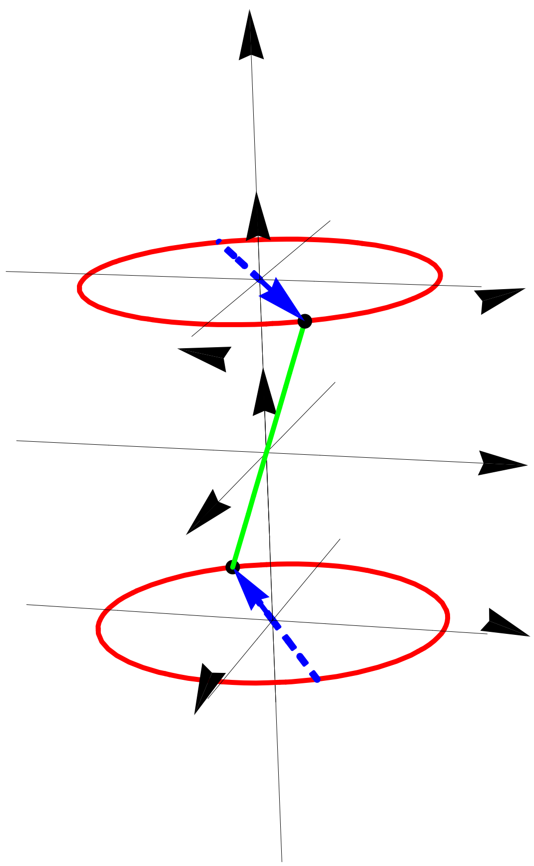
$|lm\rangle$ is an eigenket of $\hat{\pi}$:

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

From the definition of the spherical harmonics

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

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



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

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

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

and

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

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

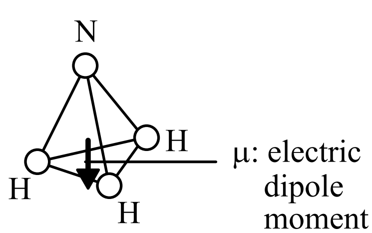
Therefore

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

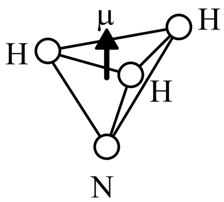
or

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

11. The state for NH_3 molecules



$|1\rangle$ when the nitrogen is up.



$|2\rangle$ when the nitrogen is down.

The property of the parity operator:

$$\hat{\pi}|\boldsymbol{r}\rangle = |-\boldsymbol{r}\rangle, \qquad \langle \boldsymbol{r}|\hat{\pi}^{+} = \langle \boldsymbol{r}|\hat{\pi} = \langle -\boldsymbol{r}|$$

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

$$\hat{\pi}^{+}\hat{\boldsymbol{r}}\hat{\pi} = -\hat{\boldsymbol{r}}$$

It is appropriate to assume that

$$\langle \boldsymbol{r}|2\rangle = \langle -\boldsymbol{r}|1\rangle = \langle \boldsymbol{r}|\hat{\pi}|1\rangle .$$

Then we get

$$|2\rangle = \hat{\pi}|1\rangle, \qquad \hat{\pi}|2\rangle = \hat{\pi}^{2}|1\rangle = |1\rangle$$

We consider the parity operator $\hat{\pi}$, such that

$$\hat{\pi}|1\rangle = |2\rangle \qquad \hat{\pi}|2\rangle = |1\rangle$$

Therefore the kets $|1\rangle$ and $|2\rangle$ are not the eigenkets of $\hat{\pi}$. Since

$$\hat{\pi} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \hat{\sigma}_{x},$$

we have the eigenkets as

$$\hat{\pi}|+x\rangle = \hat{\sigma}_{x}|+x\rangle = |+x\rangle$$

$$\hat{\pi}|-x\rangle = \hat{\sigma}_{x}|-x\rangle = -|+x\rangle$$

with

$$|+x\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix} = \frac{1}{\sqrt{2}}(|1\rangle + |2\rangle) \qquad \text{(eigenvalue +1)}$$

and

$$|-x\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\end{pmatrix} = \frac{1}{\sqrt{2}}(|1\rangle - |2\rangle) \qquad \text{(eigenvalue -1)}$$

When $\boldsymbol{r} \rightarrow \boldsymbol{r}' = -\boldsymbol{r}$,

$$|\psi\rangle \rightarrow |\psi'\rangle = \hat{\pi}|\psi\rangle, \quad \text{or} \quad \langle\psi'| = \langle\psi|\hat{\pi}$$

We assume that the Hamiltonian $\hat{H}$ is invariant under the parity change.

$$\langle\psi'|\hat{H}|\psi'\rangle = \langle\psi|\hat{H}|\psi\rangle$$

or

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

or

$$\hat{\pi}\hat{H} = \hat{H}\hat{\pi}.$$

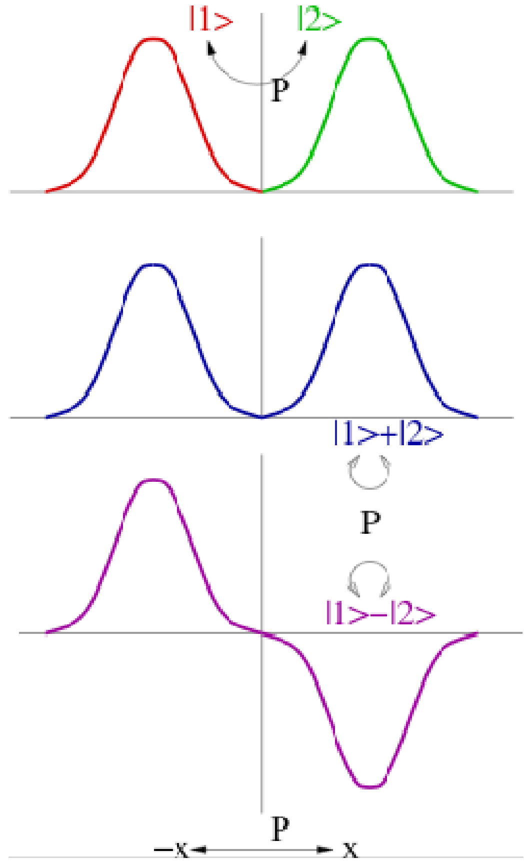
Thus $|+x\rangle$ and $|-x\rangle$ are simultaneous eigenkets of $\hat{H}$ and $\hat{\pi}$.

For NH_3 maser, the Hamiltonian $\hat{H}$ can be described by

$$\hat{H} = \begin{pmatrix}E_0 & -A\\ -A & E_0\end{pmatrix} = E_0\hat{1} - A\hat{\sigma}_x$$

In fact, $\hat{H}$ commutates with the parity operator $\hat{\pi}$, since

$$[\hat{H}, \hat{\pi}] = [E_0\hat{1} - A\hat{\sigma}_x, \hat{\sigma}_x] = 0$$



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