## 5.4. Parity and Time Reversal Transformations

Up to now we have been considering proper rotations, $\det R = +1$, when we also include improper rotations, $\det R = -1$, we must consider space-inversions also. In fact every rotation with $\det R = -1$ can be made up of a proper rotation following a parity transformation. A parity transformation is defined to invert the space coordinate axes

$$\vec{r}\,' = -\vec{r}$$

or introducing matrix notation

$$x'^i = P^{ij} x^j \quad \text{with}$$

$$P^{ij} = -\delta^{ij} = \begin{pmatrix} -1 & & 0 \\ & -1 & \\ 0 & & -1 \end{pmatrix}_{ij} .$$

Since two consecutive parity transformations bring us back to the original coordinate axes

$$\vec{r}\,'' = -\vec{r}\,'$$
$$\vec{r}\,' = -\vec{r}$$

$$\Rightarrow \vec{r}\,'' = \vec{r}$$

That is $P^2 = 1$, as can be checked directly.

The identity matrix and parity matrix $\{1, P\}$ form a 2-element, <u>discrete</u> group; the group of space inversions. $P^{-1}$ is just $P$; $P^{-1} = P$.

By Wigner's theorem, we have that the states in the parity transformed coordinate system $|\psi'\rangle$ are related to the states $|\psi\rangle$ in the original coordinate system by a unitary or anti-unitary operator $U(P) \equiv P$. (We use the same symbol for the $3\times3$ matrix $P_{ij}$ and the quantum parity operator $P$.) So

$$|\psi'\rangle = P|\psi\rangle .$$

For operators we have that the coordinates are inverted

$$P\vec{R}P^{-1} = -\vec{R}$$

$$\underline{\text{i.e.}}\quad P X^i P^{-1} = P_{ij} X^j = -X^i ,$$

further by definition

$$P\vec{P}P^{-1} = -\vec{P}$$

$$\underline{\text{i.e}}\quad P P^i P^{-1} = P_{ij} P^j = -P^i$$

The momentum is inverted since

The coordinate axes are inverted. Thus the orbital angular momentum is <u>not</u> inverted

$$\mathcal{P}\vec{L}\mathcal{P}^{-1} = \mathcal{P}\vec{R}\times\vec{P}\mathcal{P}^{-1}$$

$$= \epsilon_{ijk}\mathcal{P}X^j P^k\mathcal{P}^{-1}$$

$$= \epsilon_{ijk}\mathcal{P}X^j\underbrace{\mathcal{P}^{-1}\mathcal{P}}_{=1}P^k\mathcal{P}^{-1}$$

$$= \epsilon_{ijk}X^j P^k = \vec{L}\,.$$

Thus we define the spin operator to also be parity invariant

$$\mathcal{P}\vec{S}\mathcal{P}^{-1} \equiv \vec{S}$$

and so the total angular momentum is defined to commute with

$$\mathcal{P}\vec{J}\mathcal{P}^{-1} = \vec{J}\,.$$

To determine if $\mathcal{P}$ is unitary or anti-unitary we can consider the action of ~~a~~ parity transformation on the canonical commutation relations which should stay the same in all frames.

$$\mathcal{P}\,[X^i, P^j]\,\mathcal{P}^{-1} = \mathcal{P}(i\hbar\delta^{ij})\mathcal{P}^{-1}$$

$$\parallel$$

$$\mathcal{P} X^i \underbrace{\mathcal{P}^{-1}\mathcal{P}}_{=1} P^j \mathcal{P}^{-1} - \mathcal{P} P^j \underbrace{\mathcal{P}^{-1}\mathcal{P}}_{=1} X^i \mathcal{P}^{-1}$$

$$= X^i P^j - P^j X^i$$

$$= [X^i, P^j] = i\hbar\delta^{ij}$$

$\Rightarrow$ $\mathcal{P} i \mathcal{P}^{-1} = i$ (for the CCR to remain the same). Hence $\mathcal{P} i = i\mathcal{P}$ $\Rightarrow$ $\mathcal{P}$ is linear not anti-linear and hence $\mathcal{P}$ is unitary

$$\boxed{\mathcal{P}^\dagger = \mathcal{P}^{-1}}$$

(in the coordinate representation $\vec{r} \xrightarrow{\mathcal{P}} -\vec{r}$, $\vec{p} \xrightarrow{\mathcal{P}} -\vec{p}$ but $\vec{p} = \frac{\hbar}{i}\vec{\nabla}$ since $\vec{\nabla} \xrightarrow{\mathcal{P}} -\vec{\nabla}$ we have $i \xrightarrow{\mathcal{P}} i$, again $\mathcal{P}$ is unitary).

Since 2 parity transformations bring us back to the same coordinate system we have that

$|\psi\rangle$ and $\mathcal{P}^2|\psi\rangle$ must describe the same state, hence

$$P^2 = e^{i\varphi}\mathbb{1}, \quad \varphi \in \mathbb{R},$$

P has an arbitrary phase in its definition, $P^2$ is the identity up to a phase. Note this phase factor does not appear in the operator transformation; it is cancelled due to the appearance of P and $P^{-1}$. By convention we choose $\varphi = 0$, so

$P^2 = \mathbb{1}$. Since P is unitary we have

$P^{-1} = P^{\dagger} = P$, it is also

Hermitian.

To determine the action of P on the states of $\mathcal{H}$ consider first the action of P on the coordinate basis vectors $\{|\vec{r}\rangle\}$.

$$\begin{aligned}
P\vec{R}|\vec{r}\rangle &= \underbrace{P\vec{R}P^{-1}}_{-\vec{R}}P|\vec{r}\rangle \quad (P^{-1}P = 1)\\
P\vec{r}|\vec{r}\rangle &= -\vec{R}(P|\vec{r}\rangle)\\
\vec{r}(P|\vec{r}\rangle) &\Rightarrow \boxed{\vec{R}(P|\vec{r}\rangle) = -\vec{r}(P|\vec{r}\rangle)}
\end{aligned}$$

But
$$\vec{R}|-\vec{r}\rangle = -\vec{r}\,|-\vec{r}\rangle .$$

Thus $P|\vec{r}\rangle$ and $|-\vec{r}\rangle$ can differ by at most a phase, which again by convention we choose as zero,

$$\boxed{P|\vec{r}\rangle = |-\vec{r}\rangle .}$$

Hence for any wavefunction we have, for $|\psi'\rangle = P|\psi\rangle$,

$$\psi'(\vec{r}) = \langle\vec{r}|\psi'\rangle = \langle\vec{r}|P|\psi\rangle$$
$$= \langle-\vec{r}|\psi\rangle = \psi(-\vec{r}) .$$

Since $P^2 = 1$ this implies that $P$ has eigenvalues of $\pm 1$ only. Even functions, $\psi_{even}(\vec{r}) = \psi_{even}(-\vec{r})$ have eigenvalue of $+1$ while odd functions $\psi_{odd}(\vec{r}) = -\psi_{odd}(-\vec{r})$ have eigenvalue of $-1$. Thus for <u>eigenstates of $P$</u>

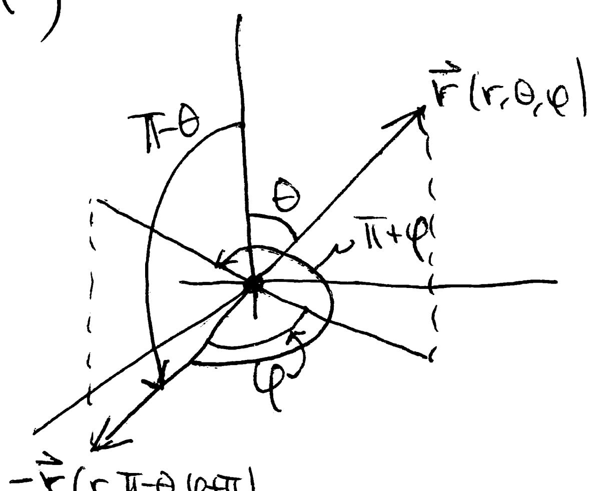
$$P|\psi\rangle = \eta_P|\psi\rangle \quad \text{with}$$

the <u>intrinsic parity</u> of the state $\eta_P = +1$ for even parity states ; $\eta_P = -1$ for odd parity states.

In spherical polar coordinates $(r, \theta, \varphi)$ space inversion $\vec{r} \to -\vec{r}$ takes

$$(r, \theta, \varphi) \to (r, \pi - \theta, \varphi + \pi)$$

But from the definition of spherical harmonics we have that




$$Y_\ell^m(\pi-\theta, \varphi+\pi) = (-1)^\ell Y_\ell^m(\theta, \varphi),$$

They are eigenfunctions of the parity operator with intrinsic parity given by $(-1)^\ell$.

Thus the orbital angular momentum eigenstates $|j=\ell, m\rangle$ are eigenstates of parity

$$P|\ell, m\rangle = (-1)^\ell |\ell, m\rangle.$$

We already knew this from our study of spin 0 particles in a central potential (ex. the hydrogen atom). Since

$$H = \frac{1}{2m}\vec{P}^2 + V(r) \quad \text{we had}$$

$\{H, \vec{L}^2, L_z\}$ as a CSCO with basis eigenstates $\{|n,l,m\rangle\}$ and their wavefunctions had the form

$$\psi_{nlm}(\vec{r}) = \langle \vec{r} | n,l,m \rangle$$

$$= R_{nl}(r) Y_l^m(\theta,\varphi)$$

where $R_{nl}(r)$ are a complete set of wavefunction solutions to the Radial equation. The point being, since $V = V(r)$, we also have

$$[P,H] = 0 = [P,\vec{L}^2] = [P,L_z]$$

The Hamiltonian is Parity invariant, hence the parity is a <u>conserved</u> quantity.

On the basis states we find

$$\psi'_{nlm}(r) = \langle \vec{r} | P | n,l,m \rangle$$

$$= \langle -\vec{r}|n,l,m\rangle = \psi_{nlm}(-\vec{r})$$

$$= \langle r, \pi-\theta, \varphi+\pi | n,l,m\rangle$$

$$= R_{nl}(r)\, Y_l^m(\pi-\theta, \varphi+\pi)$$

$$= (-1)^l R_{nl}(r)\, Y_l^m(\theta, \pi)$$

$$= (-1)^l \langle r,\theta,\varphi|n,l,m\rangle$$

$$= (-1)^l \langle \vec{r}|n,l,m\rangle = (-1)^l \psi_{nlm}(\vec{r})$$

Thus $\boxed{P|n,l,m\rangle = (-1)^l |n,l,m\rangle}$, and

The wavefunctions obey

$$\boxed{\psi_{nlm}(-\vec{r}) = (-1)^l \psi_{nlm}(\vec{r})}.$$

The central potential eigenstates of $\{H, \vec{L}^2, L_z\}$ are divided into even and odd parity eigenstates

1) even $\quad (-1)^l = 1 \Rightarrow l =$ even integer

2) odd parity $\quad (-1)^l = -1 \Rightarrow l =$ odd integer

Of course this result is not true for the total angular momentum eigenstates of a multi-particle system. For example

$$|l_1, l_2; L, M\rangle = \sum_{m_1 m_2}' |l_1, m_1\rangle \otimes |l_2, m_2\rangle \cdot$$

$$\cdot \langle l_1, l_2; m_1, m_2 | L, M\rangle$$

are total orbital angular momentum eigenstates of a 2 particle system.

$$P|l_1, l_2; L, M\rangle = (-1)^{l_1+l_2} |l_1, l_2; L, M\rangle$$

$$\neq (-1)^L |l_1, l_2; L, M\rangle .$$

The parity of ~~an~~ total angular momentum eigenstate in general is not fixed by its total angular momentum eigenvalue.

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Besides inverting the space coordinates, we can imagine a transformation that reverses the direction of time. More accurately, we can imagine that the motion of a system is reversed, momentum flowing in the opposite direction, direction of angular momentum opposite its original direction etc. This motion reversal, as we shall see, is equivalent to letting $t \to -t$ in our states.

A time reversal transformation is defined by

$$\vec{r}' = \vec{r} \quad \text{but}$$

$$t' = -t \,. \quad \text{Thus we}$$

define the operator that relates the states in these two frames as $U_T \equiv T$

$$|\psi'\rangle = T|\psi\rangle . \quad \text{The transformation}$$

is defined to leave the coordinates unchanged so we define

$$T\vec{R}T^{-1} = \vec{R} .$$

But $t \to -t$ thus velocities and hence momentum should be reversed (motion reversal), so we define

$$T \vec{P} T^{-1} = -\vec{P} .$$

Since $\vec{L} = \vec{R} \times \vec{P} \Rightarrow T \vec{L} T^{-1} = -\vec{L}$ and we define

$$T \vec{J} T^{-1} = -\vec{J} .$$

Now if the commutation relations are to be the same in each frame we must have

$$T [X^i, P^j] T^{-1} = T i\hbar \delta^{ij} T^{-1}$$

$$= T X^i T^{-1} T P^j T^{-1} - T P^j T^{-1} T X^i T^{-1}$$

$$= -X^i P^j + P^j X^i$$

$$= -[X^i, P^j]$$

$$= -i\delta^{ij}\hbar \quad = \hbar \delta^{ij} T i T^{-1}$$

$$\Rightarrow \boxed{T i T^{-1} = -i \Rightarrow T i = -i T}$$

T must be <u>anti-linear</u>, hence by Wigner's Theorem it is <u>anti-unitary</u>

Since two time reversal operations result in the original system we have that

$$T^2|\psi\rangle = e^{i\varphi}|\psi\rangle \quad ; \varphi \in \mathbb{R}.$$

Using the <u>associative property of operator multiplication</u> we find

$$T^3|\psi\rangle = T^2(T|\psi\rangle) = T(T^2|\psi\rangle)$$

$$= T(e^{i\varphi}|\psi\rangle)$$

but T is anti-linear so

$$= e^{-i\varphi}(T|\psi\rangle).$$

Now for the sum of 2 states $(|\psi\rangle + T|\psi\rangle)$ we also have

$$T^2(|\psi\rangle + T|\psi\rangle) = e^{i\varphi'}(|\psi\rangle + T|\psi\rangle)$$

$$\parallel$$

$$T^2|\psi\rangle + T^3|\psi\rangle = e^{i\varphi}|\psi\rangle + e^{-i\varphi}T|\psi\rangle$$

$$\Rightarrow e^{i\varphi}|\psi\rangle + e^{-i\varphi}T|\psi\rangle$$
$$= e^{i\varphi'}(|\psi\rangle + T|\psi\rangle)$$

$$\Rightarrow e^{i\varphi} = e^{i\varphi'} = e^{-i\varphi} \Rightarrow \boxed{\varphi = 0 \text{ or } \pi \text{ for all phases}}$$

Thus $\boxed{T^2|\psi\rangle = \pm|\psi\rangle}$. 2 successive time reversal transformations need not be the identity, just like a rotation through $2\pi$.

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Indeed consider the case where $[T, A] = 0$ for the CSCO $\{A, \vec{J}^2, J_z\}$.

Then since $T\vec{J}T^{-1} = -\vec{J}$

$$\Rightarrow T\vec{J} = -\vec{J}T \Rightarrow \{T, \vec{J}\} = 0.$$

Now using $[A, BC] = \{A, B\}C - B\{A, C\}$

we have $[T, \vec{J}^2] = 0$ but

$$\{T, J_z\} = 0 \quad \text{so}$$

$$J_z T|k,j,m\rangle = -T J_z |k,j,m\rangle$$
$$= -m\hbar T|k,j,m\rangle$$
$$\vec{J}^2 T|k,j,m\rangle = +T\vec{J}^2|k,j,m\rangle$$
$$= j(j+1)\hbar^2 T|k,j,m\rangle$$
$$A T|k,j,m\rangle = +T A|k,j,m\rangle$$
$$= a_k T|k,j,m\rangle.$$

$$\Rightarrow \quad T|k,j,m\rangle = \omega(k,j,m)|k,j,-m\rangle$$

where $|\omega(k,j,m)| = 1$.

next $J_\pm|k,j,m\rangle = \hbar\sqrt{j(j+1)-m(m\pm1)}\,|k,j,m\pm1\rangle$

but $T(J_x \pm iJ_y)T^{-1} = -(J_x \mp iJ_y)$

since $TiT^{-1} = -i$

So $\quad TJ_\pm T^{-1} = -J_\mp$

$$\Rightarrow \quad TJ_\pm = -J_\mp T.$$

So

$$-J_\mp T|k,j,m\rangle = T J_\pm |k,j,m\rangle$$

$$-J_\mp\, \omega(k,j,m)\,|k,j,-m\rangle$$

$$= \hbar\sqrt{(j\mp m)(j\pm m+1)}\, \underbrace{T|k,j,m\pm 1\rangle}_{=\,\omega(k,j,m\pm1)|k,j,-m\mp1\rangle}$$

$\Rightarrow$

$$-\hbar\sqrt{(j\mp m)(j\pm m+1)}\,\omega(k,j,m)\,|k,j,-m\mp 1\rangle$$

$$= \hbar\sqrt{(j\mp m)(j\pm m+1)}\,\omega(k,j,m\pm 1)|k,j,-m\mp 1\rangle$$

$$\Rightarrow \boxed{\omega(k,j,m\pm 1) = -\omega(k,j,m)}$$

$$\Rightarrow \boxed{\omega(k,j,m) = (-1)^m\,\omega(k,j)}$$

$\omega(k,j)$ can be chosen by convention to be $(-1)^j$

So $$\boxed{T|k,j,m\rangle = (-1)^{j+m}|k,j,-m\rangle}$$

Thus

$$T^2|k,j,m\rangle = (-1)^{j+m}\, T|k,j,-m\rangle$$
$$= (-1)^{j+m}(-1)^{j-m}\,|k,j,m\rangle$$
$$= (-1)^{2j}\,|k,j,m\rangle$$

for $\frac{1}{2}$ odd-integer angular momenta we have

$$T^2|k,j,m\rangle = -|k,j,m\rangle$$
$$j = \tfrac{1}{2}, \tfrac{3}{2}, \ldots$$

for integral $j$ we have

$$T^2|k,j,m\rangle = +|k,j,m\rangle$$
$$j = 0, 1, 2, \ldots \, .$$

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Proof that $\omega(k,j)$ is irrelevant:

redefine $|k,j\,m\rangle$ states by

$$|k,j,m\rangle' \equiv (-1)^{j+m}\,\xi(k,j)\,|k,j,-m\rangle$$

where $|\xi(k,j)| = 1$ and we will show that we could choose this phase so that $\omega(k,j)$ is cancelled from each transformation law.

$$T\,|k,j,m\rangle' = (-1)^{j+m}\,\xi^*(k,j)\,T\,|k,j,-m\rangle$$
$$= (-1)^{j+m}\,\xi^*(k,j)\,\omega(k,j)\,(-1)^{j-m} \times$$
$$\times\,|k,j,m\rangle$$

but

$$|k,j,m\rangle = (-1)^{j-m}\,\frac{1}{\xi(k,j)}\,|k,j,-m\rangle'$$

So

$$T\,|k,j,m\rangle' = (-1)^{j+m}\,\frac{\xi^*(k,j)}{\xi(k,j)}\,\omega(k,j)\,|k,j,-m\rangle'.$$

Choose $\dfrac{\xi^*(k,j)}{\xi(k,j)}\,\omega(k,j) = \left(\xi^*(k,j)\right)^2\omega(k,j)$

$$\equiv 1.$$

$$\Rightarrow \boxed{T\,|k,j,m\rangle' = (-1)^{j+m}\,|k,j,-m\rangle'}$$

with no phase $\omega(k,j)$.