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Quantum Mechanics-II

Useful Books : Quantum Mechanics
Eugen Merzbacher
Modern Quantum Mechanics
J.J. Sakurai

Chapter 4

Symmetry in Quantum Mechanics

4.1 - Symmetries, Conservation laws, and Degeneracies

In classical mechanics;

Under displacement $q_i \rightarrow q_i + \delta q_i$

if $L(q_i, \dot{q}_i, t) = L(q_i + \delta q_i, \ldots)$ (invariant)

Since $L(q_i + \delta q_i, \ldots) = L(q_i, \ldots) + \frac{\partial L}{\partial q_i}\delta q_i$

$$\rightarrow \frac{\partial L}{\partial q_i} = 0$$

Using the Lagrange equ. $\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_i}\right) - \frac{\partial L}{\partial q_i} = 0$

$$\rightarrow \frac{dP_i}{dt} = 0 \qquad \text{where } P_i = \frac{\partial L}{\partial \dot{q}_i}$$

We say:

If L has a <u>symmetry</u> under $q_i \rightarrow q_i + \delta q_i$

<u>Then</u> there exists a <u>conserved</u> quantity namely the Canonical momentum conjugate to q_i.

Similarly:

$$H(q_i, P_i, t) = \sum P_i \dot{q}_i - L(q_i, \dot{q}_i, t)$$

$$\rightarrow dH = \sum (P_i \cancel{d\dot{q}_i} + \dot{q}_i dP_i) - \sum \left(\frac{\partial L}{\partial q_i} dq_i + \cancel{\frac{\partial L}{\partial \dot{q}_i} d\dot{q}_i} \right) - \frac{\partial L}{\partial t} dt$$

$$= \left(\dot{q}_i dP_i - \frac{\partial L}{\partial q_i} dq_i \right) - \frac{\partial L}{\partial t} dt$$

$$\left\{ \begin{array}{l} \frac{\partial (P_i \dot{q}_i)}{\partial \dot{q}_i} = P_i \\ \frac{\partial (P_i \dot{q}_i)}{\partial P_i} = \dot{q}_i \end{array} \right.$$

Also $dH = \frac{\partial H}{\partial q_i} dq_i + \frac{\partial H}{\partial P_i} dP_i + \frac{\partial H}{\partial t}$

$$\longrightarrow \frac{\partial H}{\partial P_i} = \dot{q}_i \qquad \frac{\partial H}{\partial q_i} = -\frac{\partial L}{\partial q_i} = -\dot{P}_i \qquad \frac{\partial H}{\partial t} = -\frac{\partial L}{\partial t}$$

then, if $\frac{\partial H}{\partial q_i} = 0 \longrightarrow \frac{dP_i}{dt} = 0$

i.e.:

H is symmetric under $q_i \rightarrow q_i + \delta q_i \longrightarrow P_i$ is conserved

Symmetry in Q.M.:

In Q.M., translations, rotations... etc. are represented by a unitary operator ($\mathcal{S}$). ($\langle\alpha|\alpha\rangle = \langle\alpha|U^{+}U|\alpha\rangle = 1$)
Normalization

It has been customary to call these operators symmetry operators regardless of whether the physical system itself possesses the symmetry corresponding to these operators, ($\mathcal{S}$).

(Def. $U^{+}U = UU^{+} = I$ unitary op.)

For an infinitesimal transformation being unitary:

$$\mathcal{S} = 1 - \frac{i\epsilon}{\hbar} G$$

Note: $\langle\alpha|\beta\rangle = \langle\alpha|U^{+}U|\beta\rangle$
→ A unitary op. applied to all vectors of the space, preserves the length of the vectors and angles between any two of them

where;

G: Hermitian generator of symmetry operator $\mathcal{S}$

Hermitian of G is neccessary cond. for the operator $\mathcal{S}$ to be unitary.

$$\mathcal{S}\mathcal{S}^{+} = \left(1 - \frac{i\epsilon}{\hbar}G\right)\left(1 + \frac{i\epsilon}{\hbar}G^{+}\right) = 1 + \cancel{\frac{\epsilon^2}{\hbar^2} GG^{+}} + \frac{i\epsilon}{\hbar}G^{+} - \frac{i\epsilon}{\hbar}G$$

$$\mathcal{S}\mathcal{S}^{+} = 1 \longrightarrow G^{+} = G$$

Now, suppose H is invariant under $\mathcal{S}$, i.e.:

$$\mathcal{S}^{+}H\mathcal{S} = H \longrightarrow [\mathcal{S}, H] = 0$$

$$\left(1 - \frac{i\epsilon}{\hbar}G\right)H - H\left(1 - \frac{i\epsilon}{\hbar}G\right) = 0$$

$$H - \frac{i\epsilon}{\hbar}GH - H + \frac{i\epsilon}{\hbar}HG = 0 \longrightarrow [G, H] = 0$$

By virtue of the Heisenberg equ. of motion:

$$[G, H] = 0 \rightarrow [U^{+}GU, U^{+}HU] = 0 \rightarrow [G^{H}, H^{H}] = 0 \rightarrow [G^{H}, H] = 0$$

$$i\hbar \frac{dG^{H}}{dt} = [G^{H}, H] \rightarrow \frac{dG^{H}}{dt} = 0$$ Conserved quantity

$$\rightarrow \frac{dG}{dt} = 0$$

G is a const. of motion.

Note: $U \equiv U(t, t_0)$

Hence;

If H is <u>invariant</u> under symmetry operation (<u>unitary op. $\mathcal{J}$</u>) . $\longrightarrow$ The generator of the symmetry op., G <u>is conserved</u>.

Ex. - Consider an infinitesimal translation;

$$\mathcal{J}(dx) = 1 - \frac{i\,d\bar{x}}{\hbar}\cdot\bar{p}$$

If $\mathcal{J}^{+}(dx)\, H\, \mathcal{J}(dx) = H \longrightarrow \frac{d\bar{p}}{dt} = 0$ $\quad \bar{p}$ = const. of motion

Remark:

$$f(x+dx) = \sum_{n=0}^{\infty} \frac{1}{n!} f^{(n)}(x)(dx)^n \simeq f(x) + \frac{\partial f(x)}{\partial x}\,dx$$

$$= f(x) + \frac{i}{\hbar}\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right) f(x)\,dx = f(x) + \frac{i}{\hbar}\,dx\, p\, f(x)$$

In 3-dim: $\quad f(x+dx) = f(x) + \frac{i}{\hbar}\, d\bar{x}\cdot\bar{p}\, f(x)$

$$f(x+dx) = \left(1 + \frac{i\,d\bar{x}}{\hbar}\cdot\bar{p}\right) f(x)$$

Ex. - If H is invariant under rotation;

$$\mathcal{J}^{+}(\hat{n},\varphi)\, H\, \mathcal{J}(\hat{n},\varphi) = H$$

where $\mathcal{J}(\hat{n},\varphi) = 1 - \frac{i\,\delta\varphi\,\hat{n}}{\hbar}\cdot\bar{J}$ $\quad$ infinitesimal rotation

$$\longrightarrow \frac{d\bar{J}}{dt} = 0 \qquad J = \text{const. of motion}$$

Alternative point of view:

Suppose: $G|g'\rangle = g'|g'\rangle$ at t_0

and suppose $[G,H]=0$

Apply time evaluation op. on eigenket $|g'\rangle$

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

$$G[\mathcal{U}(t,t_0)|g'\rangle] = \mathcal{U}(t,t_0)\,G|g'\rangle = g'[\mathcal{U}(t,t_0)|g'\rangle]$$ due to $[G,H]=0$

Therefore:

$$\frac{dG}{dt}=0 \longrightarrow [G,H]=0 \longrightarrow g' = \text{const in time}$$

Then, $|g', t_0; t\rangle$ is an eigenket of G with the same eigenvalue of g'.

Remark:

$$\mathcal{U}(t_0+dt, t_0) = 1 - \frac{i\,dt}{\hbar} H$$

$$\mathcal{U}(t,t_0) = e^{-\frac{i}{\hbar}\int_{t_0}^{t} dt' H(t')}$$

$$\mathcal{U}(t,t_0) = e^{-\frac{i}{\hbar}(t-t_0)H}$$ for time-indep H

Degeneracies:

Suppose: $[H, \mathcal{S}] = 0$

$\mathcal{S}$: symmetry op.

and suppose $H|n\rangle = E_n|n\rangle$

$$\rightarrow H(\mathcal{S}|n\rangle) = \mathcal{S}(H|n\rangle) = E_n(\mathcal{S}|n\rangle)$$

Then $\mathcal{S}|n\rangle$ is also an energy eigenket with the same eigenvalue.

If $|n\rangle$ and $\mathcal{S}|n\rangle$ represent different states, then they are degenerate.

If $\mathcal{S} = \mathcal{S}(\lambda)$ where, λ: continuous parameter

all $\mathcal{S}(\lambda)|n\rangle$ have the same energy E_n.

Ex.- If H is rotationally invariant; i.e.;

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

where, $\mathcal{D}(R) = e^{-\frac{i\varphi\hat{n}}{\hbar}\cdot\bar{J}}$

$$\mathcal{D}(R) = 1 + \left(-\frac{i\varphi\hat{n}}{\hbar}\cdot\bar{J}\right) + \left(-\frac{i\varphi\hat{n}}{\hbar}\cdot\bar{J}\right)^2 + \ldots$$

$$\rightarrow [J, H] = 0 \qquad [J^2, H] = 0$$

Remark:

$J^2 = J_xJ_x + J_yJ_y + J_zJ_z$

$[J^2, J_k] = 0 \quad k = 1, 2, 3$

for $k = 3$

$[J^2, J_z] = J_x[J_x, J_z] + [J_x, J_z]J_x$

$+ J_y[J_y, J_z] + [J_y, J_z]J_y + 0$

$= J_x(-i\hbar J_y) + (-i\hbar J_y)J_x$

$+ J_y(-i\hbar J_x) + (i\hbar J_x)J_y = 0$

To prove for $k = 1, 2$

$(1 \rightarrow 2 \rightarrow 3 \rightarrow 1)$

Since $[J_x, J_y] \neq 0, [J_y, J_z] \neq 0, [J_z, J_x] \neq 0$

we can diagonalize one of them with J^2

This means that we can form simultaneous eigenstates of H, J^2, J_z denoted by $|n,j,m\rangle$

Also, $[\mathcal{D}(R), H] = 0 \longrightarrow$ All states of $\mathcal{D}(R)|n,j,m\rangle$ have the <u>same</u> energy

$$[\mathcal{D}(R), H] = 0 \longrightarrow H|n,j,m\rangle = E_{n,j}|n,j,m\rangle$$

(not $E_{n,j,m}$)

$$H\left(\mathcal{D}(R)|n,j,m\rangle\right) = E_{n,j}\left(\mathcal{D}(R)|n,j,m\rangle\right)$$

we know:

$$\mathcal{D}(R)|n,j,m\rangle = \sum_{m'=-j}^{j} |n,j,m'\rangle \mathcal{D}^{j}_{mm'}(R)$$

where $\mathcal{D}^{j}_{mm'}(R) = \langle j,m'|\exp(-\frac{i\varphi\hat{n}}{\hbar}\cdot\bar{J})|j,m\rangle$

If we change the continuous parameter of $\mathcal{D}(R)$ (i.e. $R: \hat{n}, \varphi$) we get different linear combination of $|n,j,m'\rangle$.

If $H\left(\mathcal{D}(R)|n,j,m\rangle\right) = E_{n,j}\left(\mathcal{D}(R)|n,j,m\rangle\right) \quad \forall \mathcal{D}(R)$

then $\longrightarrow$ each of $|n,j,m\rangle$ with different m must have the same energy.

So: The degeneracy is $2j+1$-fold

This point is also evident from the fact that:

$$J_\pm |n,j,m\rangle = N_\pm |n,j,m\pm 1\rangle$$

Since $J_\pm = J_x \pm i J_y$

$$[D(R,H] = 0 \rightarrow [J, H] = 0 \rightarrow [J_\pm, H] = 0$$

$$H\left(J_\pm |n,j,m\rangle\right) = J_\pm\left(H|n,j,m\rangle\right) = E_{n,j}\left(J_\pm |n,j,m\rangle\right)$$

Ex.- Consider an atomic electron, whose potential is written as:

$$V(r) + V_{LS}(r)\,\bar{L}\cdot\bar{S}$$

Since $[D(R), r] = 0 \rightarrow \begin{cases} [D(R), V(r)] = 0 \\ [D(R), V_{LS}(r)] = 0 \end{cases}$

and $[D(R), L\cdot S] = [D(R), \frac{1}{2}(J^2 - L^2 - S^2)]$

Since $[D(R), J^2] = 0$, $[D(R), L^2] = 0$, $[D(R), S^2] = 0$

$$\longrightarrow [D(R), S\cdot L] = 0$$

So, $V(r) + V_{LS}(r)\,\bar{L}\cdot\bar{S}$ is rotationally invariant.

Therefore there are $(2j+1)$ fold degeneracy for each atomic level.

On the other hand;

suppose there is an <u>electric</u> or <u>magnetic</u> field, say in the z-direction.

The rotational symmetry is now manifestly broken.

Ex.- Consider the extra term of interaction to be:

$$\frac{e}{2\mu c}\bar{B}\cdot(g_e\bar{L}+g_s\bar{S})$$

we see $\left[D(R), \frac{e}{2\mu c}\bar{B}\cdot(g_e\bar{L}+g_s\bar{S})\right] \neq 0$ for $g_s \neq g_e$

If $\bar{B}$ is in z-dir.

having $g_\ell = 1$ $g_s = 2$

The energy for this extra term can be obtained as:

$$\frac{e}{2\mu c}|B|\, m\hbar + \frac{e}{2\mu c}|B|\frac{j(j+1)+s(s+1)-\ell(\ell+1)}{2j(j+1)}\, m\hbar$$

where $j = \ell - \frac{1}{2}$, $\ell + \frac{1}{2}$ and $s = \frac{1}{2}$

This is Zeeman effect and the degeneracies are removed.

We conclude:

When the <u>symmetry</u> is <u>broken</u>, then the <u>degeneracies</u> <u>are removed</u>.

4-2 Discrete Symmetries

Parity, or space Inversion:

Using the continuous symmetry operators, the operations can be obtained by applying successively infinitesimal symmetry operations.

This is not the case for discrete symmetry operators.

We will consider three symmetry operators that can be considered to be discrete.

1- Parity op.
2- Lattice translation op.
3- Time reversal op.

Parity op., Π, as applied to transformation on the coord-sys., changes a right-handed (RH) system into a left-handed (LH) system.

But here we will consider a tr. on state kets rather than on the coord.-sys.

Given a state $|\alpha\rangle$;

$$|\alpha\rangle \longrightarrow \Pi|\alpha\rangle \qquad \text{space inverted state}$$

(we assume that this is possible by applying a unitary op. Π)

We require;

$$\langle\alpha|\Pi^{+} X \Pi|\alpha\rangle = -\langle\alpha|X|\alpha\rangle \qquad (X\text{: Position op.})$$

which is a reasonable requirement

This is accomplished if $\quad \Pi^{+} X \Pi = -X$

or $\longrightarrow \quad \{\bar{X}, \Pi\} = 0$

Now, $\quad \Pi|X'\rangle = ? \qquad$ ($|X'\rangle$: eigenket of position op)

A claim: $\Pi|X'\rangle = e^{i\delta}|-X'\rangle$

where $e^{i\delta}$ is a phase factor (δ: real)

Proof:

Note that: $\quad X\Pi|X'\rangle = -\Pi X|X'\rangle = (-X')\Pi|X'\rangle$

$\longrightarrow$ $-X'$ is eigenvalue of eigenket $\Pi|X'\rangle$

So, $\Pi|X'\rangle$ must be same as eigenket $|-X'\rangle$

up to a phase factor.

By convention: $\quad e^{i\delta} = 1$

Remark: Another look
If $\Pi|X'\rangle = |-X'\rangle$
$\rightarrow X|X'\rangle = X'|X'\rangle$
$\Pi X \Pi^{-1}\Pi|X'\rangle = X'|-X'\rangle = -X|-X'\rangle$
$\rightarrow \Pi X \Pi^{-1} = -X$

Remark:

Since $\langle x'|\Pi^{+} x \Pi|x'\rangle = -\langle x'|x|x'\rangle$

$$= -x'$$

$$\langle x'|\Pi^{+} x \Pi|x'\rangle = \underbrace{e^{-i\delta} e^{i\delta}} \langle -x'|x|-x'\rangle = -x'$$

then in general $\longrightarrow \Pi|x'\rangle = e^{i\delta}|-x'\rangle$

Therefore:

$$\Pi|x'\rangle = |-x'\rangle$$

$$\longrightarrow \Pi^2|x'\rangle = |x'\rangle \longrightarrow \Pi^2 = I$$

Also

$$\left\{ \begin{array}{l} \langle x'|\Pi^{+}\Pi|x'\rangle = \langle -x'|-x'\rangle = 1 \\ \langle x'|\Pi^2|x'\rangle = \langle x'|x'\rangle = 1 \end{array} \right. \longrightarrow \Pi = \Pi^{+}$$

$$\Pi^2 = I \longrightarrow \Pi = \Pi^{-1}$$

The eigenvalues are ± 1

The momentum operator:

Since $p = m\frac{dx}{dt}$ $\longrightarrow$ it is natural to expect it to be <u>odd</u> under parity, like x.

i.e. $\longrightarrow \{\Pi, P\} = 0$

More satisfactory argument:

P is the generator of translation

From the Fig. it is evident that, for an infinitesimal translation:

$$\Pi\, \mathcal{T}(d\bar{x}') = \mathcal{T}(-d\bar{x}')\,\Pi$$

$$\longrightarrow \Pi\left(1-\frac{i\bar{P}}{\hbar}\cdot d\bar{x}'\right) = \left(1+\frac{i\bar{P}}{\hbar}\cdot d\bar{x}'\right)\Pi \longrightarrow \Pi\left(1-\frac{i\bar{P}}{\hbar}\cdot d\bar{x}'\right)\Pi^{+} = 1+\frac{i\bar{P}}{\hbar}\cdot d\bar{x}'$$

$$\longrightarrow \{\Pi, P\} = 0 \quad \text{or} \quad \Pi^{+} P\, \Pi = -P$$

Spin operator:

$J = L + S$

$L = \bar{X} \wedge \bar{P}$

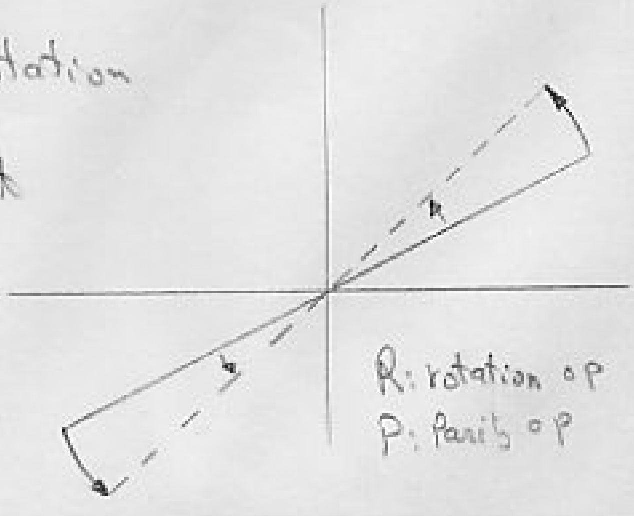
Since X and P are <u>odd</u> under parity, then L will be even under parity:

$$[\Pi, L] = 0$$

J is the generator of rotation

From the Fig. it is evident that

$$\begin{cases} PR = RP \\ P = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \end{cases}$$



R: rotation op

P: parity op

Therefore it is natural to postulate the corresponding relation for the unitary operators in Q.M.;

$$\Pi\, \mathcal{D}(R) = \mathcal{D}(R)\,\Pi$$

where $\mathcal{D}(R) = 1 - \frac{i\delta\varphi\,\hat{n}}{\hbar}\cdot J$

$\longrightarrow \quad [\Pi, J] = 0 \quad$ or $\quad \Pi^{+} J \Pi = J$

Now:

$$\left\{\begin{array}{l} [L,\Pi]=0 \\ [J,\Pi]=0 \end{array}\right. \longrightarrow \quad [S,\Pi]=0$$

Remark:

Under rotations $\bar{x}$ and $\bar{J}$ transform <u>in the same</u> way.

$\langle\psi'|x_i|\psi'\rangle = \langle x_i\rangle' = \sum a_{ij}\langle x_j\rangle \qquad \langle J_i\rangle' = \sum a_{ij}\langle J_j\rangle$

$\xrightarrow{\text{so}}$ they are vectors (spherical tensors of rank 1)

However $\bar{x}$ (or $\bar{P}$) is <u>odd</u> under parity, while J is <u>even</u> under parity.

$$\left\{\begin{array}{l}\text{Vectors that are odd under parity, are called polar vectors.} \\ \text{" \quad " \quad " even \quad " \quad " \quad " \quad " } \underbrace{\text{axial}}_{\text{pseudo vectors}} \text{ ".}\end{array}\right.$$

Remark:

Under rotations, the operators like $S \cdot x$ transform like ordinary scalars, (such as $S \cdot L$ or $x \cdot p$).

$$\langle \alpha' | S \cdot x | \alpha' \rangle = \sum_i \langle \alpha' | S_i X_i | \alpha' \rangle = \sum_i \sum_{\beta'} \langle \alpha' | S_i | \beta' \rangle \langle \beta' | X_i | \alpha' \rangle$$

$$= \sum_i \sum_\beta \sum_j \sum_k a_{ij} \langle \alpha | S_j | \beta \rangle a_{ik} \langle \beta | X_k | \alpha \rangle$$

$$= \sum_i \sum_\beta \sum_j \sum_k a_{ij} a_{ik} \langle \alpha | S_j | \beta \rangle \langle \beta | X_k | \alpha \rangle$$

$$= \sum_\beta \sum_j \sum_k \delta_{jk} \langle \alpha | S_j | \beta \rangle \langle \beta | X_k | \alpha \rangle = \sum_\beta \sum_k \langle \alpha | S_k | \beta \rangle \langle \beta | X_k | \alpha \rangle$$

$$= \sum_k \langle \alpha | S_k X_k | \alpha \rangle = \langle \alpha | S \cdot x | \alpha \rangle$$

Similarly for the others.

Yet under space inversion, we have

$$\Pi^+ (\vec{S} \cdot \vec{x}) \Pi = - S \cdot x$$

while for ordinary scalars, we have

$$\Pi^+ (L \cdot S) \Pi = L \cdot S \qquad , \quad \Pi^+ (P \cdot x) \Pi = P \cdot x$$

and so on.

The operators like $\bar{L}\cdot\bar{S}$ are called Scalar operators.
" " " $\bar{S}\cdot\bar{x}$ " " Pseudoscalar " .

Wave Functions Under Parity:

Let ψ be the wave-func. of spinless particle whose state ket is $|\alpha\rangle$

$$\psi(x') = \langle x'|\alpha\rangle$$

The wave-func of the space-inverted state, represented by the state ket $\pi|\alpha\rangle$, is

$$\langle x'|\pi|\alpha\rangle = \langle -x'|\alpha\rangle = \psi(-x')$$

Suppose $|\alpha\rangle$ is an eigenket of Parity

Since the eigenvalue of Parity must be ± 1
(because $\pi^2|\alpha\rangle = |\alpha\rangle \rightarrow (\pi^2 - 1)|\alpha\rangle = 0$)
$\longrightarrow \pi|\alpha\rangle = \pm|\alpha\rangle$ Sym./Antisym. sols.

The corresponding wave func. $\langle x'|\pi|\alpha\rangle = \pm\langle x'|\alpha\rangle$
On the other hand we obtained $\langle x'|\pi|\alpha\rangle = \langle -x|\alpha\rangle$

$$\longrightarrow \langle -x'|\alpha\rangle = \pm \langle x'|\alpha\rangle$$

or $$\psi(-x') = \pm\psi(x') \begin{cases} + & \text{even parity} \\ - & \text{odd} \ '' \end{cases}$$

Remark: Not all wave funcs. of Physical interest have definite parities.

Ex. – Consider, the momentum eigenket, we have;

$\{\Pi, P\} = 0 \longrightarrow$ the momentum eigenket is not expected to be parity eigenket

$$\langle x|P\rangle = N e^{\frac{i}{\hbar}P\cdot x} \qquad P = -i\hbar\frac{\partial}{\partial x}$$

$$\underline{P}|P\rangle = p|P\rangle$$

but $\Pi|P\rangle \neq k|P\rangle$ $\qquad$ k: cont

$$\longrightarrow \langle -x'|P\rangle \neq \pm\langle x'|P\rangle$$

or $$\psi(-x') \neq \pm\psi(x')$$

Ex.— An eigenket of orbital angular momentum is expressed to be parity eigenket.

Because: $\qquad [\Pi, L] = 0$

The eigenket of L^2 and L_z is $|\alpha; l, m\rangle$

The wave func.: $\langle x' | \alpha, l, m\rangle = R_\alpha(r)\, Y_l^m(\theta,\varphi)$

Under space inversion:

$$\vec{x}' \to -\vec{x}' \Longrightarrow \begin{cases} r \to r \\ \theta \to \pi - \theta & (\cos\theta \longrightarrow -\cos\theta) \\ \varphi \to \pi + \varphi & (e^{im\varphi} \longrightarrow (-1)^m e^{im\varphi}) \end{cases}$$

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

$$P_l^m(x) = \frac{(-1)^m}{2^l l!}(1-x^2)^{m/2} \frac{d^{l+m}}{dx^{l+m}}(x^2-1)^l \qquad \forall m\ (\pm)$$

$$P_l^{-m}(x) = (-1)^m \frac{(l-m)!}{(l+m)!} P_l^m(x)$$

$$Y_l^{-m}(\theta,\varphi) = (-1)^m Y_l^{m*}(\theta,\varphi)$$

$$P_l^m(x) = (-1)^m (1-x^2)^{m/2} \frac{d^m}{dx^m} P_l(x)$$

where $P_l(x) = \dfrac{1}{2^l l!} \dfrac{d^l}{dx^l}(x^2-1)^l$

$$\int_{-1}^{+1} P_{l'}(x)\, P_l(x)\, dx = \frac{2}{2l+1}\delta_{ll'}$$

$$\int_0^{2\pi} d\varphi \int_0^{\pi} \sin\theta\, d\theta\, Y_{l'}^{m'}(\theta,\varphi)\, Y_l^m(\theta,\varphi) = \delta_{ll'}\,\delta_{mm'}$$

$$\sum_{l=0}^{\infty} \sum_{m=-l}^{l} Y_l^{m*}(\theta',\varphi')\, Y_l^m(\theta,\varphi) = \delta(\varphi-\varphi')\,\delta(\cos\theta-\cos\theta')$$

Completeness relation

$$\begin{cases} \varphi \longrightarrow \pi+\varphi \\ \theta \longrightarrow \pi-\theta \end{cases} \longrightarrow \begin{cases} e^{im\varphi} \longrightarrow (-1)^m e^{im\varphi} \\ P_l^m(\cos\theta) \longrightarrow (-1)^{l+m} P_l^m(\cos\theta) \end{cases}$$

$$\Longrightarrow \quad Y_l^m(\theta,\varphi) \longrightarrow (-1)^l\, Y_l^m(\theta,\varphi)$$

Hence;

$$\Pi|\alpha,l,m\rangle = (-1)^l|\alpha,l,m\rangle$$

Alternative investigation:

$$[\Pi, L] = 0 \longrightarrow [\Pi, L_\pm] = 0 \quad \longrightarrow [\Pi, L_\pm^r] = 0 \quad (r=0,1,\dots l)$$

To obtain the state $|\alpha,l,m\rangle$:

$$|\alpha,l,m\rangle = \underbrace{L_\pm L_\pm \cdots L_\pm}_{m\text{-number}} |\alpha, l, m=0\rangle$$

Therefore it is enough to determine the parity of $|\alpha,l,m=0\rangle$ instead of $|\alpha,l,m\rangle$, because $[\Pi, L_\pm^r]=0$ and both $|\alpha,l,m=0\rangle$ and $|\alpha,l,m\rangle$ have the same parity.
(i.e. it is sufficient to work with $Y_l^{m=0}$).

Parity properties of Energy Eigenstates:

Theorem:

Suppose: $[H, \Pi] = 0$

and $|n\rangle$ to be a nondegenerate eigenket of H

$$H|n\rangle = E_n|n\rangle$$

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

Proof. —

Consider the state $\frac{1}{2}(1 \pm \Pi)|n\rangle$

This is a parity eigenket with eigenvalues: ± 1

$$\Pi\left[\tfrac{1}{2}(1 \pm \Pi)|n\rangle\right] = \tfrac{1}{2}\Pi|n\rangle \pm \tfrac{1}{2}\Pi^2|n\rangle = \tfrac{1}{2}\Pi|n\rangle \pm \tfrac{1}{2}|n\rangle$$

$$= \tfrac{1}{2}(\Pi \pm 1)|n\rangle = \pm\tfrac{1}{2}(\pm\Pi + 1)|n\rangle = \pm\tfrac{1}{2}(1 \pm \Pi)|n\rangle$$

Furthermore, this is also an energy eigenket:

$$H\left[\tfrac{1}{2}(1 \pm \Pi)|n\rangle\right] = \tfrac{1}{2}H|n\rangle \pm \tfrac{1}{2}H(\Pi|n\rangle)$$

$$= \tfrac{1}{2}H|n\rangle \pm \tfrac{1}{2}\Pi H|n\rangle = \tfrac{1}{2}E_n|n\rangle \pm \tfrac{1}{2}E_n\Pi|n\rangle$$

$$= E_n\left[\tfrac{1}{2}(1 \pm \Pi)|n\rangle\right]$$

But since the states are nondegenerate, then $|n\rangle$ and $\frac{1}{2}(1\pm\Pi)|n\rangle$ must represent the same state.

$$\longrightarrow |n\rangle = K\left(\tfrac{1}{2}(1\pm\Pi)|n\rangle\right)$$

$K \to$ const.

$$\longrightarrow \Pi|n\rangle = \pm|n\rangle$$

Remark: $H\Pi = \Pi H \to H(\Pi|n\rangle) = E_n(\Pi|n\rangle)$

$\to \Pi|n\rangle$ and $|n\rangle$ have E_n energy

But there is no degeneracy, because they are in the same vector axis.

Ex.- Consider a Simple Harmonic Oscillator (SHO);

the ground state $|0\rangle$ has <u>even</u> parity.

$$\psi_0(x') = \langle x'|0\rangle = \left(\frac{1}{\pi x_0^2}\right)^{1/4} e^{-\frac{1}{2}\left(\frac{x'}{x_0}\right)^2} \quad \text{(Gaussian wave-func.)}$$

Because $\psi_0(x')$ is <u>even</u> under $x' \longrightarrow -x'$

The first excited state $|1\rangle = a^\dagger|0\rangle$ must have an <u>odd</u> parity,

Because $a^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\left(x - \frac{iP}{m\omega}\right)$ is linear in x and P, which are both <u>odd</u>

In general the parity of SHO $= (-1)^n$

Thus the states are also eigenstates of parity OP.

Note that nondegenerate assumption is essential.

Ex. — Consider the hydrogen atom in nonrelativistic limit;

The energy eigenvalues are given by

$$E_n = -\frac{1}{2}\mu\,\frac{(Z\alpha c)^2}{n^2} \qquad \alpha = \frac{e^2}{\hbar c}$$

and depend on only principal quantum number n.

(for example 2P, and 2S states are degenerate)

Coulomb potential is obviously invariant under parity

i.e. $$[\Pi, -\frac{Ze^2}{r}] = 0$$

But the energy eigenket $c_p|2P\rangle + c_s|2S\rangle$

which satisfies;

$$H\left(c_p|2P\rangle + c_s|2S\rangle\right) = E_n\left(c_p|2P\rangle + c_s|2S\rangle\right)$$

is not a parity eigenket

Because;

$$\varphi(\vec{r}) = R_{n\ell}(r)\,Y_\ell^m(\theta,\varphi)$$

$$\begin{cases} \text{For s-state} & \ell = 0 \\ \text{" } \ell\text{- "} & \ell = 1 \end{cases}$$

So, $l=0$, and $l=1$ give different parities, and the combination of these two states does not have a definite parity.

$$\Pi\left(c_p|2P\rangle + c_s|2S\rangle\right) \neq \pm\left(c_p|2P\rangle + c_s|2S\rangle\right)$$

Ex. — Consider a momentum eigenket $|p'\rangle$

we know $\{\Pi, P\} = 0$

$H = \frac{P^2}{2m}$ for free particle

$$\rightarrow [H,\Pi] = \frac{1}{2m}[P^2,\Pi] = \frac{1}{2m}\left(P\{P,\Pi\} - \{P,\Pi\}P\right) = 0$$

$$[AB,C] = A\{B,C\} - \{A,C\}B$$

$$\longrightarrow \Pi^{+} H \Pi = H$$

The momentum eigenket (though obviously an energy eigenket, $[H,P]=0$) is not a parity eigenket.

$\langle x|p\rangle = N e^{\frac{i}{\hbar} p \cdot x'}$

$H|p'\rangle = \frac{P^2}{2m}|p'\rangle = \frac{p'^2}{2m}|p'\rangle \qquad E = \frac{p'^2}{2m}$

But

$$\Pi|p'\rangle = \int dx' \, \Pi|x'\rangle\langle x'|p'\rangle$$
$$= \int dx' \, |-x'\rangle\langle x'|p'\rangle$$

$$\longrightarrow \langle x|\Pi|p\rangle = \int dx' \langle x|-x'\rangle\langle x'|p'\rangle$$

$$= \int dx' \, \delta(x+x')\langle x'|p'\rangle = \langle -x|p'\rangle$$

Since $\langle x|p\rangle = N e^{\frac{i}{\hbar}\vec{p}\cdot\vec{x}}$

$$\longrightarrow \langle -x|p\rangle = N e^{-\frac{i}{\hbar}\vec{p}\cdot\vec{x}}$$

$$\longrightarrow \Pi|p'\rangle \neq \pm|p'\rangle \qquad !$$

Our theorem remains intact, because, in the theorem non-degeneracy requirement is essential, but here we have degeneracy between $|p'\rangle$ and $|-p'\rangle$ (both give the same eigenvalue of energy)

But the linear combination $\frac{1}{\sqrt{2}}(|p'\rangle \pm |-p'\rangle)$ are Parity eigenket.

$$\Pi\left(\frac{1}{\sqrt{2}}(|p'\rangle \pm |-p'\rangle)\right) = \pm\frac{1}{\sqrt{2}}(|p'\rangle \pm |-p'\rangle)$$

In terms of wave-func. language;

while → $e^{i\frac{p\cdot x}{\hbar}}$: does not have a definite parity

but → $\left\{\begin{array}{l} \cos\frac{p\cdot x}{\hbar} \\ \sin\frac{p\cdot x}{\hbar} \end{array}\right.$: do " " "

$$\left(e^{i\frac{p\cdot x}{\hbar}} \pm e^{-i\frac{p\cdot x}{\hbar}}\right)$$

Symmetrical Double-well Potential:

For a single-well: $$\frac{d^2u(x)}{dx^2}+\frac{2m}{\hbar^2}(E-V(x))\,u(x)=0$$

$$\frac{2m}{\hbar^2}V(x)=-\frac{\lambda}{a}\delta(x)$$

And for $E<0$, $$\frac{d^2u(x)}{dx^2}-k^2u(x)=-\frac{\lambda}{a}\delta(x)u(x)$$

where $k^2=\frac{2m}{\hbar^2}|E|$

$$\rightarrow u(x)=\begin{cases} e^{-kx} & x>0 \\ e^{kx} & x<0 \end{cases}$$ (the sol. of $\frac{d^2u(x)}{dx^2}-k^2u(x)=0$ for all x except $x=0$)

$$\left(\frac{du(x)}{dx}\right)_{x=0^+}-\left(\frac{du(x)}{dx}\right)_{x=0^-}=-\frac{\lambda}{a}u(0)$$ (the derivative is not continuous)

Recall:
$$\left(\frac{du}{dx}\right)_{\epsilon}-\left(\frac{du}{dx}\right)_{-\epsilon}=\int_{-\epsilon}^{\epsilon}dx\,\frac{d}{dx}\frac{du}{dx}$$
$$=\int_{-\epsilon}^{\epsilon}dx\,\frac{2m}{\hbar^2}(V(x)-E)u(x)=0$$
If $V=V_0\delta(x-a)$
$$\left(\frac{du}{dx}\right)_{a+\epsilon}-\left(\frac{du}{dx}\right)_{a-\epsilon}=\frac{2m}{\hbar^2}\int_{a-\epsilon}^{a+\epsilon}dx\,V_0\,\delta(x-a)u(x)$$
$$=\frac{2m}{\hbar^2}V_0\,u(a)$$

$$\rightarrow -k-k=-\frac{\lambda}{a} \quad\rightarrow k=\frac{\lambda}{2a}$$

For double-well

$$\frac{2m}{\hbar^2}V(x)=-\frac{\lambda}{a}\left[\delta(x-a)+\delta(x+a)\right]$$

Since $V(x)=V(-x)$ $\longrightarrow$ there will be sols. with definite parity
i.e. $[V(x),\Pi]=0$

i) Even Sol.

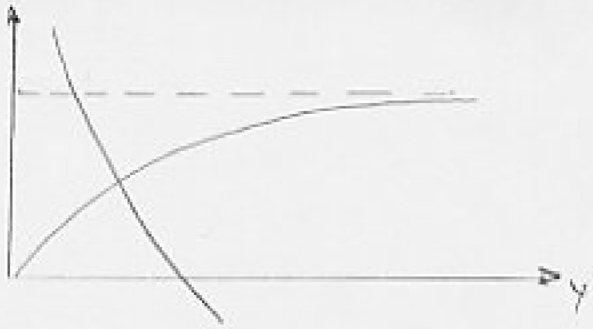
$$u(x)=\begin{cases} e^{-kx} & x>a \\ A\cosh kx & -a<x<a \\ e^{kx} & x<-a \end{cases}$$

$$e^{-ka}=A\cosh kx$$ (continuity of the wave-func.)

$$-ke^{-ka}-kA\sinh ka=-\frac{\lambda}{a}e^{-ka}$$ (discontinuity at $x=a$)

$$\rightarrow \tanh ka=\frac{\lambda}{ka}-1$$ eigenvalue cond.

$$K > \frac{\lambda}{2a}$$



$\tanh y = \frac{\lambda}{y} - 1 \qquad (y \equiv ka)$

$E \rightarrow$ larger negative number compared with single-well case (remember: $K \sim |E|$ and $E < 0$)

ii) Odd sol.

$$u(x) = \begin{cases} e^{-kx} & x > a \\ A \sinh kx & -a < x < a \\ -e^{+kx} & x < -a \end{cases}$$

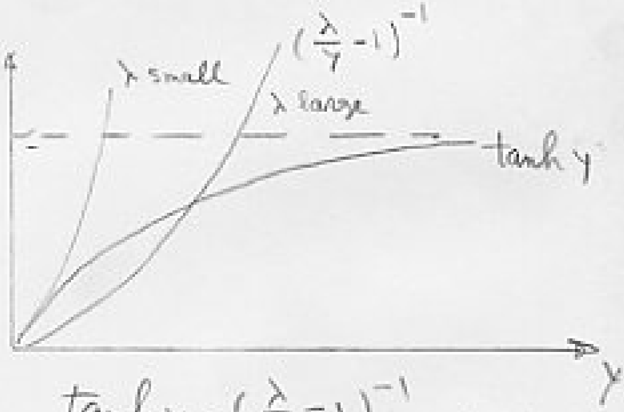
$$A \sinh ka = e^{-ka} \qquad \text{(continuity cond. at } a)$$

$$-k e^{-ka} - kA \cosh ka = -\frac{\lambda}{a} e^{-ka} \qquad \text{(discontinuity at } x = a)$$

$$\rightarrow \coth ka = \frac{\lambda}{ka} - 1 \rightarrow \tanh ka = \left(\frac{\lambda}{ka} - 1\right)^{-1}$$

$$\rightarrow \quad k < \frac{\lambda}{2a}$$

$\longrightarrow$ less strongly bound than even sol.



$\tanh y = \left(\frac{\lambda}{y} - 1\right)^{-1} \qquad y = ka$

$\longrightarrow E_o > E_e$

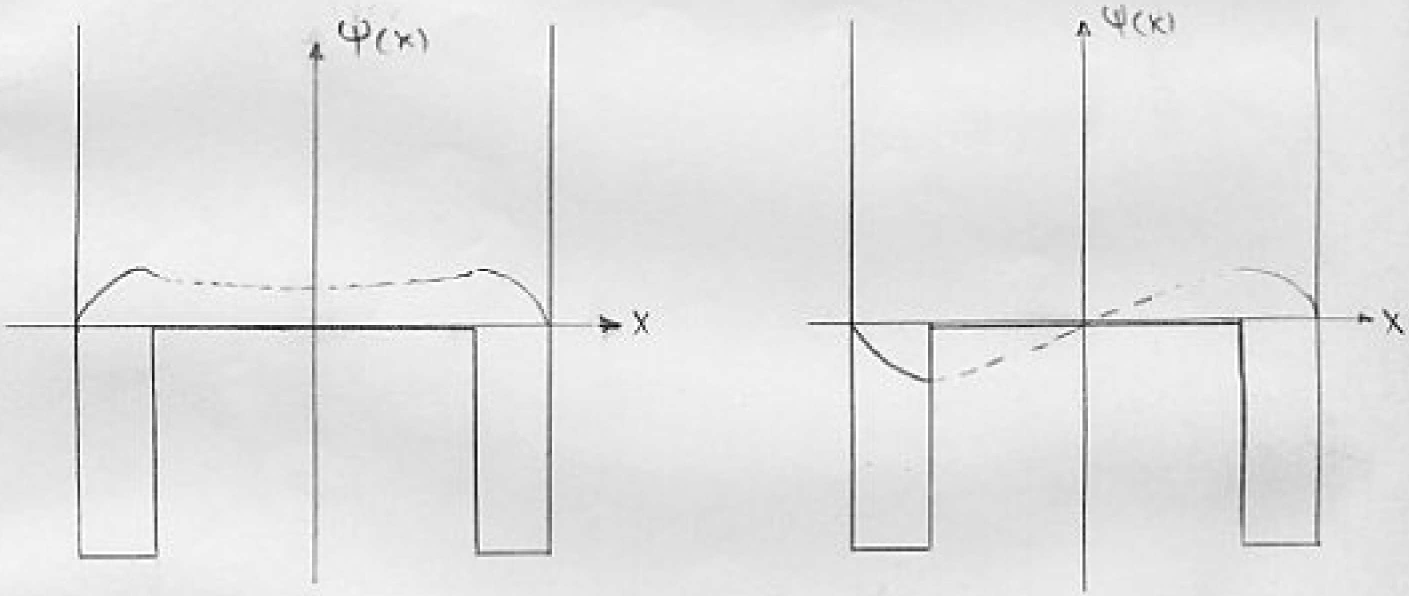
We designate:

Odd sols. $\xrightarrow{\text{as}}$ Anti-Sym. Sols. (A)

Even " $\xrightarrow{\text{as}}$ Sym. sol. (S)

$\longrightarrow E_A > E_S$ where $E_A - E_S$ $\left\{\begin{array}{l}\text{is very small when} \\ \text{the middle barrier is high}\end{array}\right.$

In general: Min energy ~ Smallest No. of nodes.



Sym. Sol. Ant. Sym. Sol.

$|S\rangle$ $|A\rangle$

Of course since $[H, \Pi] = 0$ (for $|S\rangle$ or $|A\rangle$)

$$H \begin{Bmatrix} |S\rangle \\ |A\rangle \end{Bmatrix} = \begin{Bmatrix} E_S |S\rangle \\ E_A |A\rangle \end{Bmatrix}$$ & (see the Fig. for V(x)) Remark: There is no degeneracy either or $|S\rangle$ or $|A\rangle$.

$$\Pi \begin{Bmatrix} |S\rangle \\ |A\rangle \end{Bmatrix} = \begin{Bmatrix} +|S\rangle \\ -|A\rangle \end{Bmatrix}$$

By superposition of states we can form;

$$|R\rangle = \frac{1}{\sqrt{2}}\left(|S\rangle + |A\rangle\right)$$ Wave func. consentrated at the right

$$|L\rangle = \frac{1}{\sqrt{2}}\left(|S\rangle - |A\rangle\right)$$ " " " left

Obviously: $\begin{cases} \Pi|R\rangle \neq \pm|R\rangle \\ \Pi|L\rangle \neq \pm|L\rangle \end{cases}$

In fact; $\begin{cases} \Pi|R\rangle = |L\rangle \\ \Pi|L\rangle = -|R\rangle \end{cases}$

($|R\rangle$ and $|L\rangle$ are neigther the eigen states of H nor Π.)

Also; $\begin{cases} H|R\rangle \neq E|R\rangle \\ H|L\rangle \neq E|L\rangle \end{cases}$

But:

Let us consider the behaviour of system as t increases;

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

$$= \frac{1}{\sqrt{2}} e^{-iE_S t/\hbar}\left(|S\rangle + e^{-i(E_A - E_S)t/\hbar}|A\rangle\right)$$

At time $t = \frac{T}{2} = \frac{\pi\hbar}{(E_A - E_S)}$, the system is found in <u>pure</u> $|L\rangle$.

At $t = T$, we are back to pure $|R\rangle$, and so forth.

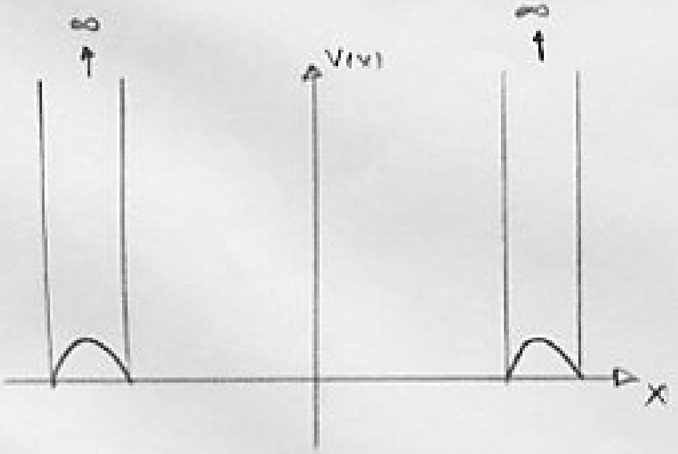
Thus we have oscillation between $|R\rangle$ and $|L\rangle$ with the frequency:

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

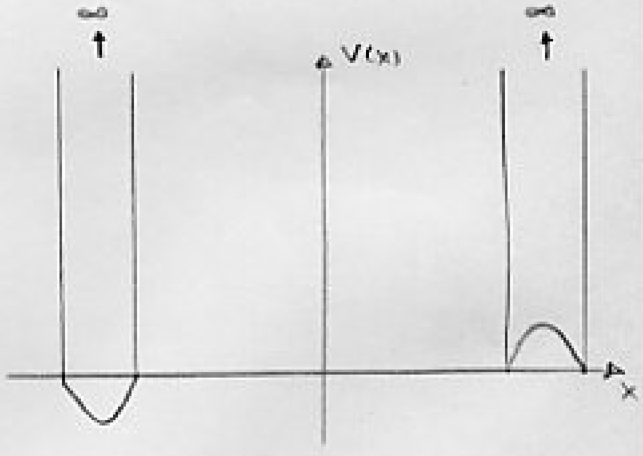
This is a tunneling effect.

The particle passes through classically forbiden region from right to left and vice versa

If the middle barrier become infinitely high, the $|S\rangle$ and $|A\rangle$ states become degenerate.



Sym. sol.



Anti. sym. sol.

$E_A = E_S = E$

$\longrightarrow H|S\rangle = E|S\rangle$

$H|A\rangle = E|A\rangle$

$\longrightarrow \begin{cases} H|R\rangle = E|R\rangle \\ H|L\rangle = E|L\rangle \end{cases}$

There is degeneracy

But still:

$$\Pi|R\rangle \neq \pm|R\rangle$$

$$\Pi|L\rangle \neq \pm|L\rangle$$

Our theorem remains valid (since we have degeneracy here)

Once the system is found, say in $|R\rangle$, it remains so forever.

$$\omega = \frac{E_A - E_S}{\hbar} = 0 \longrightarrow T \longrightarrow \infty$$

There is no possibility of tunneling.

Thus, when there is a degeneracy, the physically realizable energy eigenkets need not be parity eigenkets.

Remark:

Parity - Selection Rule (Wigner)

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

$$\Pi|\alpha\rangle = \epsilon_\alpha|\alpha\rangle$$
$$\Pi|\beta\rangle = \epsilon_\beta|\beta\rangle$$

where $\epsilon_\alpha, \epsilon_\beta = \pm 1$

We can show $\langle\beta|X|\alpha\rangle = 0$ unless $\epsilon_\alpha = -\epsilon_\beta$

i.e.: Parity odd operator X connects states of opposite parity.

Proof. —

$$\langle\beta|X|\alpha\rangle = \langle\beta|\Pi^{-1}\Pi X \Pi^{-1}\Pi|\alpha\rangle = \epsilon_\alpha\epsilon_\beta\langle\beta|\Pi X\Pi^{-1}|\alpha\rangle$$

$$= -\epsilon_\alpha\epsilon_\beta\langle\beta|X|\alpha\rangle$$

$$\longrightarrow \begin{cases} \langle\beta|X|\alpha\rangle = 0 \\ \text{or } \epsilon_\alpha\epsilon_\beta = -1 \longrightarrow \epsilon_\alpha = -\epsilon_\beta \end{cases}$$

We remember that: $\int \psi_\beta^*(x)\, x\, \psi_\alpha(x)\, dx = 0$

when ψ_β and ψ_α have the same parity.
(when the total parity becomes odd).

This selection rule is of importance in discussing <u>radiative transitions</u> between atomic states.
(transitions between states of opposite parity are allowed)

If $\begin{cases} [H,\Pi]=0 \\ \text{no-degeneracy} \end{cases}$ $\quad H|n\rangle = E_n|n\rangle \longrightarrow \Pi|n\rangle = \pm|n\rangle$

$\longrightarrow$ $|n\rangle$ has definite parity $(+)$ or $(-)$

$\longrightarrow$ $\langle n|X|n\rangle = 0$

But if $\Pi|n\rangle \neq \pm|n\rangle$, we may have <u>non-vanishing terms</u>.

Ex. — If $|\alpha\rangle = a|n_1\rangle + b|n_2\rangle$

where $\Pi|n_1\rangle = +|n_1\rangle$
$\Pi|n_2\rangle = -|n_2\rangle$

$$\longrightarrow \langle\alpha|X|\alpha\rangle = |a|^2 \cancel{\langle n_1|X|n_1\rangle} + |b|^2 \cancel{\langle n_2|X|n_2\rangle} + ab^* \langle n_2|X|n_1\rangle + a^*b\langle n_1|X|n_2\rangle$$

$$\langle\alpha|X|\alpha\rangle = ab^*\langle n_2|X|n_1\rangle + a^*b\langle n_1|X|n_2\rangle$$

Note – In multipole expansion of electric dipole transition we encounter with such an operator (X) between initial and final states.

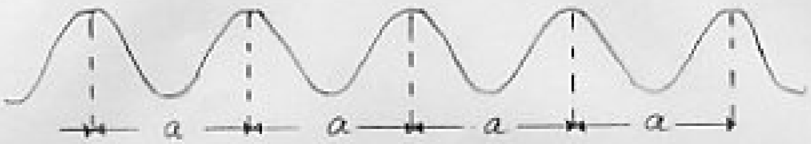
Conclusion: Odd operators under parity, like P or $S \cdot x$ have nonvanishing matrix elements only between states of opposite parity.

In contrast, operators that are even under parity, connect states of the same parity.

4.3 - Lattice Translation as a Discrete Symmetry

Consider a periodic potential in one dimension:

$$V(X \pm a) = V(x)$$



Ex. - The motion of an electron in a chain of regulary spaced positive ions.

In general: $[H, \tau] \neq 0 \quad \forall\, \tau(l)$, l: arbitrary

Note that: $\begin{cases} \tau^\dagger(l)\, X\, \tau(l) = x + l \\ \tau(l)|x'\rangle = |x'+l\rangle \end{cases}$ $\left([x_i, \tau(\vec{l})] = l_i\, \tau(\vec{l}) \right.$

Remark: $X\left(\tau(dx')|x'\rangle\right) = X|x'+dx'\rangle = (x'+dx')|x'+dx'\rangle$

$$\tau(dx')\, X|x'\rangle = x'\,\tau(dx')|x'\rangle = x'|x'+dx'\rangle$$

$$[X, \tau(dx')]\,|x'\rangle = dx'|x'+dx'\rangle \simeq dx'|x'\rangle \quad \underline{\forall |x'\rangle}$$

Second order approx.

$$\Rightarrow [x, \tau(dx')] = dx'$$

$$\rightarrow \tau^\dagger(dx')\, X\, \tau(dx') - x = dx'$$

Now for our periodic potential:

$$\tau^{\dagger}(a)\, V(x)\, \tau(a) = V(x+a) = V(x)$$

$$\rightarrow [V(x), \tau(a)] = 0$$

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

$$\left[\frac{p^2}{2m}, \tau(a)\right] = 0 \qquad \left(\text{because } \tau(a) = e^{-\frac{i\bar{P}\cdot\bar{a}}{\hbar}}\right)$$

$$\longrightarrow \tau^{\dagger}(a)\, H\, \tau(a) = H$$

$$\longrightarrow [H, \tau(a)] = 0$$

$\longrightarrow$ H and $\tau(a)$ can be simultaneously diagonalized.

Remark: Although $\tau(a)$ is <u>unitary</u>, it <u>is not Hermition</u>, so we expect the eigenvalue to be complex number of <u>modulus 1</u>.

Remark: $\tau(dx')$ should be unitary, because it is reasonable if a state ket $|\alpha\rangle$ is normalized to unity, then $\tau(dx')|\alpha\rangle$ must be normalized to unity.

$$\langle\alpha|\alpha\rangle = \langle\alpha|\tau^{\dagger}(dx')\,\tau(dx')|\alpha\rangle = 1$$

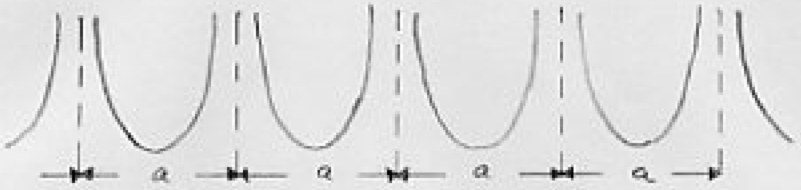
Remark: Hermitian op.; $\int (F\psi_1)^* \psi_2\, d\tau = \int \psi_1^* F \psi_2\, d\tau$

or $\langle Ax, y\rangle = \langle x, Ay\rangle$

Def. of Hermitain adjoint op $\int (F\psi_1)^* \psi_2\, d\tau = \int \psi_1^* F^{\dagger} \psi_2\, d\tau$

First consider a special case:

Consider the barrier height between two adjecent latice site goes to infinity:



Clearly a state in which, the particle is completely localized in one of the lattice sites can be a candidate for the ground state

let: $|n\rangle$ the ket of particle at the nth site.

$$H|n\rangle = E_0|n\rangle$$

The wave-func. $\langle x'|n\rangle$ is finite only in the nth site.

A similar state localized at some other site, also has the same energy E_0.

$\longrightarrow$ there exist denumerably infinite ground states n,

$$-\infty < n < \infty$$

obviously:

$$\tau(a)|n\rangle = |n+1\rangle$$

So despite:

$$[H, \tau(a)] = 0$$

$$H|n\rangle = E_0|n\rangle$$

but $$\tau(a)|n\rangle \neq C|n\rangle$$

This is consistant with our earlier Theorem (since we have infinite-fold degeneracy).

When there is, such degeneracy, the symmetry of the world need not be the symmetry of the energy eigenkets.

Our task is to find a <u>simultaneous</u> eigenket of H and $\tau(a)$.

Let us form a linear combination:

$$|\theta\rangle = \sum_{n=-\infty}^{\infty} e^{in\theta}|n\rangle \qquad \text{where } -\pi \leq \theta \leq \pi$$

Remark: This is analogous with the case of $|R\rangle$ and $|L\rangle$ in double-well potential.

We assert that $|\theta\rangle$ is simultaneous eigenket of H and $\tau(a)$.

$$H|\theta\rangle = \sum_{n=-\infty}^{\infty} e^{in\theta} H|n\rangle$$

but $\quad H|n\rangle = E_0|n\rangle \qquad \forall n$

$$\longrightarrow \quad H|\theta\rangle = E_0|\theta\rangle$$

Now

$$\tau(a)|\theta\rangle = \sum_{n=-\infty}^{\infty} e^{in\theta}\tau(a)|n\rangle = \sum_{n=-\infty}^{\infty} e^{in\theta}|n+1\rangle$$

Since, $\sum$ is from $-\infty$ to ∞;

$n \longrightarrow n-1$ gives the same result

$$\longrightarrow \tau(a)|\theta\rangle = \sum_{n=-\infty}^{\infty} e^{i(n-1)\theta}|n\rangle = e^{-i\theta}|\theta\rangle$$

Note that $\begin{cases} \theta : \text{continuous} \\ E_0 : \text{indep. of } \theta \end{cases}$

$$\begin{cases} \theta : \text{lables degeneracy } (\infty\text{-fold}) \\ \frac{\partial}{\partial\theta} E_0 = 0 \end{cases}$$

Remark: Since $[H, \tau(a)] = 0$, it means we can find simultaneous eigenket of H and $\tau(a)$. But since there is degeneracy, the eigenkets of H (i.e. $|n\rangle$) are not eigenkets of $\tau(a)$, but still we could introduce the parameter θ to form simultaneous eigenkets of H and $\tau(a)$.

More Realistic Situation

We return to the first case;

The potential barrier is not infinitely high.

As before;

$$\tau(a)|n\rangle = |n+1\rangle$$

However, now there is some leakage possible, into, neighbouring lattice sites. (due to quantum mechanical tunneling).

In other words; the wave-func.

$$\langle x'|n\rangle$$

has a tail extending to sites other than nth site.

$$\longrightarrow \langle n|n+1\rangle \neq 0 \quad \left(\int \langle n|x\rangle \langle x|n+1\rangle dx \neq 1 \right)$$

Because of translational invariance; $\left(\langle n|\tau^{\dagger} H \tau|n\rangle = \langle n|H|n\rangle \right)$

$$\langle n|H|n\rangle = E_0 \qquad \forall n \quad \text{(diagonal elements of } H)$$

However H is not completely diagonal in the $\{|n\rangle\}$ basis due to leakage.

$$H|n\rangle \neq E_0|n\rangle$$

Remark: In the previous case we had;

$$\langle m|H|n\rangle = E_0 \delta_{mn}$$

but, here $\quad \langle m|H|n\rangle \neq 0 \quad \forall\ m\neq n$

Now, suppose the barriers are high enough but not infinite.

Then we expect;

$$\langle n'|H|n\rangle \neq 0 \quad \text{if} \quad n' = \begin{cases} n \\ n\pm 1 \end{cases}$$

This assumption is known as "tight-binding approximation". (in solid state phys.)

define; $\quad \langle n\pm 1|H|n\rangle = -\Delta \quad \forall n \qquad (1)$

Also $\quad \langle n|n'\rangle \approx \delta_{nn'} \qquad (2)$

Δ is indep. of n, due to translation invariance of H.

In the earlier case $\quad |n\rangle \doteq \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ \langle n|n\rangle \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}$ $\qquad$ Now $|n\rangle \doteq \begin{pmatrix} 0 \\ 0 \\ 0 \\ \langle n-1|n\rangle \\ \langle n|n\rangle \\ \langle n+1|n\rangle \\ 0 \\ 0 \\ 0 \end{pmatrix}$ (or the same as before)

$$\left\{ H = \begin{pmatrix} E_0 & 0 & 0 & 0 & \cdots \\ 0 & E_0 & 0 & 0 & 0 \\ 0 & 0 & E_0 & 0 & 0 \\ & & - & & - \end{pmatrix} \right.$$

old

$$(\text{new}) \quad H = \begin{pmatrix} & - & - & - & - & - & \\ \cdots & E_0 & -\Delta & 0 & 0 & 0 & \cdots \\ \cdots & -\Delta & E_0 & -\Delta & 0 & 0 & \cdots \\ \cdots & 0 & -\Delta & E_0 & -\Delta & 0 & \cdots \\ \cdots & 0 & 0 & -\Delta & E_0 & -\Delta & \cdots \\ & - & - & - & - & - & \\ & - & - & - & - & - & \end{pmatrix}$$

$$H|n\rangle = \begin{pmatrix} - - - \\ E_0\langle n-1|n\rangle - \Delta\langle n|n\rangle \\ -\Delta\langle n-1|n\rangle + E_0\langle n|n\rangle - \Delta\langle n+1|n\rangle \\ -\Delta\langle n|n\rangle + E_0\langle n+1|n\rangle \\ - - - - \end{pmatrix}$$

$$H|n\rangle = \overbrace{\left(E_0\langle n-1|n\rangle - \Delta\langle n|n\rangle\right)|n-1\rangle}^{\text{new}(-\Delta)}$$

$$+\left(-\Delta\underbrace{\langle n-1|n\rangle}_{\text{2nd order}} + E_0\langle n|n\rangle - \Delta\langle n+1|n\rangle\right)|n\rangle$$

$$+\left(-\Delta\langle n|n\rangle + E_0\langle n+1|n\rangle\right)|n+1\rangle$$

$$\simeq E_0|n\rangle - \Delta\left(|n-1\rangle + |n+1\rangle\right)$$

Remark: Note that;

$|\alpha\rangle = \sum_{a'} C_{a'}|a'\rangle \qquad \langle a''|\alpha\rangle = \sum_{a'} C_{a'}\langle a''|a'\rangle \rightarrow C_{a'} = \langle a'|\alpha\rangle$ if $\langle a''|a'\rangle = \delta_{a'a''}$

$\rightarrow |\alpha\rangle = \sum_{a'}|a'\rangle\langle a'|\alpha\rangle \quad \rightarrow \sum_{a'}|a'\rangle\langle a'| = I$

However if $\langle a'|a''\rangle \neq \delta_{a'a''} \quad \rightarrow \sum_{a'}|a'\rangle\langle a'| \neq I$

So in our case $\sum_{n'}|n'\rangle\langle n'| \simeq I$ and also $H \simeq \sum_{n''}\sum_{n'}|n''\rangle\langle n''|H|n'\rangle\langle n'|$

$$H|n\rangle = \sum_{n'}|n'\rangle\langle n'|H|n\rangle \quad (3)$$

$$(1)(2)(3) \rightarrow H|n\rangle = E_0|n\rangle - \Delta\left(|n-1\rangle + |n+1\rangle\right) \quad (4)$$

Let us for a linear combination:

$$|\theta\rangle = \sum_{n=-\infty}^{\infty} e^{in\theta}|n\rangle$$

As before $\tau(a)|\theta\rangle = e^{-i\theta}|\theta\rangle$

What about $H|\theta\rangle \overset{?}{=} c|\theta\rangle$

$$H|\theta\rangle = H\sum e^{in\theta}|n\rangle = \sum e^{in\theta} H|n\rangle$$

$$= \sum e^{in\theta}\left(E_0|n\rangle - \Delta(|n-1\rangle + |n+1\rangle)\right)$$

$$= E_0\sum e^{in\theta}|n\rangle - \Delta\sum e^{in\theta}|n-1\rangle - \Delta\sum e^{in\theta}|n+1\rangle$$

$$= E_0\sum e^{in\theta}|n\rangle - \Delta\sum\left(e^{i(n+1)\theta} + e^{i(n-1)\theta}\right)|n\rangle$$

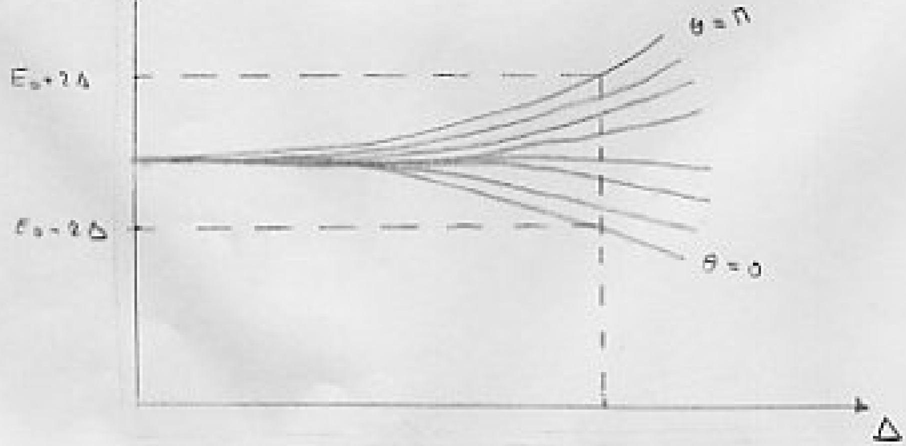
$$= (E_0 - 2\Delta\cos\theta)\sum e^{in\theta}|n\rangle$$

$$\longrightarrow \quad H|\theta\rangle = (E_0 - 2\Delta\cos\theta)|\theta\rangle$$

This time, the eigenvalue $(E_0 - 2\Delta\cos\theta)$ depends on the continuous real parameter θ.

$$\frac{\partial}{\partial\theta}(E_0 - 2\Delta\cos\theta) \neq 0$$

The degeneracy is lifted as Δ becomes finite.
We have a continuous distribution of energy eigenvalues between $E_0-2\Delta$ and $E_0+2\Delta$.



The Physical meaning of θ:

let us study the wave func. $\langle x'|\theta\rangle$

The wave func. of the lattice-translated state is:

$$\tau(a)|\theta\rangle \qquad \text{lattice-translated state}$$

$$\langle x'|\tau(a)|\theta\rangle = \langle x'-a|\theta\rangle$$

because; $\tau^{+}(a)\,X\,\tau(a) = X+a \quad \to \tau(a)|x'\rangle = |x'+a\rangle$

$\tau(a)\,X\,\tau^{+}(a) = X-a \quad \to \tau^{+}(a)\,|x'\rangle = |x'-a\rangle$

At the same time we have;

$$\langle x'|\tau(a)|\theta\rangle = e^{-i\theta}\langle x'|\theta\rangle$$

$$\to \langle x'-a|\theta\rangle = \langle x'|\theta\rangle\, e^{-i\theta}$$

let; $\begin{cases} \theta = ka \\ \langle x'|\theta\rangle = e^{ikx'}\,u_k(x') \end{cases}$

where $u_k(x')$: Periodic func. with periodicity of a

$\to u_k(x'+a) = u_k(x')$ as we can see below;

Substituting:

$$e^{ik(x'-a)} u_k(x'-a) = e^{ikx'} u_k(x') \, e^{-ika}$$

$$\longrightarrow \quad u_k(x'-a) = u_k(x')$$

Thus we get the important cond. as:

Bloch's Theorem:

The wave-func of $|\theta\rangle$, which is an eigenket of $\tau(a)$, can be written as a plane wave $e^{ikx'}$ times a periodic func. with periodicity a.

Therefore;

Where $\quad V(x) = V(x+a)$

The sol. $\longrightarrow \quad \psi_k(x') = e^{ikx'} u_k(x')$

Remark: The only fact we have used, is that $|\theta\rangle$ is an eigenket of $\tau(a)$ with the eigenvalue $e^{-i\theta}$. In particular — the theorem holds even if <u>tight-binding</u> approximation <u>breaks down</u>.

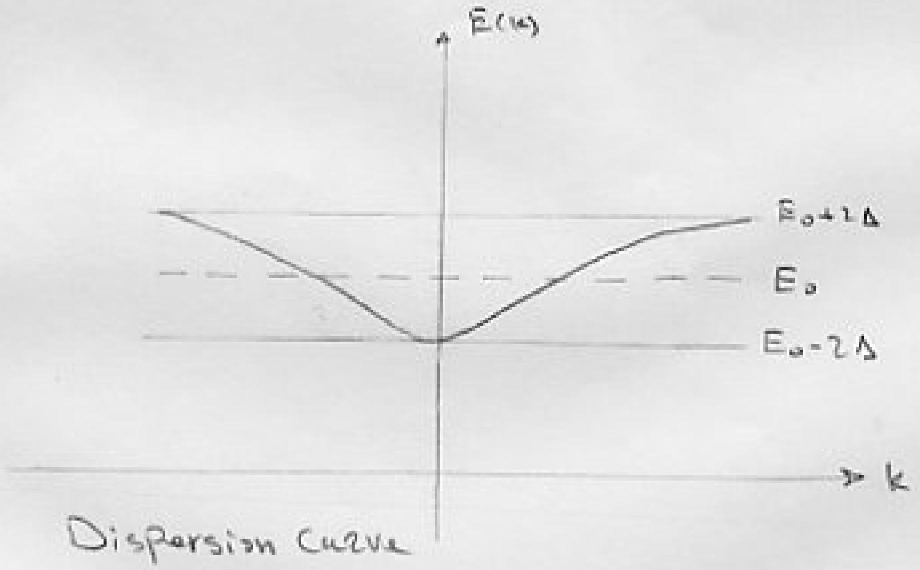
We obtained:

$$\langle x' | \theta \rangle = e^{ikx'} u_k(x')$$

$E = E_0 - 2\Delta \cos\theta$ energy eigen-value

$\theta = ka \longrightarrow E(k) = E_0 - 2\Delta \cos ka$

Since $-\pi \leq \theta \leq \pi \longrightarrow -\frac{\pi}{a} \leq k \leq \frac{\pi}{a}$



Dispersion curve

Notice that:

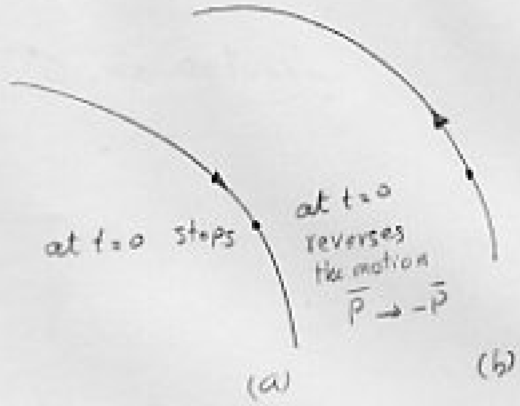
1- This energy eigen-value problem is independent of the detailed shape of potential (as long as the tight-binding approx. is valid.)

2- There is a cut-off in the wave vector k of Bloch wave-func. $\langle x' | \theta \rangle = e^{ikx'} u_k(x')$

given by $|k| = \frac{\pi}{a}$

As a result of tunneling, the denumerably infinitefold degeneracy is now completely lifted, and the allowed energy values form a continuous band between $E_0 - 2\Delta$ and $E_0 + 2\Delta$ known as Brillouim Zone.

4-4 The Time Reversal Discrete Symmetry



Classical Case:

Consider a particle subject to a certain force field.

Suppose its trajectory is given by (a).

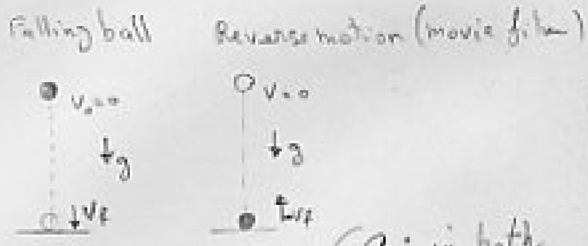
At $t=0$ it stops and reverses its motion (b).

$$\bar{p} \longrightarrow -\bar{p} \qquad (\text{at } t=0)$$

More formally:

If $X(t)$ is a sol. to $\quad m\ddot{X}(t) = -\nabla V(x)$

$X(-t)$ is also a possible sol. in the <u>same force field</u> derivable from $V(x)$.



Ex.- If $X(t) = at^2 + vt + x_0$

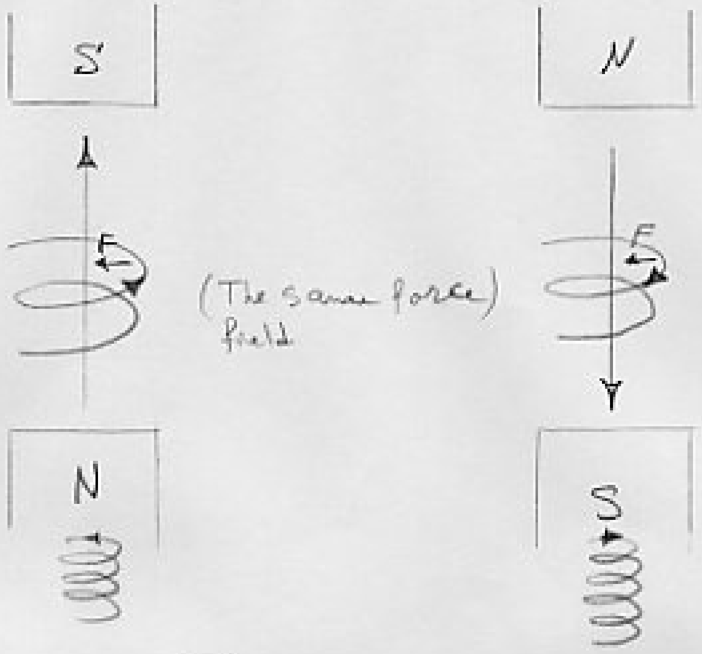
We observe; $X(-t) = a(-t)^2 + (-v)(-t) + x_0$

$\left\{ \begin{array}{l} a: \text{in both cases in the same direction} \\ a = \frac{dv}{dt} \end{array} \right.$

is invariant under $\left\{ \begin{array}{l} t \longrightarrow -t \\ \bar{p} \longrightarrow -\bar{p} \end{array} \right. \Longrightarrow \bar{V} \longrightarrow -\bar{V}$

Remark: We don't discuss about the <u>dissipative</u> forces (like friction force).

Ex. —



Symmetric Motion
$(t \longrightarrow -t)$

More formally:

The Maxwell eqns.

$$\begin{cases} \nabla\cdot E = \rho \\ \nabla\times E = -\dfrac{\partial B}{\partial t} \\ \nabla\times B - \dfrac{1}{c}\dfrac{\partial E}{\partial t} = \dfrac{j}{c} \\ \nabla\cdot B = 0 \end{cases}$$

and Lorentz force $F = e\left[E + \frac{1}{c}(v\times B)\right]$

are invariant under: $t \longrightarrow -t$, provided also let;

$$\begin{cases} E \longrightarrow E \\ B \longrightarrow -B \\ \rho \longrightarrow \rho \\ j \longrightarrow -j \\ v \longrightarrow -v \end{cases}$$

Time Reversal in Quantum Mechanics:

If $\psi(x,t)$ is a sol. of the Schrödinger equ.:

$$i\hbar \frac{\partial \psi}{\partial t} = \left(-\frac{\hbar^2}{2m}\nabla^2 + V\right)\psi$$

we see that $\psi(x,-t)$ is not, a sol. (we obtain a minous sign.)

because the Schrödinger equ. is linear in $\frac{\partial}{\partial t}$ (first order time derivative)

But $\psi^*(x,-t)$ is a sol.

If $\psi(x,t) = U(x)\, e^{-\frac{iEt}{\hbar}}$

$\psi^*(x,-t) = U^*(x)\, e^{-\frac{iEt}{\hbar}}$ $\longrightarrow$ $\begin{cases} E\,U(x) = \left(-\frac{\hbar^2}{2m}\nabla^2 + V\right) U(x) \\ E\,U^*(x) = \left(-\frac{\hbar^2}{2m}\nabla^2 + V\right) U^*(x) \end{cases}$

Thus, we conjecture that time reversal must have something to do with complex conjugation.

If $\psi = \langle x|\alpha\rangle$ at $t=0$ $\longrightarrow$ $\psi^* = \langle x|\alpha\rangle^*$ corresponding time-reversal state

Antilinear Operators:

A: antilinear op

$$A\,(c_1|\alpha\rangle + c_2|\beta\rangle) = c_1^* A|\alpha\rangle + c_2^* A|\beta\rangle \quad \text{(Def.)}$$

$$\forall\ |\alpha\rangle, |\beta\rangle$$
$$\forall\ c_1, c_2$$

Obviously, then $cA = Ac^*$

If A, B: antilinear ops.,

$$(AB)(c_1|\alpha\rangle + c_2|\beta\rangle) = c_1 AB|\alpha\rangle + c_2 AB|\beta\rangle$$

$\rightarrow$ AB: linear op

Also; $AA^{-1} = I = A^{-1}A$

Since I: linear op $\rightarrow A^{-1}$: antilinear op.

Linear Vector space:

A linear vector space V is defined by a set S of elements $x, y, z, \ldots$ called vectors and a field F of numbers $a, b, c, \ldots$ called scalars, with the following properties:

i) The space is closed under vector addition

$x + y = z$ where $z \in V$ and is unique.

Also $x + y = y + x$ (vector addition is commutative)

$$x + (y+z) = (x+y) + z \quad (\quad " \quad " \quad " \text{ associative})$$
$$= x + y + z$$

ii) There is a null vector

$$x + 0 = x \qquad \forall x$$

iii) There is an additive inverse $(-x)$ such that

$$x + (-x) = 0$$

iv) The space is closed under multiplication by scalars.

i.e. $\quad cx \in V \qquad \forall x$

also, $\quad cx = xc \qquad$ (commutative)

$$a(bx) = (ab)x = abx \quad \text{(associative)}$$

$$\left\{\begin{aligned} (a+b)x &= ax + bx \\ a(x+y) &= ax + ay \end{aligned}\right. \quad \text{distributive}$$

Example: The set of all n-tuples of numbers $(x_1, x_2 \ldots x_n)$, when addition of vectors and multiplication of a vector by a scalar are defined by

$$(x_1, x_2 \ldots x_n) + (y_1, y_2 \ldots y_n) = (x_1 + y_1, \ldots x_n + y_n)$$

$$a(x_1, x_2 \ldots x_n) = (ax_1, \ldots ax_n)$$

n-dim Euclidean space

v) A linear vector space is unitary if a scalar product is defined if;

$\forall\, x, y$ there corresponds a unique scalar (x, y) such that;

pre-factor Post-factor

$$(x,y) = (y,x)^*$$

$$(x, y+z) = (x,y) + (x,z)$$

$$(x,cy) = c(x,y)$$

$$(x,x) \geqslant 0 \qquad ((x,x) = 0 \text{ if } x = 0)$$

$(x, ay+bz) = a(x,y) + b(x,z)$ (The scalar product is linear w.r.t. the post-factor)

$(ax+by, z) = a^*(x,z) + b^*(y,z)$ (" " " anti-linear " " pre-factor)

For linear ops.:

$$(y, Ax)^* = (Ax, y) = (x, A^\dagger y)$$

In bra-ket notation: $\langle y|A|x\rangle^* = \langle Ax|y\rangle = \langle x|A^\dagger|y\rangle$

For antilinear ops:

$$(y, Ax)^* = (Ay, x) = (A^\dagger x, y) = (x, A^\dagger y)^* \qquad (a)$$

In bra-ket notation;

$$\langle y|A|x\rangle^* = \langle Ay|x\rangle = \langle A^\dagger x|y\rangle = \langle x|A^\dagger|y\rangle^* \qquad (b)$$

From this $\longrightarrow$

If A, B, C: anti linear

$(ABCy, x) = ((ABC)^\dagger x, y)$ (1) (since ABC is anti-linear op.)

But since AB and BC are linear ops.

$$(ABCy, x) = (Cy, (AB)^\dagger x) = (C^\dagger (AB)^\dagger x, y) \qquad (2)$$

and $(ABCy, x) = (A^{+}x, BCy) = ((BC)^{+}A^{+}x, y)$ (3)

(1)(2)(3) $\rightarrow$ $(ABC)^{+} = C^{+}B^{+}A^{+}$ (4)

Note that it is important to explicitly specify in a scalar product, whether an antilinear op. is operating on a ket vector to the right or on the bra vector to the left.

Antiunitary ops.:

An antilinear op A is said to be antiunitary if

$$A^{+} = A^{-1}$$

i.e.: $AA^{+} = A^{+}A = I$

If A, B, C, D: antiunitary:

$\rightarrow$ ABC: antiunitary
$ABCD$: unitary

Remark: A similarity tr. by an antiunitary op. also preserves the Hermitian character of a linear op.

i.e. if A: antiunitary op.
B: linear op.

$$(ABA^{-1})^{+} = ABA^{-1} \qquad \text{where } B = B^{+}$$

This follows from (4)

Remark: The cond. for U to be unitary is that

$$(UBU^{-1})^{+} = UBU^{-1} \qquad \text{where } B = B^{+} \text{ (linear op.)}$$

A linear op. U is unitary if it preserves the Hermitian character of an op. under a similarity tr.

Remark:

(a) $\Rightarrow$ $$(x, y) \xrightarrow[\text{antiunitary}]{A} (\tilde{x}, \tilde{y}) = (\tilde{x}, Ay) = (y, A^{+}\tilde{x})$$

$$= (y, A^{+}Ax) = (y, x) = (x, y)^{*} \qquad (c)$$

or

$$\langle x | y \rangle \xrightarrow{A} \langle \tilde{x} | \tilde{y} \rangle = \langle \tilde{x} | A | y \rangle = \langle y | A^{+} | \tilde{x} \rangle$$

$$= \langle y | A^{+}A | x \rangle = \langle y | x \rangle = \langle x | y \rangle^{*} \qquad (d)$$

Thus, only the absolute value of the scalar product is preserved under an antiunitary tr..

$$|(\tilde{x}, \tilde{y})| = |(x, y)^{*}| = |(x, y)|$$

Remark: The absolute value of the scalar product is also preserved by the unitary tr.

$$(x', y') = (Ux, Uy) = (x, U^+Uy) = (x, y)$$

The properties of an antiunitary tr.:

i) A: antiunitary

$$|\tilde{x}\rangle = A|x\rangle$$

ii) $\langle\tilde{x}| = \langle A^+x|$

Proof:

(c) $\rightarrow$ $\langle\tilde{x}|\tilde{y}\rangle = \langle\tilde{x}|Ay\rangle = \langle x|y\rangle^*$

(a) $\rightarrow$ $\langle\tilde{x}|Ay\rangle = \langle A\tilde{x}|y\rangle^*$

$\rightarrow$ $\langle A\tilde{x}| = \langle x|$

$\rightarrow$ $\langle\tilde{x}| = \langle A^+x|$

iii) A linear op. B transforms into

$$\tilde{B} = ABA^+ \qquad (A\text{: antiunitary})$$

Proof: let $|y\rangle = B|x\rangle$

$$A|y\rangle = AB|x\rangle = (ABA^+)A|x\rangle$$

$$\rightarrow |\tilde{y}\rangle = \tilde{B}|\tilde{x}\rangle$$

iv) A complex number c transforms into

$$\tilde{C} = ACA^{+} = C^{*}$$

Remark:

$$B_{jk} \equiv \langle u_j|B|u_k\rangle \xrightarrow[\text{antiunitary}]{A} B^{*}_{jk}$$

$$\langle u_j|B|u_k\rangle \xrightarrow{A} \langle \tilde{u}_j|\tilde{B}|\tilde{u}_k\rangle$$

$$= (\langle A^{+}u_j|)(ABA^{+})(A|u_k\rangle)$$

$$= (\langle A^{+}u_j|)(ABA^{+}A|u_k\rangle) = [(\langle \underset{\sim}{AA^{+}}u_j|)(B\underset{\sim}{A^{+}A}|u_k\rangle)]^{*}$$

$$= \langle u_j|B|u_k\rangle^{*}$$

Remark:

Let, $|\alpha\rangle = (a+ib)|a'\rangle \qquad |\beta\rangle = (c-id)|a'\rangle$

A: antiunitary

$|\tilde{\alpha}\rangle = A|\alpha\rangle = (a-ib)|a'\rangle \rightarrow \langle\tilde{\alpha}| = (a+ib)\langle a'|$

$|\tilde{\beta}\rangle = A|\beta\rangle = (c+ib)|a'\rangle$

$\langle\tilde{\alpha}|\tilde{\beta}\rangle = (a+ib)(c+id)$

But the following is <u>wrong</u>:

$\langle\alpha|A^{+}A|\beta\rangle \neq \langle\alpha|\beta\rangle = (a-ib)(c-id)$

because $\underset{\alpha}{\underbrace{A^{+}A}} \neq I$

Change of Basis

$$\{|a_k\rangle\} \qquad \{|b_k\rangle\}$$

$$|b_k\rangle = U|a_k\rangle = \sum_i |a_i\rangle\langle a_i|U|a_k\rangle$$

$$|\alpha\rangle = \sum_i |a_i\rangle\langle a_i|\alpha\rangle = \sum_k |b_k\rangle\langle b_k|\alpha\rangle$$

$$= \sum_i\sum_k |a_i\rangle\langle a_i|U|a_k\rangle\langle b_k|\alpha\rangle$$

$$\to \langle a_i|\alpha\rangle = \sum_k \langle a_i|\underbrace{U|a_k\rangle}\langle b_k|\alpha\rangle$$

$$\to \begin{pmatrix} \langle a_1|\alpha\rangle \\ \langle a_2|\alpha\rangle \\ \vdots \\ \vdots \end{pmatrix} = U \begin{pmatrix} \langle b_1|\alpha\rangle \\ \langle b_2|\alpha\rangle \\ \vdots \\ \vdots \end{pmatrix}$$

Also;

$$A|b_j\rangle = \sum_i |b_i\rangle\langle b_i|A|b_j\rangle = \sum_i\sum_k |a_k\rangle\langle a_k|U|a_i\rangle\langle b_i|A|b_j\rangle$$

on the other hand

$$A|b_j\rangle = A\sum_\ell |a_\ell\rangle\langle a_\ell|U|a_j\rangle = \sum_\ell\sum_k |a_k\rangle\langle a_k|A|a_\ell\rangle\langle a_\ell|U|a_j\rangle$$

$$\to \sum_i \langle a_k|U|a_i\rangle\langle b_i|A|b_j\rangle = \sum_\ell \langle a_k|A|a_\ell\rangle\langle a_\ell|U|a_j\rangle$$

$$\to UA' = AU \quad \to \quad A' = U^{-1}AU$$

In classical Mechanics:

We keep the basis <u>fixed</u> and the unitary op. acts on the vectors;

let $G = AX \;\to UG = UAX \;\to UG = \underline{UAU^{-1}}UX \;\to A' = UAU^{-1}$

In Q.M.: Let $|\psi'\rangle = S|\psi\rangle \quad A'|\psi'\rangle \overset{\text{must}}{=\!=} S(A|\psi\rangle) \to A' = SAS^{-1}$

Note that $S^{-1} = S^{+} = U$

Digression on Symmetry Operations;

Consider a symmetry operation;

$$|\alpha\rangle \longrightarrow |\tilde{\alpha}\rangle \quad , \quad |\beta\rangle \longrightarrow |\tilde{\beta}\rangle$$

We may expect the following requirements (Past experience, shows);

$$\langle\tilde{\beta}|\tilde{\alpha}\rangle = \langle\beta|\alpha\rangle \qquad (1)$$

Indeed for symmetry operations such as <u>rotations</u>, <u>translations</u>, and even <u>parity</u> this is indeed the case.

This arises from the <u>unitary nature</u> of the symmetry operations;

$$\langle\tilde{\beta}|\tilde{\alpha}\rangle = \langle\beta|\underbrace{U^{\dagger}U}_{I}|\alpha\rangle = \langle\beta|\alpha\rangle$$

But requirement (1) is very restorictive;
For time-reversal (time translation) we impose a <u>weaker</u> cond.

$$|\langle\tilde{\beta}|\tilde{\alpha}\rangle| = |\langle\beta|\alpha\rangle| \quad (2)$$

Remark: The absolute value of the scalar product of the vectors is <u>preserved</u> either by <u>unitary</u> or <u>antiunitary</u> trs.

If (1) holds $\longrightarrow$ (2) also holds

But if (2) holds $\longrightarrow$ (1) may or may not hold.

Instead of (1) if $\langle\tilde{\beta}|\tilde{\alpha}\rangle = \langle\beta|\alpha\rangle^{*} \equiv \langle\alpha|\beta\rangle$

$\longrightarrow$ (2) holds

$$\rightarrow \begin{matrix} \langle\tilde{\beta}|\tilde{\alpha}\rangle = \langle\beta|\alpha\rangle \\ \langle\tilde{\beta}|\tilde{\alpha}\rangle = \langle\beta|\alpha\rangle^{*} \end{matrix} \xrightarrow{\text{in both cases}} (2) \text{ holds}$$

Def. – The transformation;

$$|\alpha\rangle \longrightarrow |\tilde{\alpha}\rangle = \theta|\alpha\rangle$$

$$|\beta\rangle \longrightarrow |\tilde{\beta}\rangle = \theta|\beta\rangle$$

is said to be <u>anti</u>unitary if,

$$\begin{cases} \langle\tilde{\beta}|\tilde{\alpha}\rangle = \langle\beta|\alpha\rangle^* \\ \\ \theta\left(c_1|\alpha\rangle + c_2|\beta\rangle\right) = c_1^*\,\theta|\alpha\rangle + c_2^*\,\theta|\beta\rangle \end{cases}$$

and (the second line) (antilinear cond.) Def for antilinear op.

Claim:

An antiunitary op. can be written as:

$$\theta = KU \quad \text{where} \begin{cases} U: \text{unitary op.} \\ K: \text{complex conjugate op.} \end{cases}$$

i.e. $Kf = f^* \longrightarrow K^2 f = f \rightarrow K^2 = I \rightarrow K = K^{-1}$

$\rightarrow \theta^{-1} = U^{+}K$ (for special case $U = I$, then K itself is antiunitary op.)

Properties of K op.:

1 – $\quad K(c|\alpha\rangle) = c^*\,(K|\alpha\rangle)$

2 – $\quad$ If $|\alpha\rangle = \sum_{a'} |a'\rangle\langle a'|\alpha\rangle$

where $\{|a'\rangle\}$ base kets

Then $\xrightarrow{K}$ $K\sum_{a'} |a'\rangle\langle a'|\alpha\rangle$

$$= \sum_{a'} \langle a'|\alpha\rangle^*\, K|a'\rangle = \sum_{a'} \langle a'|\alpha\rangle^*\, |a'\rangle$$

Note that:

$$K|a'\rangle = |a'\rangle$$

Because, the explicit representation of $|a'\rangle$ is:

$$|a'\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

and there is nothing to be changed by K.

Illustrative Ex.—

For spin $\frac{1}{2}$, suppose we choose the eigenkets of S_z as the base;

$$\{|a'\rangle\} = \left\{ |+\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \ |-\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \right\}$$

It is obvious;

$$K|+\rangle = |+\rangle \quad , \quad K|-\rangle = |-\rangle$$

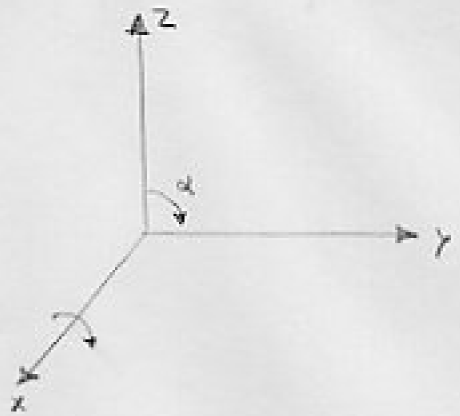
In this base, S_y-eigenkets are;

$$|+\,S_y\rangle = |+\rangle_y = \frac{1}{\sqrt{2}}\left(|+\rangle + i|-\rangle\right)$$

$$|-\,S_y\rangle = |-\rangle_y = \frac{1}{\sqrt{2}}\left(|+\rangle - i|-\rangle\right)$$

Remark:

$$|+S_y\rangle = e^{+i\sigma_x \frac{\alpha}{2}} |+\rangle$$



$$|+S_y\rangle = \begin{pmatrix} \cos\frac{\alpha}{2} & +i\sin\frac{\alpha}{2} \\ +i\sin\frac{\alpha}{2} & \cos\alpha/2 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

We see that:

$$K|+\rangle_y = |-\rangle_y$$
$$K|-\rangle_y = |+\rangle_y$$

The answer is that:

Here we used S_z eigenkets (for S_y), then we have to change the S_y eigenkets.

But if S_y-eigenkets themselves are used as the base kets, we don't change the S_y-eigenkets under the action of K.

Thus, the effect of K changes with the basis. As a result the form of U in $\Theta = UK$ also depends on the particular representation (that is, the choice of base kets).

Now;

1- $\Theta(c_1|\alpha\rangle + c_2|\beta\rangle) = UK(c_1|\alpha\rangle + c_2|\beta\rangle)$

$= c_1^* UK|\alpha\rangle + c_2^* UK|\beta\rangle$

$= c_1^* \Theta|\alpha\rangle + c_2^* \Theta|\beta\rangle$

2- $|\tilde{\alpha}\rangle = \Theta|\alpha\rangle = \Theta \sum_{a'} |a'\rangle\langle a'|\alpha\rangle$

$= UK \sum_{a'} |a'\rangle\langle a'|\alpha\rangle = \sum_{a'} \langle a'|\alpha\rangle^* UK|a'\rangle$

$= \sum_{a'} \langle\alpha|a'\rangle U|a'\rangle$

As for $|\beta\rangle$, we have

$$|\tilde{\beta}\rangle = \sum_{a''} \langle a''|\beta\rangle^* U|a''\rangle \xleftrightarrow{DC} \langle\tilde{\beta}| = \sum_{a''} \langle a''|\beta\rangle\langle a''|U^+$$

$$\longrightarrow \langle\tilde{\beta}|\tilde{\alpha}\rangle = \sum_{a'}\sum_{a''} \langle a''|\beta\rangle \underbrace{\langle a''|U^+U|a'\rangle}_{\delta_{a'a''}} \langle\alpha|a'\rangle$$

$$= \sum_{a'} \langle a'|\beta\rangle\langle\alpha|a'\rangle = \sum_{a'} \langle\alpha|a'\rangle\langle a'|\beta\rangle = \langle\alpha|\beta\rangle$$

$$\langle\tilde{\beta}|\tilde{\alpha}\rangle = \langle\alpha|\beta\rangle \longrightarrow \langle\tilde{\beta}|\tilde{\alpha}\rangle = \langle\beta|\alpha\rangle^*$$

Thus $\Theta = UK$, works (Indeed we mentioned before that time-reversal must have something to do with complex conjugate!.

But; it is always safer to work with the <u>action of Θ</u> on Kets only.

In order, for $|\langle\tilde{\beta}|\tilde{\alpha}\rangle| = |\langle\beta|\alpha\rangle|$ to be satisfied, it is of physical interest to consider just two types of tr. – unitary and antiunitary –

Other possibilities are related to either of the preceding, via trivial phase change.

Ex. – For the state $|\alpha\rangle = |\bar{p}\rangle$

$$\Theta|\bar{p}\rangle = |-\bar{p}\rangle \qquad \text{motion reversed state (up to a phase)}$$

Also for $|\alpha\rangle = |\bar{J}\rangle$

$$\Theta|\bar{J}\rangle = |-\bar{J}\rangle$$

when Θ is time-reversal op.

Time-Reversal Operator;

Consider time-reversal op. Θ

then $|\tilde{\alpha}\rangle = \Theta|\alpha\rangle$ is time-reversed state
or motion- " "

If at $t=0$ the state is $|\alpha\rangle$

then $\longrightarrow$ $|\alpha, t_0=0; t=\delta t\rangle = \left(1 - \frac{iH}{\hbar}\delta t\right)|\alpha\rangle$ at $t=\delta t$

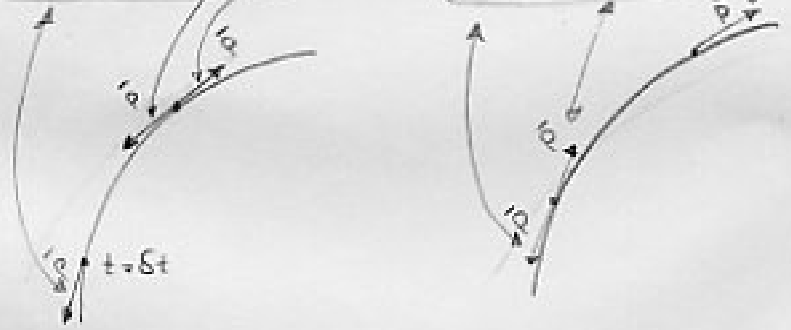
Instead if we apply the op. Θ on $|\alpha\rangle$ at $t=0$ and then let the system to evolve under the influence of H, we obtain:

$$\left(1-\frac{iH}{\hbar}\delta t\right)\Theta|\alpha\rangle$$

If the motion obeys symmetry under time-reversal, we expect the preceding state ket to be the <u>same</u> as:

$$\Theta|\alpha, t_0=0; t=-\delta t\rangle = \Theta\left(1-\frac{iH}{\hbar}(-\delta t)\right)|\alpha\rangle$$

$$\longrightarrow \left(1-\frac{iH}{\hbar}\delta t\right)\Theta|\alpha\rangle = \Theta\left(1-\frac{iH}{\hbar}(-\delta t)\right)|\alpha\rangle \qquad \forall |\alpha\rangle$$



$$\longrightarrow -iH\Theta|\;\rangle = \Theta iH|\;\rangle \qquad \forall |\;\rangle$$

Now, we show that Θ cannot be unitary if the notion of time-reversal is to make sense.

1- If Θ is unitary

$$-iH\Theta = \Theta iH \longrightarrow -iH\Theta = i\Theta H$$

$$\rightarrow \; -H\Theta = H\Theta$$

Now consider the energy eigenket $|n\rangle$ with the energy eigenvalue E_n,

and the corresponding time-reversal state would be $\Theta|n\rangle$, then;

$$H(\Theta|n\rangle) = H\Theta|n\rangle = -\Theta H|n\rangle$$
$$= (-E_n)\,\Theta|n\rangle$$

$\longrightarrow$ the energy eigenvalue of $\Theta|n\rangle$ is $-E_n$, but this is nonsencical.

Because, the energy spectrum of a free particle is positive, semidefinite. (0 to $+\infty$).

This is clear from;

$$-H\Theta = \Theta H \longrightarrow \Theta^{-1} H \Theta = -H$$

if $H = \frac{p^2}{2m}$ (free particle)

$$\Theta^{-1}\frac{p^2}{2m}\Theta = -\frac{p^2}{2m}$$

We expect, under Θ, the sign of p be changed but not p^2.

2- If Θ is antiunitary:

$$-iH\Theta|\,\rangle = \Theta iH|\,\rangle$$

$$\longrightarrow -iH\Theta|\,\rangle = -i\Theta H|\,\rangle$$

$$\longrightarrow \Theta H = H\Theta \longrightarrow [\Theta, H] = 0$$

Now $H(\Theta|n\rangle) = E_n(\Theta|n\rangle$

Remark: It is best <u>to avoid</u> an antiunitary op. acting on bras from the left, that is:

$$\langle\beta|\Theta|\alpha\rangle = (\langle\beta|)\cdot(\Theta|\alpha\rangle)$$

and we never define: $(\langle\beta|\Theta)\cdot|\alpha\rangle$

Operators:

The behaviour of operators under time-reversal:

consider

$$|\tilde{\alpha}\rangle = \Theta|\alpha\rangle$$
$$|\tilde{\beta}\rangle = \Theta|\beta\rangle$$

and consider a linear operator L

define: $|\gamma\rangle = L^{+}|\beta\rangle \xleftrightarrow{DC} \langle\gamma| = \langle\beta|L$

Then,

$$\langle \beta | L | \alpha \rangle = \langle \gamma | \alpha \rangle = \langle \alpha | \gamma \rangle^* = \langle \tilde{\alpha} | \tilde{\gamma} \rangle$$

$$= \langle \tilde{\alpha} | \theta | \gamma \rangle = \langle \tilde{\alpha} | \theta L^+ | \beta \rangle = \langle \tilde{\alpha} | \theta L^+ \theta^{-1} \theta | \beta \rangle$$

$$= \langle \tilde{\alpha} | \theta L^+ \theta^{-1} | \tilde{\beta} \rangle$$

$$\rightarrow \langle \beta | L | \alpha \rangle = \langle \tilde{\alpha} | \theta L^+ \theta^{-1} | \tilde{\beta} \rangle$$

Remark:
$\langle \tilde{\alpha} | \theta L^+ \theta^{-1} | \tilde{\beta} \rangle =$
$\langle \tilde{\alpha} | \theta L^+ | \beta \rangle$
$= \langle \alpha | L^+ | \beta \rangle$
Because from (a, p 47/3)
$\rightarrow \langle \tilde{\alpha} | \theta (L^+ | \beta \rangle) =$
$\langle \theta \tilde{\alpha} | (L^+ | \beta \rangle)^* =$
$\langle \theta^{-1} L^+ \beta | \tilde{\alpha} \rangle^* =$
$(\langle \beta | L) \theta^{-1} | \tilde{\alpha} \rangle =$
$\langle \beta | L | \alpha \rangle$

Compare

For the observables: $A = A^+$

$$\langle \beta | A | \alpha \rangle = \langle \tilde{\alpha} | \theta A \theta^{-1} | \tilde{\beta} \rangle$$

Def. - We say that an observable is <u>even</u> or <u>odd</u> under time-reversal, acc. to whether we have the <u>upper</u> or <u>lower</u> sign in:

$$\theta A \theta^{-1} = \pm A$$

or $\quad [\theta, A] = 0$

$\quad \{\theta, A\} = 0$

Remark:
$\langle \tilde{\alpha} | \theta | \beta \rangle \neq \langle \alpha | \beta \rangle$
because from (a, p 47/3)
$\rightarrow \langle \tilde{\alpha} | \theta | \beta \rangle = \langle \theta \tilde{\alpha} | \beta \rangle^*$
$= \langle \theta^{-1} \beta | \tilde{\alpha} \rangle^* = \langle \beta | \theta^{-1} | \tilde{\alpha} \rangle$
$= \langle \beta | \alpha \rangle$

Using the last identity:

$$\langle \beta | A | \alpha \rangle = \pm \langle \tilde{\alpha} | A | \tilde{\beta} \rangle = \pm \langle \tilde{\beta} | A | \tilde{\alpha} \rangle^*$$

if $\alpha = \beta \rightarrow \langle \alpha | A | \alpha \rangle = \pm \langle \tilde{\alpha} | A | \tilde{\alpha} \rangle$

Ex.— let $A=P$

since $\bar{P} \xrightarrow{\theta} -P$ $\left(\begin{array}{l} P = \frac{\hbar}{i}\frac{\partial}{\partial x} \rightarrow \Theta P = -P\Theta \\ \rightarrow \Theta P \Theta^{-1} = -P \end{array} \right)$

$\langle\alpha|P|\alpha\rangle = -\langle\tilde{\alpha}|P|\tilde{\alpha}\rangle$ (we expect)

$\Theta P \Theta^{-1} = -P \quad \longrightarrow \quad \{\Theta, P\} = 0$

This implies that;

$P(\Theta|P'\rangle) = (-\Theta P \Theta^{-1})\Theta|P'\rangle = -(\Theta P)|P'\rangle$

$= -P'(\Theta|P'\rangle)$

This is in accordance with the assertion that $\Theta|P'\rangle$ is a momentum eigenket with eigenvalue $-P'$

$\Theta|P'\rangle = |-P'\rangle$ up to a phase

$P|-P\rangle = -P'|-P'\rangle$

Ex.— let $A=X$

$\langle\alpha|X|\alpha\rangle = +\langle\tilde{\alpha}|X|\tilde{\alpha}\rangle$

because the position is expected to be the same;

$\Theta X \Theta^{-1} = X \quad \longrightarrow \quad [\Theta, X] = 0$

$\Theta|X'\rangle = |X'\rangle$ up to a phase.

The invariance of the fundamental commutation relation:

1- $$[x_i, P_j]\,|\alpha\rangle = i\hbar\,\delta_{ij}\,|\alpha\rangle \qquad \forall\,|\alpha\rangle$$

$$\longrightarrow \quad \Theta\,[x_i, P_j]\,\Theta^{-1}\Theta\,|\alpha\rangle = \Theta\, i\hbar\,\delta_{ij}\,|\alpha\rangle$$

$$[\Theta x_i \Theta^{-1}, \Theta P_j \Theta^{-1}]\,\Theta\,|\alpha\rangle = \Theta\, i\hbar\,\delta_{ij}\,|\alpha\rangle$$

$$[x_i, -P_j]\,\Theta\,|\alpha\rangle = -i\hbar\,\delta_{ij}\,\Theta\,|\alpha\rangle$$

$$-[x_i, P_j]\,\Theta\,|\alpha\rangle = -i\hbar\,\delta_{ij}\,\Theta\,|\alpha\rangle$$

$$[x_i, P_j]\,\Theta\,|\alpha\rangle = i\hbar\,\delta_{ij}\,\Theta\,|\alpha\rangle$$

So, commutator is preserved under Θ

$$\longrightarrow \quad [x_i, P_j] = i\hbar\,\delta_{ij}$$

2- Similarly:

$$[J_i, J_j]\,|\alpha\rangle = i\hbar\,\epsilon_{ijk}\,J_k\,|\alpha\rangle \qquad \forall\,|\alpha\rangle$$

$$\Theta\,[J_i, J_j]\,\Theta^{-1}\Theta\,|\alpha\rangle = \Theta\, i\hbar\,\epsilon_{ijk}\,J_k\,|\alpha\rangle$$

$$[\Theta J_i \Theta^{-1}, \Theta J_j \Theta^{-1}]\,\Theta\,|\alpha\rangle = \Theta\, i\hbar\,\epsilon_{ijk}\,J_k\,|\alpha\rangle$$

Now if: $\Theta J_i \Theta^{-1} = -J_i$

$$\longrightarrow \quad [-J_i, -J_j]\,\Theta\,|\alpha\rangle = -i\hbar\,\epsilon_{ijk}\,\Theta\,J_k\,|\alpha\rangle$$

$$[J_i, J_j]\,\Theta|\alpha\rangle = -i\hbar\,\epsilon_{ijk}\,(-J_k\Theta)|\alpha\rangle$$

$$[J_i, J_j]\,\Theta|\alpha\rangle = i\hbar\,\epsilon_{ijk}\,J_k\Theta|\alpha\rangle$$

$\longrightarrow$ $[J_i, J_j] = i\hbar\,\epsilon_{ijk}J_k$ is preserved under Θ

Therefore, $\Theta\bar{J}\Theta^{-1} = -J \longrightarrow \{\Theta, J\} = 0$

(to preserve the commutation relation)

Then, the angular momentum must be <u>odd</u> under Θ.

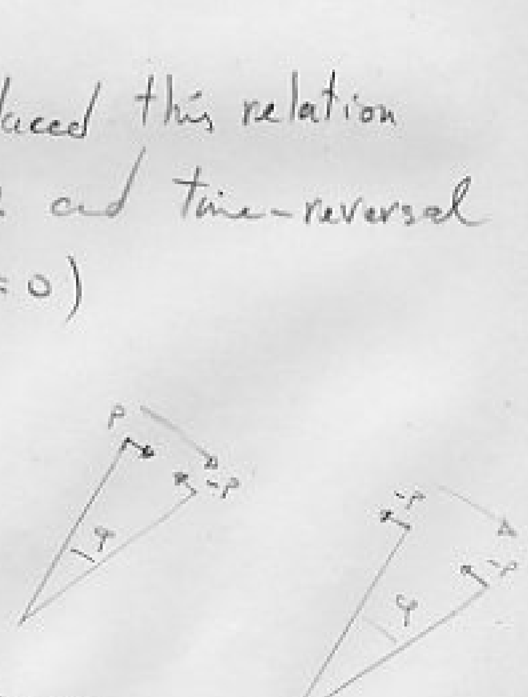
This is consistent for <u>spinless</u> systems where

$\bar{J} = \bar{X}\wedge\bar{P}$

Alternatively, we could have deduced this relation by noting that the rotational op. and time-reversal op. commute. ($[D(R), \Theta] = 0$)

$[e^{-\frac{i}{\hbar}\varphi\hat{n}\cdot J}, \Theta] = 0$ $\quad\bar{J} = \bar{L} + \bar{S}$

For spinless system $\bar{J} = \bar{L}$



$D(R)\,\Theta = \Theta\,D(R)$

Wave Function:

Suppose at some given time, say at $t=0$, a spinless single particle system is found in a state, $|\alpha\rangle$.

We may write:

$$|\alpha\rangle = \int d^3x' \, |x'\rangle\langle x'|\alpha\rangle$$

$$\Theta|\alpha\rangle = \int d^3x' \, \Theta|x'\rangle\langle x'|\alpha\rangle^* = \int d^3x' \, |x'\rangle\langle x'|\alpha\rangle^*$$

where we have chosen the phase convention so that;

$$\Theta|x'\rangle = |x'\rangle$$

Since $\langle x'|\alpha\rangle^* = \psi^*(x')$ $\qquad \left(\langle x|(\Theta|\alpha\rangle) = \langle x|\alpha\rangle^* \right)$

we then recover the rule:

$$\psi(x') \xrightarrow{\Theta} \psi^*(x')$$

Ex.- The angular part of the wave-func. is given by $Y_\ell^m(\theta,\varphi)$:

then: $Y_\ell^m(\theta,\varphi) \xrightarrow{\Theta} Y_\ell^{*m}(\theta,\varphi) = (-1)^m Y_\ell^{-m}(\theta,\varphi)$

Now, $Y_\ell^m(\theta,\varphi)$ is the wave-func. for $|\ell,m\rangle$

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

$$\rightarrow \Theta|\ell,m\rangle = (-1)^m|\ell,-m\rangle$$

$$\left\{ \begin{aligned} \Theta|\ell,m\rangle &= \Theta\int d\Omega\,|\hat{n}\rangle\langle\hat{n}|\ell,m\rangle \\ &= \int d\Omega\,|\hat{n}\rangle\langle\hat{n}|\ell,m\rangle^* \\ &= \int d\Omega\,|\hat{n}\rangle(-)^m\langle\hat{n}|\ell,-m\rangle \\ &= (-)^m|\ell,-m\rangle \end{aligned} \right.$$

Ex. - For the wave-func.

$$\langle x' | n, l, m \rangle = R_{nl}(r)\, Y_l^m(\theta, \varphi)$$

the probability density;

$$j(x,t) = -\frac{i\hbar}{2m}\left[\psi^* \nabla\psi - (\nabla\psi^*)\psi\right] = \frac{\hbar}{m}\, I_m(\psi^* \nabla \psi)$$

gives that, for $m > 0$ the current flows in the counterclockwise direction, as seen from the positive z-axis.

The wave-func. for the corresponding time-reversed state has its probability current flowing in the opposite direction (because the sing of m is reversed.)

Theorem;

Suppose the Hamiltonian is invariant under time-reversal

$$[\Theta, H] = 0$$

and energy eigenket $|n\rangle$ is <u>nondegenerate</u>, then the corresponding eigenfunc. is <u>real</u> (or more generally a <u>real func.</u> times a <u>phase factor</u> independent of $\vec{x}$)

Proof –

Note that; $H\theta|n\rangle = \theta H|n\rangle = E_n\theta|n\rangle$

So $|n\rangle$ and $\theta|n\rangle$ have the same energy.

Then $|n\rangle$ and $\theta|n\rangle$ are degenerate unless they represent the same state (an obvious contradiction).

The wave-func. for $|n\rangle$ is $\langle x'|n\rangle$

and $\langle x'|n\rangle \xrightarrow{\theta} \langle x'|n\rangle^*$ (1)

We had; $\theta|x'\rangle = |x'\rangle$ $\quad \widetilde{|x'\rangle} = \theta|x'\rangle = |x'\rangle \xleftrightarrow{DC} \widetilde{\langle x'|} = \langle x'|$

(more generally $\theta|x'\rangle = e^{i\delta}|x'\rangle$)

and we obtained $\theta|n\rangle = |n\rangle$

The wave-func. for $\theta|n\rangle$: $\langle x'|\theta|n\rangle = \langle x'|n\rangle$ (2)

(1), (2) $\longrightarrow \langle x'|n\rangle = \langle x'|n\rangle^*$

for all practical purposes.

Or more precisely, they can differ at most by a phase factor independent of $\bar{x}$.

Ex. — In the Hydrogen atom with $l \neq 0$ and $m \neq 0$, the energy eigenfunctions characterized by definite (n, l, m) quantum numbers is <u>complex</u>, because $Y_l^m(\theta, \varphi)$ is <u>complex</u>.

This doesn't contradict the theorem, because $|n, l, m\rangle$ and $|n, l, -m\rangle$ are degenerate.

Ex. — Similarly, the wave-func. of a plane-wave $e^{\frac{i p \cdot x}{\hbar}}$ is complex, but it is degenerate with $e^{-\frac{i p \cdot x}{\hbar}}$.

Conclusion;

1- For a spinless system;

$$\psi(x') \xrightarrow{\Theta} \psi^*(x') \qquad \text{(expansion in the coord. space.)}$$

or $\langle x'|\alpha\rangle \xrightarrow{\Theta} \langle x'|\alpha\rangle^*$

(say at $t=0$)

Since;

$$|\alpha\rangle = \sum_{a'} |a'\rangle\langle a'|\alpha\rangle \xrightarrow[\Theta]{K} [|\tilde{\alpha}\rangle] = K_\Theta|\alpha\rangle = \sum_{a'} \langle a'|\alpha\rangle^* K_\Theta |a'\rangle$$
$$= \sum_{a'} \langle a'|\alpha\rangle^* |a'\rangle$$

$$|\alpha\rangle = \int d^3x' |x'\rangle\langle x'|\alpha\rangle \xrightarrow[\Theta]{K} K_\Theta|\alpha\rangle = \int d^3x' K_\Theta|x'\rangle\langle x'|\alpha\rangle^*$$
$$= \int d^3x' |x'\rangle\langle x'|\alpha\rangle^*$$

$\longrightarrow \Theta \equiv K$

because, K and Θ have the same effect when acting on the base ket $|a'\rangle$ (or $|x'\rangle$).

2- We may note, however that, the situation is quite different when ket $|\alpha\rangle$ is expanded in terms of the momentum eigenket, because Θ must change $|p'\rangle$ into $|-p'\rangle$ as follows;

$$|\alpha\rangle = \int d^3p'\, |p'\rangle\langle p'|\alpha\rangle \xrightarrow{\Theta} \Theta|\alpha\rangle = \int d^3p'\, |-p'\rangle\langle p'|\alpha\rangle^*$$

$$= \int d^3p'\, |+p'\rangle\langle -p'|\alpha\rangle^*$$

Therefore;

$$\varphi(p') \xrightarrow{\Theta} \varphi^*(-p')$$

Thus particular form of Θ depends on the particular representation used.

Remark:

$$\bar{p}' \to -\bar{p}' \Rightarrow \begin{cases} \theta \to \pi - \theta & \Rightarrow d(\cos\theta) \to -d(\cos\theta),\ \int_{-1}^{1} \to \int_{1}^{-1} \\ \varphi \to \pi + \varphi & \Rightarrow d\varphi \to d\varphi,\ \int_0^{2\pi} \to \int_{\pi}^{2\pi} \end{cases}$$

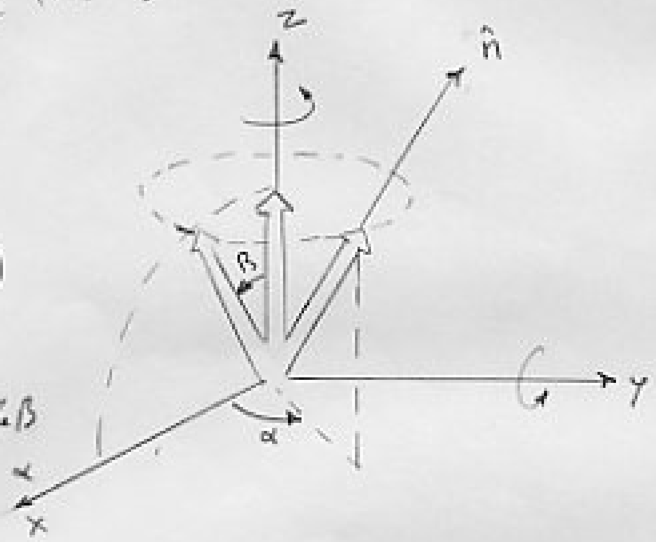
$$\Rightarrow \int d^3p' \to \int d^3p' \quad \text{unchanged}$$

Time Reversal for Spin $\frac{1}{2}$ system:

The eigenket of $\bar{S}\cdot\hat{n}$ with eigenvalue $\frac{\hbar}{2}$ can be written as:

$$|\hat{n};+\rangle = e^{-iS_z\frac{\alpha}{\hbar}}\, e^{-iS_y\frac{\beta}{\hbar}}\, |+\rangle$$

where $\quad S\cdot\hat{n}\,|\hat{n};+\rangle = \frac{\hbar}{2}\,|\hat{n};+\rangle$



$\hat{n}\begin{cases}\beta & \text{Polar angle}\\ \alpha & \text{Azimuthal} \ "\end{cases}$

$|+\rangle = \begin{pmatrix}1\\0\end{pmatrix}$ (in the z-dir.)

1- First rotate about y-axis by angle β
2- Subsequently " " z- " " " α

In Pauli spinor language:

$$\chi = e^{-i\sigma_z\frac{\alpha}{2}}\, e^{-i\sigma_y\frac{\beta}{2}}\, |+\rangle$$

or $\quad |\hat{n};+\rangle = e^{-iS_z\frac{\alpha}{\hbar}}\, e^{-iS_y\beta/\hbar}\, |+\rangle$

But: $\quad e^{-iS_z\frac{\alpha}{\hbar}} = I + (-iS_z\frac{\alpha}{\hbar}) + \frac{1}{2!}(-iS_z\frac{\alpha}{\hbar})^2 + \frac{1}{3!}(-iS_z\frac{\alpha}{\hbar})^3 + \cdots$

$$S_z^2 = (\tfrac{\hbar}{2}\sigma_z)^2 = \frac{\hbar^2}{4}\begin{pmatrix}1&0\\0&-1\end{pmatrix}\begin{pmatrix}1&0\\0&-1\end{pmatrix} = \frac{\hbar^2}{4}\begin{pmatrix}1&0\\0&1\end{pmatrix} = \frac{\hbar^2}{4} I$$

$$\rightarrow e^{-iS_z\frac{\alpha}{\hbar}} = I - iS_z\frac{\alpha}{\hbar} - \frac{1}{2!}\left(\frac{\hbar^2}{4}I\right)\frac{\alpha^2}{\hbar^2} + \frac{1}{3!}\left(S_z\frac{\hbar^2}{4}\right)\frac{\alpha^3}{\hbar^3}$$

$$= \left(1 - \frac{1}{2!}\left(\frac{\alpha}{2}\right)^2 + \cdots\right) I - i\frac{2}{\hbar}\left(\frac{\alpha}{2} - \frac{1}{3!}\left(\frac{\alpha}{2}\right)^3 + \cdots\right) S_z$$

$$e^{-iS_z\frac{\alpha}{\hbar}} = \cos\frac{\alpha}{2} - i\frac{2}{\hbar}S_z\sin\frac{\alpha}{2} = \cos\frac{\alpha}{2} - i\sigma_z\sin\frac{\alpha}{2}$$

Similarly: $e^{-iS_y\frac{\beta}{\hbar}} = \cos\frac{\beta}{2} - i\sigma_y\sin\frac{\beta}{2}$

Therefore;

$$|\hat{n},+\rangle = e^{-iS_z\frac{\alpha}{\hbar}}\, e^{-iS_y\frac{\beta}{\hbar}}|+\rangle = \left(\cos\frac{\alpha}{2} - i\sigma_z\sin\frac{\alpha}{2}\right)\left(\cos\frac{\beta}{2} - i\sigma_y\sin\frac{\beta}{2}\right)\begin{pmatrix}1\\0\end{pmatrix}$$

$$= \begin{pmatrix}\cos\frac{\alpha}{2} - i\sin\frac{\alpha}{2} & 0\\ 0 & \cos\frac{\alpha}{2} + i\sin\frac{\alpha}{2}\end{pmatrix}\begin{pmatrix}\cos\frac{\beta}{2} & -\sin\frac{\beta}{2}\\ \sin\frac{\beta}{2} & \cos\frac{\beta}{2}\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix}$$

$$= \begin{pmatrix}\cos\left(\frac{\beta}{2}\right)e^{-i\frac{\alpha}{2}}\\ \sin\left(\frac{\beta}{2}\right)e^{i\frac{\alpha}{2}}\end{pmatrix}$$

Now, since; $\Theta\vec{J}\Theta^{-1} = -\vec{J} \rightarrow \{\Theta, \vec{J}\} = 0$

$$\Theta|\hat{n},+\rangle = \Theta\left(e^{-iS_z\frac{\alpha}{\hbar}}\, e^{-iS_y\frac{\beta}{\hbar}}\, |+\rangle\right)$$

$$= \left(\Theta e^{-iS_z\frac{\alpha}{\hbar}}\Theta^{-1}\right)\left(\Theta e^{-iS_y\frac{\beta}{\hbar}}\Theta^{-1}\right)\Theta|+\rangle$$

$$\Theta e^{-iS_k\alpha_k/\hbar}\Theta^{-1} = e^{\Theta(-iS_k\alpha_k/\hbar)\Theta^{-1}} = e^{+i\frac{\alpha}{\hbar}\Theta S_k\Theta^{-1}}$$

$$= e^{\frac{i\alpha_k}{\hbar}(-S_k\Theta)\Theta^{-1}} = e^{-iS_k\alpha_k/\hbar}$$

$$\Theta |\hat{n},+\rangle = e^{-iS_z\frac{\alpha}{\hbar}} e^{-iS_y\frac{\beta}{\hbar}} \Theta |+\rangle \quad (1)$$

But $\Theta|\hat{n},+\rangle \sim |\hat{n},-\rangle$ due to motion reversal

$$\longrightarrow \Theta|\hat{n},+\rangle \equiv \eta |\hat{n},-\rangle \quad (2)$$

On the other hand;

$$|\hat{n};-\rangle = e^{-iS_z\frac{\alpha}{\hbar}} e^{-iS_y\frac{(\pi+\beta)}{\hbar}} |+\rangle \quad (3)$$

$$(1),(2),(3) \longrightarrow e^{-iS_z\frac{\alpha}{\hbar}} e^{-iS_y\frac{\beta}{\hbar}} \Theta|+\rangle = \eta\left(e^{-iS_z\frac{\alpha}{\hbar}} e^{-iS_y\frac{(\pi+\beta)}{\hbar}} |+\rangle\right)$$

$$\longrightarrow \Theta|+\rangle = \eta\, e^{-i\frac{\pi}{\hbar}S_y} |+\rangle$$

Now, set $\Theta = KU$, where $K|+\rangle = |+\rangle$

$$UK|+\rangle = \eta\, e^{-i\frac{\pi}{\hbar}S_y} |+\rangle$$

$$U|+\rangle = \eta\, e^{-i\frac{\pi}{\hbar}S_y} |+\rangle \qquad \forall\, |+\rangle$$

$$\longrightarrow U = \eta\, e^{-i\frac{\pi}{\hbar}S_y} \qquad \left(e^{-i\frac{\pi}{\hbar}S_y} = C\frac{\pi}{2} - i\,\sigma_y\, S\frac{\pi}{2}\right)$$

$$\Theta = UK = \eta\, e^{-i\frac{\pi}{\hbar}S_y} K = -i\eta\left(\frac{2S_y}{\hbar}\right)K$$

$$\longrightarrow U = -i\eta\,\sigma_y$$

η: a complex number of modulus unity $|\eta|=1$ ($UU^{\dagger}=I$)

We can show that:

$$\theta|\hat{n};+\rangle = -i\eta\sigma_y K|\hat{n};+\rangle = \eta\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix}K\begin{pmatrix}\cos\frac{\beta}{2}\, e^{-i\alpha/2}\\ \sin\beta_{/2}\, e^{i\alpha/2}\end{pmatrix} = \eta|\hat{n};-\rangle$$

$$|\hat{n};-\rangle = \begin{pmatrix}\cos\left(\frac{\beta+\pi}{2}\right)e^{-i\alpha/2}\\ \sin\left(\frac{\beta+\pi}{2}\right)e^{+i\alpha/2}\end{pmatrix} = \begin{pmatrix}-\sin\frac{\beta}{2}\, e^{-i\alpha/2}\\ \cos\frac{\beta}{2}\, e^{+i\alpha/2}\end{pmatrix}$$

$$|n;+\rangle = \begin{pmatrix}\cos\frac{\beta}{2}\, e^{-i\alpha/2}\\ \sin\frac{\beta}{2}\, e^{+i\alpha/2}\end{pmatrix} = \cos\beta_{/2}\, e^{-i\alpha/2}\begin{pmatrix}1\\0\end{pmatrix} + \sin\frac{\beta}{2}\, e^{+i\alpha/2}\begin{pmatrix}0\\1\end{pmatrix}$$

$$\theta = \eta\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix}K$$

$$\theta|\hat{n};+\rangle = \eta\left\{\cos\frac{\beta}{2}\, e^{+i\alpha/2}\begin{pmatrix}0\\1\end{pmatrix} - \sin\frac{\beta}{2}\, e^{-i\alpha/2}\begin{pmatrix}1\\0\end{pmatrix}\right\} = \eta\begin{pmatrix}-\sin\frac{\beta}{2}\, e^{-i\alpha/2}\\ \cos\beta_{/2}\, e^{+i\alpha/2}\end{pmatrix}$$

Remark: $\bar{\sigma}\cdot\hat{n} = ?$

$$\begin{cases} n_x = \sin\theta\cos\varphi\\ n_y = \sin\theta\sin\varphi\\ n_z = \cos\theta\end{cases}$$

$$\sigma_1 = \begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix} \qquad \sigma_2 = \begin{pmatrix}0 & -i\\ i & 0\end{pmatrix} \qquad \sigma_3 = \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$$

$$\bar{\sigma}\cdot\hat{n} = \begin{pmatrix}\cos\theta & \sin\theta\, e^{-i\varphi}\\ \sin\theta\, e^{i\varphi} & -\cos\theta\end{pmatrix}$$

$$n_\pm = n_x \pm i n_y = \sin\theta(\cos\varphi \pm i\sin\varphi) = \sin\theta\, e^{\pm i\varphi}$$

Θ^2 operator -

Apply θ on the most general spin $\frac{1}{2}$ ket:

$$\theta\left(c_+|+\rangle + c_-|-\rangle\right) = UK\left(c_+|+\rangle + c_-|-\rangle\right)$$

$$= U\left(c_+^*|+\rangle + c_-^*|-\rangle\right) = -i\eta\sigma_y\left(c_+^*|+\rangle + c_-^*|-\rangle\right)$$

$$= +\eta c_+^*|-\rangle - \eta c_-^*|+\rangle$$

because $\begin{cases} U|+\rangle = -i\eta\sigma_y|+\rangle = +\eta|-\rangle \\ U|-\rangle = -i\eta\sigma_y|-\rangle = -\eta|+\rangle \end{cases}$

Apply θ once again;

$$\theta^2\left(c_+|+\rangle + c_-|-\rangle\right) = \theta\left(\eta c_+^*|-\rangle - \eta c_-^*|+\rangle\right)$$

$$= -|\eta|^2 c_+|+\rangle - |\eta|^2 c_-|-\rangle = -\left(c_+|+\rangle + c|-\rangle\right)$$

because $\begin{cases} \theta\eta = \eta^*\theta \\ |\eta|^2 = 1 \end{cases}$ $\quad \forall\ \left(c_+|+\rangle + c_-|-\rangle\right)$

$\longrightarrow\ \theta^2 = -I$ $\quad$ for any spin orientation

This result is indep. of the choice of phase factor η, and is valid for any <u>half-integer</u> spin.

On the other hand for the integer spin case we have;

$$\Theta^2 = I$$

For spinless system say, $|l,m\rangle$, we have;

$$\Theta |l,m\rangle = (-1)^m |l,-m\rangle$$

$$\Theta^2 |l,m\rangle = (-1)^{2m} |l,-(-m)\rangle = +|l,m\rangle$$

$$\rightarrow \quad \Theta^2 = I$$

More Generally; (We now prove),

$$\Theta^2 |j \text{ half-integer}\rangle = -|j \text{ half-integer}\rangle$$

$$\Theta^2 |j \text{ integer}\rangle = +|j \text{ integer}\rangle$$

The eigenvalue of $\Theta^2 = (-1)^{2j}$

$$\Theta^2 |j\rangle (-1)^{2j} |j\rangle$$

Thus Θ is given in general: (we generalize)

$$\Theta = \eta\, e^{-i\pi J_y/\hbar} K$$

Now consider state ket $|\alpha\rangle$ expanded in terms of $|j,m\rangle$ eigenkets:

$$|\alpha\rangle = \sum_{j,m} |j,m\rangle\langle j,m|\alpha\rangle$$

$$\Theta|\alpha\rangle = \sum_{jm} \langle j,m|\alpha\rangle^* \eta e^{-i\pi J_y/\hbar} K|j,m\rangle$$

$$= \sum_{j,m} \langle jm|\alpha\rangle^* \eta e^{-i\pi J_y/\hbar} |jm\rangle$$

$$\Theta^2|\alpha\rangle = \sum_{jm} \langle jm|\alpha\rangle \underbrace{|\eta|^2}_{1} e^{-2\pi i J_y/\hbar} |jm\rangle \qquad \left(\begin{matrix}\text{Note:}\\ \{\Theta, J\} = 0\end{matrix}\right)$$

$$\Theta^2|\alpha\rangle = e^{-2\pi i J_y/\hbar} \sum_{jm} |jm\rangle\langle jm|\alpha\rangle$$

It can be shown $e^{-2\pi i J_y/\hbar} |jm\rangle = (-1)^{2j} |jm\rangle$ {from the properties of ang. moment. eigenstates under rotation by 2π

$$\rightarrow \Theta^2|\alpha\rangle = \sum_{jm} (-1)^{2j} \langle jm|\alpha\rangle |jm\rangle$$

$$\longrightarrow \quad \Theta^2 \rightarrow (-1)^{2j} \quad \text{on states } |jm\rangle$$

Since j always change by unit steps, in summation, $2j$ remains even or odd.

Ex. - In $\Theta^2|j \text{ integer}\rangle = +|j \text{ integer}\rangle$, the state ket may stands for the spin state of two electron system

$$|\ \rangle = \frac{1}{\sqrt{2}}\left(|+,-\rangle \pm |-,+\rangle\right)$$

i.e. $|\ \rangle = \frac{1}{\sqrt{2}}\left(\psi_\alpha(1)\psi_\beta(2) \pm \psi_\alpha(2)\psi_\beta(1)\right)$

Ex.- The state ket $|j \text{ integer}\rangle$ can also be an orbital state:

$$|\rangle = |l, m\rangle$$

Ex.- In $\Theta^2 |j \text{ half-int.}\rangle = -|j \text{ half-int.}\rangle$, the state ket may stands for three electron system.

Remark - For a system made up exclusively of electrons, any system with an odd (even) number of electrons, regardless of their spatial orientation (for example relative orbital angular momentum) is odd (even) under Θ^2, they need not even be J^2 eigenstates.

Phase Convention:

In position representation, we saw that, with the usual convention for spherical harmonics it is natural to choose, the arbitrary phase for $|l, m\rangle$ under time-reversal, so that:

$$\Theta |l, m\rangle = (-1)^m |l, -m\rangle$$

Some authors find it attractive to generalize this to obtain.

$$\Theta|j,m\rangle = (-1)^m |j,-m\rangle \quad (j \text{ an integer})$$

regardless of whether j refers to $\underline{l}$ or $\underline{S}$ (for integer spin systems)

Is this compatible with

$$\Theta^2 |j \text{ half-int.}\rangle = -|j \text{ half-int.}\rangle$$

for a spin $\frac{1}{2}$ system? (i.e. $|jm\rangle$ built up spin $\frac{1}{2}$ objects).

This is consistent provided we choose η in

$$\Theta = \eta\, e^{-i\pi J_y/\hbar} K$$

to be $+i$. In fact in general, we can take;

$$\Theta|j,m\rangle = (i)^{2m} |j,-m\rangle \qquad \left((i)^{2m} \equiv (-1)^m\right)$$

for j: either half-int. or an integer.

It is compatible, if if η to be $+i$.

Expectation values -

let $A = A^{\dagger}$

For a Hermitian op. we obtained;

$$\langle \alpha | A | \alpha \rangle = \pm \langle \tilde{\alpha} | A | \tilde{\alpha} \rangle$$

$$\rightarrow \langle \alpha, j, m | A | \alpha, j, m \rangle = \pm \langle \widetilde{\alpha, j, m} | A | \widetilde{\alpha, j, m} \rangle$$

where $|\widetilde{\alpha, j, m}\rangle = \Theta |\alpha, j, m\rangle = (i)^{2m} |\alpha, j, -m\rangle$

$$\xrightarrow{\text{D.C.}} \langle \widetilde{\alpha, j, m} | = (-i)^{2m} \langle \alpha, j, -m |$$

$$\rightarrow \langle \alpha, j, m | A | \alpha, j, m \rangle = \pm \langle \alpha, j, -m | A | \alpha, j, -m \rangle \quad (1)$$

Now suppose A is a component of spherical tensor T_q^k;

Due to Wigner-Eckart theorem;

$$\langle \alpha', j', m' | T_q^k | \alpha, j, m \rangle = (j m, k q / j' m') \frac{\langle \alpha' j' \| T^k \| \alpha j \rangle}{\sqrt{2j+1}}$$

it is sufficient to examine just the matrix element of $T_{q=0}^k$ component.

If $\langle | T_{q=0}^k | \rangle$ is known $\longrightarrow \langle \| T^k \| \rangle$ can be obtained

$\longrightarrow$ other $\langle | T_q^k | \rangle$ may be calculated using Clebsch-Gordan coeffs.

T^k (assumed to be Hermitian) is said to be <u>even</u> or <u>odd</u>, if

$$\Theta T^k_{q=0} \Theta^{-1} = \pm T^k_{q=0}$$

Remark: General Def.: $\Theta T^k_q \Theta^{-1} = \pm(-1)^q T^k_{-q}$ r: Hermitian
Ex.: $\Theta r^{(1)}_q \Theta^{-1} = +(-1)^q r^{(1)}_{-q}$
where $r^{(1)}_{\pm 1} = \pm\frac{1}{\sqrt{2}}(x \pm iy)$, $r^{(1)}_0 = z$
Remember $\Theta \vec{x} \Theta^{-1} = +x$

For $A = T^k_0$;

(1) $\rightarrow \langle \alpha, j, m | T^k_0 | \alpha, j, m \rangle = \pm \langle \alpha, j, -m | T^k_0 | \alpha, j, -m \rangle$ (2)

Due to; $|\hat{n}\rangle = \mathcal{D}(R)|\hat{z}\rangle = \sum_{l,m} \mathcal{D}(R)|l,m\rangle\langle l,m|\hat{z}\rangle$

$$\longrightarrow \langle l, m' | \hat{n} \rangle = \sum_{\substack{m \\ \text{only}}} \mathcal{D}^l_{m'm}(\alpha = \varphi, \beta = \theta, \gamma = 0)\langle l, m | \hat{z} \rangle$$

$(\langle l, m | \hat{z} \rangle = Y^m_l(0, \varphi))$

we expect $\rightarrow |\alpha, j, -m\rangle = \mathcal{D}(0, \pi, 0)|\alpha, j, m\rangle$ (up to a phase)

Also due to $\mathcal{D}^\dagger(R)\, T^k_q\, \mathcal{D}(R) = \sum_{q'=-k}^{k} \mathcal{D}^{k*}_{qq'}(R)\, T^k_{q'}$

$\rightarrow \mathcal{D}^\dagger(0,\pi,0)\, T^k_0\, \mathcal{D}(0,\pi,0) = (-1)^k T^k_0 + (q \neq 0 \text{ components})$
(where $\mathcal{D}^K_{00}(0,\pi,0) = P_k(\cos\pi) = (-1)^k$)

(2) $\rightarrow \langle \alpha, j, m | T^k_0 | \alpha, j, m \rangle = \pm(-1)^k \langle \alpha, j, m | T^k_0 | \alpha, j, m \rangle + 0$

(due to $m' = m + q$ cond.)

Conclusion:

<u>Ex.</u> $\langle \alpha, j, m | X | \alpha, j, m \rangle = 0$ $(k = 1)$

Note that $|\alpha, j, m\rangle$ <u>need not</u> to be <u>parity eigenket</u>.

For example $|\alpha, j, m\rangle = C_s|S_{1/2}\rangle + C_p|P_{1/2}\rangle$
for spin $\frac{1}{2}$ particles.

Interaction with Electrical and Magnetic Fields;

Kramers Degeneracy:

The int. of a charged particle with a static electric field is;

$$V(x) = e\varphi(x)$$

Since $V = V(x)$ (where x is time-reversal even op)

$$\rightarrow [\Theta, H] = 0$$

$\longrightarrow$ This does not lead to an interesting conservation law.

$\xrightarrow{\text{Because}}$ $\Theta U(t,t_0) \neq U(t,t_0)\Theta$

The reason: Θ passing over $U(t,t_0) = e^{-\frac{i}{\hbar}H(t-t_0)}$ changes the sign of imaginary parts.

If an operation is const. of motion, it will commute with $U(t,t_0)$. Since $[\Theta, U] \neq 0$, Θ does not contain any conserved term.

Remark: Θ is antiunitary. At the beginning of this chapter we discussed the conserved quantities related to the unitary operators.
(i.e. $[\mathcal{S}, H] = 0 \rightarrow [\mathcal{S}, U] = 0$ if $\mathcal{S}$ is unitary)

Kramers Degeneracy -

suppose $[\Theta, H] = 0$

and let $H|n\rangle = E_n|n\rangle$ $\qquad |n\rangle$ energy eigenket

$\rightarrow H(\Theta|n\rangle) = \Theta(H|n\rangle) = E_n(\Theta|n\rangle)$

Does $|n\rangle$ represent the same state as $\Theta|n\rangle$?

If it does, $|n\rangle$ and $\Theta|n\rangle$ can differ at most by a phase factor. Hence.

$$\Theta|n\rangle = e^{i\delta}|n\rangle$$

$$\rightarrow \Theta^2|n\rangle = \Theta e^{i\delta}|n\rangle = e^{-i\delta}\Theta|n\rangle = e^{-i\delta}e^{+i\delta}|n\rangle = +|n\rangle$$

This is <u>impossible</u> for half-int. j systems. for which $\Theta^2 = -1$ (always)

$\xrightarrow{\text{Then}}$ $|n\rangle$ and $\Theta|n\rangle$ are distinct states
(in the case of j = half-int)

$\longrightarrow$ there exist degeneracy.

Ex.- Odd number of electron systems in an external electric field E are at least <u>two-fold</u> degenerate, no matter how complicated E may be.

Ex.- Odd-electron and even-electron system in crystals exhibit very different behaviors.

Kramer inferred degeneracy of this kind by looking at explicit sols. of the Schrödinger eqn..
Later Wigner pointed out that Kramers degeneracy is a consequence of time-reversal invariance.

Now consider a magnetic field; H may contain terms like;

$$S\cdot B \;,\quad P\cdot A + A\cdot P \qquad (B = \nabla \times A)$$

where, B: external

Since P and S are odd under time-reversal, then;

$$[\Theta, H] \neq 0$$

As a trivial example for a spin $\frac{1}{2}$ system;

$$|+\rangle \xrightarrow{\Theta} |-\rangle \qquad \text{(distinct states)}$$

$|+\rangle$ and $\Theta|+\rangle = |-\rangle$ have no longer the same energy at the presence of an external magnetic field B.

$$[\Theta, B] = 0 \qquad \text{since } B \text{ is external}$$

This should not be confused with our earlier remarks concerning the invariance of Maxwell equs. and Lorentz force under;

$$t \longrightarrow -t$$

and

$$\begin{cases} E \to E, & B \to -B, \quad \rho \to \rho \\ j \to -j & v \longrightarrow -v \end{cases}$$

There, we were to apply time-reversal to the whole world, for example, even to the currents in the wire that produces the B field!

i.e. The equs. should be invariant either in our internal system or external system.