COLLEGE OF ARTS AND SCIENCES
HOMER L. DODGE
DEPARTMENT OF PHYSICS AND ASTRONOMY
The UNIVERSITY of OKLAHOMA

Quantum Mechanics 2

CH. 4 SYMMETRY IN QUANTUM MECHANICS LECTURE NOTES

STUDENT
Taylor Larrechea

PROFESSOR
Dr. Bruno Uchoa

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Symmetries In Quantum Mechanics

A symmetry transformation is represented by a unitary operator $\tilde{\mathcal{U}}\tilde{\mathcal{U}}^{-1} = \mathbb{1}$. For a continuous symmetry, the infinitesimal operator is:

$$\tilde{\mathcal{U}} = \mathbb{1} - \frac{i\varepsilon\tilde{G}}{\hbar}$$

Where $\tilde{G} = \tilde{G}^{\dagger}$ is the infinitesimal generator of the transformation.

The system is <u>invariant</u> under a symmetry transformation when the Hamiltonian satisfies

$$\tilde{\mathcal{U}}^{\dagger}\tilde{H}\tilde{\mathcal{U}} = \tilde{H}$$

or equivalently

$$[\tilde{H},\tilde{G}] = 0$$

$\therefore$ $\tilde{G}$ is conserved (constant of the motion).

Examples:

$$\tilde{G} = \tilde{P}_i, \tilde{X}_i, \tilde{H}, \tilde{J}_m \quad ; \quad \varepsilon = x_i, p_i, \Delta t, \varphi$$

In the Heisenberg picture, if $\tilde{G}$ is a constant of motion

$$\frac{\partial \tilde{G}}{\partial t} = 0$$

In the Schrödinger version, if g is an eigenvalue of $\tilde{G}$ at $t = t_0$,

$$\tilde{G}|g,t_0\rangle = g|g,t_0\rangle$$

then the time evolution

$$|g,t_0;t\rangle = \tilde{\mathcal{U}}(t,t_0)|g,t_0\rangle$$

$$\tilde{G}|g,t_0;t\rangle = \tilde{G}\tilde{\mathcal{U}}(t,t_0)|g,t_0\rangle = g|gt_0,t\rangle$$

$|g,t_0;t\rangle$ is an eigenket of $\tilde{G}$ for all time, with time independent eigenvalues.

Symmetries and Degeneracies

Suppose the Hamiltonian is invariant under a symmetry transformation $\tilde{\mathcal{U}}$,

$$[\tilde{H},\tilde{\mathcal{U}}] = 0$$

If $|m\rangle$ is an eigenstate of $\tilde{H}$,

$$\tilde{H}|m\rangle = E_m|m\rangle$$

then

$$\tilde{H}(\tilde{u}|m\rangle) = \tilde{u}(\tilde{H}|m\rangle)$$
$$= E_m(\tilde{u}|m\rangle)$$

$\Rightarrow$ $u|m\rangle$ is also an eigenstate of $\tilde{H}$ with energy E_m $\therefore$ $|m\rangle$ and $\tilde{u}|m\rangle$ are degenerate states if $\tilde{u}|m\rangle \neq |m\rangle$!

Discrete Symmetries

Some symmetry operators cannot be described in terms of infinitesimal generators. For these symmetry operations we call them <u>discrete</u>

Parity Operator

The parity operator $\tilde{\pi}$ is related to the inversion of the spacial co-ordinate.

$$\vec{x} \xrightarrow{\tilde{\pi}} -\vec{x}$$

The wigner definition of parity is:

$$\tilde{\pi}\psi(\vec{x}) \equiv \langle\vec{x}|\tilde{\pi}|\psi\rangle$$
$$= \psi(I^{-1}\vec{x}) = \psi(-\vec{x}) = \langle-\vec{x}|\psi\rangle$$

we can also further say

$$\tilde{\pi}^{+}|\vec{x}\rangle = |-\vec{x}\rangle$$

we have also,

$$\int \psi^*(\vec{x})\tilde{\pi}\psi(\vec{x})\,d\vec{x} = \int \varphi^*(\vec{x})\psi(-\vec{x})\,dx$$

Changing the variables

$$\vec{\xi} = -\vec{x}\ , \quad d\vec{\xi} = d\vec{x}\left\|\frac{d\vec{\xi}}{d\vec{x}}\right\|$$

Since the volume of the space does not change under inversion then,

$$I = \int \varphi^*(-\vec{\xi})\psi(\vec{\xi})\,d\vec{\xi} = \int (\tilde{\pi}\varphi(\vec{\xi}))^*\psi(\vec{\xi})\,d\vec{\xi} = \int (\tilde{\pi}\varphi(\vec{x}))^*\psi(\vec{x})\,d\vec{x}$$

$$\Rightarrow \varphi^*\pi = (\pi\varphi)^* \Rightarrow \tilde{\pi} = \tilde{\pi}^{+}$$

Where we have finally

$$\tilde{\pi}|\vec{x}\rangle = \tilde{\pi}^{+}|\vec{x}\rangle = |-\vec{x}\rangle$$

This way,

$$\langle\varphi|(\tilde{\pi}|\psi\rangle) = (\langle\varphi|\tilde{\pi})|\psi\rangle = \langle\psi|\tilde{\pi}^{+}|\varphi\rangle^{*} = \langle\psi|\pi|\varphi\rangle^{*}$$

Finally,

$$\langle\vec{x}|\tilde{\pi}\vec{x}\tilde{\pi}|\vec{y}\rangle = (\langle\vec{x}|\tilde{\pi}^{+})\,\vec{x}\,(\tilde{\pi}|\vec{y}\rangle) = \langle-\vec{x}|\vec{x}|-\vec{y}\rangle = -\vec{x}\langle-\vec{x}|-\vec{y}\rangle = -\langle\vec{x}|\vec{x}|\vec{y}\rangle$$

From this we conclude

$$\tilde{\pi}\vec{x}\tilde{\pi} = -\vec{x}$$

or equivalently

$$\tilde{\pi}\vec{x} = -\vec{x}\tilde{\pi}$$

$\therefore$ $\tilde{\pi}$ and $\vec{x}$ anti-commute

Determining the translation operator

$$\tilde{\mathcal{U}}(d\vec{x}') = \mathbb{1} - \frac{i}{\hbar}\vec{P}\,d\vec{x}'$$

Translation followed by parity is the same thing as parity followed by translation in the opposite direction,

$$\tilde{\pi}\tilde{\mathcal{U}}(d\vec{x}') = \tilde{\mathcal{U}}(-d\vec{x}')\tilde{\pi}$$

Finessing this we get

$$\Rightarrow \tilde{\pi}\left(\mathbb{1} - \frac{i}{\hbar}\vec{P}\cdot d\vec{x}'\right)\tilde{\pi}^{+} = \mathbb{1} + \frac{i}{\hbar}\vec{P}\cdot d\vec{x}'$$

Where finally we have

$$\tilde{\pi}\vec{P}\tilde{\pi} = -\vec{P} \quad \text{or} \quad \tilde{\pi}\vec{P} = -\vec{P}\tilde{\pi}$$

However, since $\vec{L} = \vec{x}\times\vec{p}$ then we can say

$$\tilde{\pi}\vec{L}\tilde{\pi} = \vec{L} \Rightarrow [\tilde{\pi}, \vec{L}] = 0$$

The above tells us angular momentum is invarient under parity

<u>Theorem</u>: If $[\tilde{H}, \pi] = 0$, with $|m\rangle$ a non-degenerate eigenstate of $\tilde{H}$ with energy E_m, then $|m\rangle$ has a well defined parity.

Proof: If $\tilde{H}|m\rangle = E_m|m\rangle$ then

$$\tilde{\pi}\underbrace{\left(\frac{1}{2}(\mathbb{1}\pm\tilde{\pi})|m\rangle\right)}_{|\alpha\rangle} = \frac{1}{2}(\tilde{\pi}\pm\tilde{\pi}^2)|m\rangle = \pm\frac{1}{2}(\mathbb{1}\pm\tilde{\pi})|m\rangle$$

Therefore we can say $|\alpha\rangle$ is an eigenstate of $\tilde{\pi}$ with eigenvalues ± 1. Since:

$$\tilde{H}|\alpha\rangle = \frac{1}{2}(\mathbb{1}\pm\tilde{\pi})|m\rangle = E_m|\alpha\rangle \quad \therefore \quad |\alpha\rangle = |m\rangle$$

If $|\alpha\rangle \neq |m\rangle$ the spectrum would be degenerate.

$$\pi|m\rangle = \pm|m\rangle$$

From the above we can deduce and say that $|m\rangle$ has a <u>well-defined parity</u>.

In general, if $|\alpha\rangle$ is a parity eigenket,

$$\pi|\alpha\rangle = \pm|\alpha\rangle$$

then

$$\langle\vec{x}|\tilde{\pi}|\alpha\rangle = \pm\langle\vec{x}'|\alpha\rangle = \langle-\vec{x}'|\alpha\rangle$$

Therefore the corresponding wave function must have a well-defined parity

$$\psi(-\vec{x}) = \pm\psi(\vec{x})$$

with $+$ for even parity and $-$ for odd parity.

<u>Example</u>: Spherical Harmonics

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

which follows from the fact

$$Y_l^m \xrightarrow{I} (-1)^l Y_l^m \quad \text{under} \quad \vec{r} \to -\vec{r}$$

<u>Parity Selection Rule</u>

If $|\alpha\rangle$ and $|\beta\rangle$ are parity eigenstates

$$\tilde{\pi}|\alpha\rangle = \varepsilon_\alpha|\alpha\rangle\ , \ \tilde{\pi}|\beta\rangle = \varepsilon_\beta|\beta\rangle$$

with $\varepsilon_\alpha, \varepsilon_\beta = \pm 1$, then

$$\langle\beta|\vec{x}|\alpha\rangle = \langle\beta|\tilde{\pi}^{-1}(\tilde{\pi}\vec{x}\tilde{\pi})\tilde{\pi}|\alpha\rangle$$

Carrying the above out we find

$$\langle\beta|\hat{\vec{x}}|\alpha\rangle = E_\alpha E_\beta(-\langle\beta|\hat{\vec{x}}|\alpha\rangle)$$

This tells us that $E_\alpha E_\beta = -1$ and $\therefore$ $|\alpha\rangle$ and $|\beta\rangle$ must have opposite parities.

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Unitary and Anti-Unitary Operators

Given two kets $|\alpha\rangle$ and $|\beta\rangle$, and S a symmetry operation:

$$|\alpha\rangle \xrightarrow{S} |\tilde{\alpha}\rangle \,, \quad |\beta\rangle \xrightarrow{S} |\tilde{\beta}\rangle$$

where S should typically leave inner products invariant,

$$\langle\tilde{\beta}|\tilde{\alpha}\rangle = \langle\beta|\alpha\rangle .$$

This is satisfied if the symmetry operation is represented by a unitary operator,

$$\tilde{S}: \tilde{U}_s \,, \quad \tilde{U}_s^\dagger \tilde{U}_s = \tilde{U}_s \tilde{U}_s^\dagger = \mathbb{1} \Rightarrow |\tilde{\alpha}\rangle = \tilde{U}_s|\alpha\rangle \,, \quad |\tilde{\beta}\rangle = U_s|\beta\rangle$$

$$\langle\tilde{\beta}|\tilde{\alpha}\rangle = (\langle\beta|\tilde{U}_s^\dagger)(\tilde{U}_s|\alpha\rangle) = \langle\beta|\tilde{U}_s^\dagger\tilde{U}_s\rangle = \langle\beta|\alpha\rangle$$

The physical requirement for invariance of inner products is the conservation of transition probabilities

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

Definition: Anti unitary transformation

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

Θ is anti-unitary if

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

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

From ii) an anti-unitary operator is also anti-linear

Definition: Conjugation K

For a complete basis $\{|a'\rangle\}$, we can express an arbitrary ket as:

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

We define conjugation K as

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

<u>Theorem</u>: Every anti unitary operator can be written as:

$$\tilde{\Theta} = \tilde{u}\check{K}$$

where K is conjugation (and a generator of anti-unitary operators).

<u>Proof</u>:

$$\Theta(c_1|\alpha_1\rangle + c_2|\alpha_2\rangle) = \tilde{u}[K(c_1|\alpha_1\rangle + c_2|\alpha_2\rangle)] = \tilde{u}(c_1^* K|\alpha_1\rangle + c_2^* K|\alpha_2\rangle)$$
$$= c_1^*\tilde{u}K|\alpha_1\rangle + c_2^*\tilde{u}K|\alpha_2\rangle = c_1^*\Theta|\alpha_1\rangle + c_2^*\Theta|\alpha_2\rangle$$

Θ is therefore Anti-Linear. Also,

$$\Theta|\alpha\rangle = |\tilde{\alpha}\rangle = \tilde{u}(K|\alpha\rangle) = \sum_{a'}\langle a'|\alpha\rangle^*\tilde{u}|a'\rangle = \sum_{a'}\langle\alpha|a'\rangle\tilde{u}|a'\rangle$$

In the same way,

$$|\tilde{\beta}\rangle = \Theta|\beta\rangle = \tilde{u}(K|\beta\rangle) = \sum_{a''}\langle a''|\beta\rangle^*\tilde{u}|a''\rangle \Rightarrow \langle\tilde{\beta}| = \sum_{a''}\langle a''|\beta\rangle\langle a''|\tilde{u}^\dagger$$

Finally,

$$\langle\tilde{\beta}|\tilde{\alpha}\rangle = \sum_{a'a''}\langle a''|\beta\rangle\langle a'|\alpha\rangle^*\underbrace{\langle a''|\tilde{u}^\dagger\tilde{u}|a'\rangle}_{\delta_{a'a''}}$$
$$= \sum_{a'}\langle\alpha|a'\rangle\langle a'|\beta\rangle = \langle\alpha|\beta\rangle = \langle\beta|\alpha\rangle^*$$

which satisfies property i).

The conjugation operator K is the most elementary anti unitary operator $K^2 = \mathbb{1}$, in general, the operator K does not commute with other operators

If Ω is some arbitrary operator. Let's define:

$$\tilde{\Omega} \equiv K\tilde{\Omega}K,$$

Calculating the matrix elements of $\tilde{\Omega}$ in the $\{|a'\rangle\}$ basis,

$$\langle a'|\tilde{\Omega}|a''\rangle = \langle a'|K\tilde{\Omega}|a''\rangle = \langle a'|K\sum_{a'''}|a'''\rangle\langle a'''|\tilde{\Omega}|a''\rangle = \sum_{a'''}\underbrace{\langle a'|a'''\rangle}_{\delta_{a',a'''}}\langle a'''|\tilde{\Omega}|a''\rangle^*$$
$$= \langle a'|\tilde{\Omega}|a''\rangle^* = \langle a'|\tilde{\Omega}^*|a''\rangle$$

We can conclude $\tilde{\Omega} = K\tilde{\Omega}K = \tilde{\Omega}^*$ which in turn tells us

$$K\tilde{\Omega} = \tilde{\Omega}^* K$$

We have shown that $\Theta = \tilde{u}K$ have all the properties of anti unitary operators. To show that it is also required for Θ to be in this form. We show that ΘK is unitary.

If

$$|\tilde{\alpha}\rangle = K|\alpha\rangle \ , \ |\tilde{\beta}\rangle = K|\beta\rangle$$

and

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

then :

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

Hence, ΘK is unitary,

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

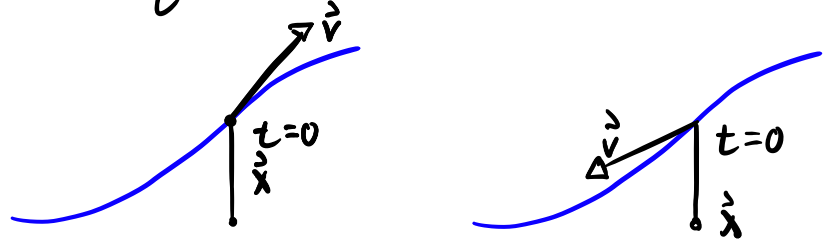
$$\langle\tilde{\tilde{\beta}}|\tilde{\tilde{\alpha}}\rangle = \langle\beta|\alpha\rangle \Rightarrow \Theta K = \tilde{U} \ (\text{unitary})$$

Where $\tilde{U}$ and $\tilde{K}$ do not commute,

$$K\tilde{U} = \tilde{U}^* K \ \therefore \ K\tilde{U}K = \tilde{U}^* \Rightarrow \tilde{U}K = K\tilde{U}^*$$

Time Reversed Operation

Time reversed operation is equivalent to the reversal of the motion of a physical system.



namely

$$\vec{x} \rightarrow \vec{x} \ , \ \vec{v} \rightarrow -\vec{v}$$

In open systems with applied external fields, the external magnetic field breaks time reversed symmetry. In the absence of a $\vec{B}$ field, $\tilde{T}$ is a conserved quantity and hence is a symmetry of the system.

We would like to build a $\tilde{T}$ operator that

$$\tilde{T}\vec{x}\tilde{T}^{-1} = \vec{x} \ , \ \tilde{T}\vec{p}\tilde{T}^{-1} = -\vec{p}$$

Since

$$\vec{L} = \vec{x} \times \vec{p} \Rightarrow \tilde{T}\vec{L}\tilde{T}^{-1} = -\vec{L}$$

In the same way, since the spin is an intrinsic angular momentum,

$$\tilde{T}\vec{S}\tilde{T}^{-1} = -\vec{S}$$

Schrödinger picture: A given ket $|\alpha\rangle$ describes a trajectory parametrized in time in the Hilbert Space. Let us define

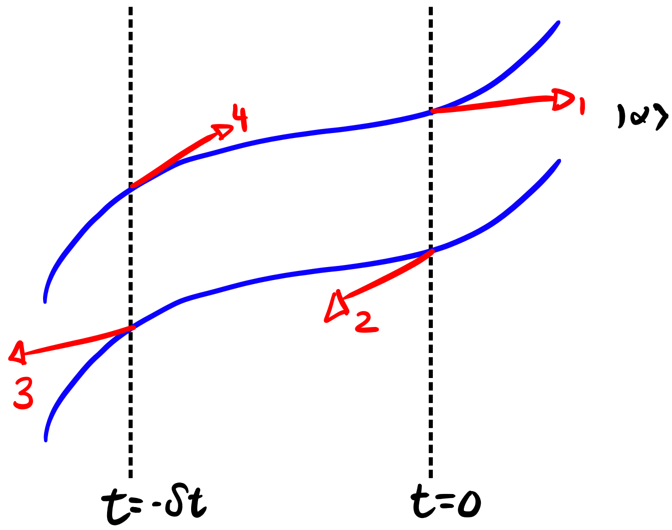
$$\tilde{T}|\alpha\rangle$$

as a time reversed ket.

From $t=0$, the time evolved ket is,

$$|\alpha, t_0=0; t\rangle = \left(\mathbb{1} - \frac{i}{\hbar}\tilde{\mathcal{H}}\delta t\right)|\alpha\rangle$$

Let's operate $\tilde{T}$ on $|\alpha\rangle$ at $t=0$, and then let it evolve to $t=\delta t$.



In (3), we have:

$$\left(\mathbb{1} - \frac{i}{\hbar}\tilde{\mathcal{H}}\delta t\right)\tilde{T}|\alpha\rangle$$

However, in (4)

$$|\alpha, t_0=0; t=-\delta t\rangle = \left(\mathbb{1} + \frac{i}{\hbar}\tilde{\mathcal{H}}\delta t\right)|\alpha\rangle$$

we can go from (4) to (3) with $\tilde{T}$

$$\tilde{T}\left(\mathbb{1} + \frac{i}{\hbar}\tilde{\mathcal{H}}\delta t\right) = \left(\mathbb{1} - \frac{i}{\hbar}\tilde{\mathcal{H}}\delta t\right)\tilde{T}$$

Where $\hbar$ and δt are real scalars. $\Rightarrow$ $\tilde{T}(i\tilde{\mathcal{H}}) = (-i\tilde{\mathcal{H}})\tilde{T}$

i) If $\tilde{T}$ is linear and unitary we can cancel the i^{th} vector,

$$\tilde{T}\tilde{\mathcal{H}} = -\tilde{\mathcal{H}}\tilde{T}$$

Therefore $\tilde{T}$ and $\tilde{\mathcal{H}}$ anti-commute. $\Rightarrow$ $\tilde{T}$ reverses the energy spectrum

$$\tilde{T}\tilde{\mathcal{H}}\tilde{T}^{-1}|m\rangle = -\tilde{\mathcal{H}}|m\rangle = -E_m|m\rangle$$

For $\tilde{\mathcal{H}}|m\rangle = E_m'|m\rangle$ $\Rightarrow$ no ground state and not possible.

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Previous class

$$\tilde{T}(i\tilde{\mathcal{H}}) = (-i\tilde{\mathcal{H}})\tilde{T}$$

i) If $\tilde{T}$ is unitary:

$$\tilde{T}\tilde{\mathcal{H}} = -\tilde{\mathcal{H}}\tilde{T} \Rightarrow \tilde{T}\tilde{\mathcal{H}}\tilde{T}^{-1}$$

$\tilde{\mathcal{H}}$ for the kinetic energy of a free particle

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

becomes negative and unbound from below!

ii) Alternatively, one can require that $\tilde{T}$ and $\tilde{\mathcal{H}}$ commute

$$[\tilde{\mathcal{H}}, \tilde{T}] = 0$$

$\Rightarrow$ $\tilde{T}$ is a conserved quantity $\therefore$

$$\tilde{T}(i)\tilde{\mathcal{H}} = (-i)\tilde{T}\tilde{\mathcal{H}}$$

With

$$\tilde{T}(i) = (-i)\tilde{T} = (i)^*\tilde{T}$$

$\Rightarrow$ $\tilde{T}$ is an antilinear operator.

Since

$$\tilde{T}\vec{x}\tilde{T}^{-1} = \vec{x} \text{ (commute)}$$
$$\tilde{T}\vec{p}\tilde{T}^{-1} = -\vec{p} \text{ (anti commute)}$$

Considering the basis:

$$\{|\vec{x}'\rangle\}, \{|\vec{p}'\rangle\}$$

Then

$$\vec{p}(\tilde{T}|\vec{p}'\rangle) = -\tilde{T}\tilde{p}|\vec{p}'\rangle = -\vec{p}'\tilde{T}|\vec{p}'\rangle = |-\vec{p}\rangle$$

$\tilde{T}|\vec{p}'\rangle$ is an eigenstate of $\vec{p}$ with eigenvalue $-\vec{p}'$ $\therefore$ up to a phase,

$$\tilde{T}|\vec{p}'\rangle = |-\vec{p}'\rangle$$

In the same way,

$$\vec{x}(\tilde{T}|\vec{x}'\rangle) = \tilde{T}\vec{x}|\vec{x}'\rangle = \vec{x}'(\tilde{T}|\vec{x}'\rangle) \Rightarrow \tilde{T}|\vec{x}'\rangle = |\vec{x}'\rangle$$

Up to a phase.

The anti-linearity of $\tilde{T}$ preserves commutation relations among canonically related operators,

$$[\tilde{x}_i, \tilde{p}_j] = i\hbar\delta_{ij}$$

$$\Rightarrow \qquad \tilde{T}[\tilde{x}_i, \tilde{p}_j]\tilde{T}^{-1} = \tilde{T}(i\hbar)\delta_{ij}\tilde{T}^{-1} = -i\hbar\delta_{ij} \quad \Rightarrow [\tilde{x}_i, -\tilde{p}_j] = -i\hbar\delta_{ij}$$

and hence $[\tilde{x}_i, \tilde{p}_j] = i\hbar\delta_{ij}$ is unchanged.

Besides, if $\tilde{T}$ represents a symmetry it <u>must</u> be anti unitary. Since

$$\tilde{T}\vec{J}\tilde{T}^{-1} = -\vec{J} \quad (\text{and}) \quad [\vec{J}_i, \vec{J}_j] = i\hbar\epsilon_{ijk}\vec{J}_k$$

$$\Rightarrow \qquad \tilde{T}[\vec{J}_i, \vec{J}_j]\tilde{T}^{-1} = \tilde{T}(i\hbar)\epsilon_{ijk}\vec{J}_k\tilde{T}^{-1}, \quad [-\vec{J}_i, -\vec{J}_j] = -i\hbar\epsilon_{ijk}(-\vec{J}_k)\tilde{T}\tilde{T}^{-1}$$

$\Rightarrow$ The signs cancel (invariance). As an anti-unitary operator,

$$\tilde{T} = \tilde{u}\tilde{k}$$

With $\tilde{u}$ unitary

$$\tilde{T}^2 = c\,\mathbb{1} = \tilde{u}\tilde{k}\cdot\tilde{u}\cdot\tilde{k} = \tilde{u}\cdot\tilde{u}^*$$

Where c is a complex number

$$\tilde{u}^* = (\tilde{u}^\dagger)^t = (\tilde{u}^{-1})^t = (u^t)^{-1}$$

$$c\cdot\mathbb{1} = \tilde{u}(\tilde{u}^t)^{-1} \Rightarrow \tilde{u} = c\tilde{u}^t$$

Taking the transpose,

$$\tilde{u}^t = c\tilde{u} \Rightarrow \tilde{u} = c\tilde{u}^t = c(c\tilde{u})$$

$$\tilde{u} = c^2\tilde{u} \Rightarrow c^2 = 1 \Rightarrow c = \pm 1$$

Or, equivalently,

$$\tilde{T}^2 = \pm\mathbb{1}$$

When

$$C=\pm 1 \Rightarrow \tilde{u}^{t}=\tilde{u} \text{ (symmetric)}$$
$$C=-1 \Rightarrow \tilde{u}^{t}=-\tilde{u} \text{ (anti-symmetric)}$$

<u>Particle with no spin</u>

In co-ordinate representation

$$\tilde{T}\vec{x}\tilde{T}^{-1}=\vec{x} \Rightarrow \tilde{T}\vec{x}=\vec{x}\tilde{T}$$

$\therefore$ $$\tilde{u}\tilde{k}\vec{x}=\vec{x}\tilde{u}\tilde{k} \Rightarrow \tilde{u}\vec{x}\tilde{k}=\vec{x}\tilde{u}\tilde{k} \Rightarrow \tilde{u}\vec{x}=\vec{x}\tilde{u} \quad \therefore \quad [\tilde{u},\vec{x}]=0$$

Also,

$$\tilde{T}\vec{P}=-\vec{P}\tilde{T}=T(-i\hbar\vec{\nabla})=(i\hbar\vec{\nabla})\tilde{T}$$

$\therefore$ $$\tilde{u}\tilde{k}(-i\hbar\vec{\nabla})=i\hbar\vec{\nabla}\tilde{u}\tilde{k} \Rightarrow \tilde{u}(i\hbar\vec{\nabla})\tilde{k}=(i\hbar\vec{\nabla}\tilde{u})\tilde{k} \Rightarrow [\tilde{u},\vec{\nabla}]=0$$

From this we can say that $\tilde{u}$ does not depend either on $\vec{x}$ or $\vec{\nabla}$ $\therefore$

$$\tilde{u}=e^{i\alpha}$$

We assume $e^{i\alpha}=\mathbb{1}$ $\therefore$ $\tilde{T}\equiv\tilde{k}$ (For spinless particle)

For the wavefunction,

$$\tilde{T}|\alpha\rangle=\tilde{T}\int d\vec{x}'|\vec{x}'\rangle\langle\vec{x}'|\alpha\rangle=\int d\vec{x}'\langle\vec{x}'|\alpha\rangle^{*}T|\vec{x}'\rangle$$

Therefore,

$$\langle\vec{x}'|\tilde{T}|\alpha\rangle=\langle\vec{x}'|\alpha\rangle^{*}=\psi_\alpha^{*}(\vec{x}')$$

With,

$$\tilde{T}\psi_\alpha(\vec{x}')=\psi_\alpha^{*}(\vec{x}')$$

Is the time reversed wavefunction. In the schrödinger equation

$$(i\hbar)\partial_t\psi(\vec{x},t)=\tilde{\mathcal{H}}\psi(\vec{x},t) \rightarrow \tilde{T}(i\hbar)\partial_t\psi(\vec{x},t)=\tilde{T}\tilde{\mathcal{H}}\psi(x,t)=\tilde{\mathcal{H}}\tilde{T}\psi(\vec{x},t)$$

$\Rightarrow$ $$(-i\hbar)\psi^{*}(\vec{x},t)=\tilde{\mathcal{H}}\psi^{*}(\vec{x},t)$$

Taking $t\rightarrow -t$,

$$(i\hbar)\partial_{t'}\psi^{*}(\vec{x},t)=\tilde{\mathcal{H}}\psi^{*}(\vec{x},-t')$$

The Schrödinger equation becomes invariant under

$$\Psi(\vec{x},t) \xrightarrow{\tilde{T}} \Psi^*(\vec{x},-t) \iff \tilde{T}\Psi(\vec{x},t) = \Psi^*(\vec{x},-t)$$

In the stationary state,

$$\Psi(\vec{r},t) = u_n(\vec{x})e^{-iE_nt/\hbar}, \quad \Psi^*(\vec{r},t) = u_n^*(\vec{x})e^{iE_nt/\hbar}$$

$\Rightarrow$

$$\Psi^*(\vec{r},-t) = u_n^*(\vec{x})e^{-iE_nt/\hbar}$$

$\therefore$ $\Psi(\vec{x},t)$ and $\tilde{T}\Psi(\vec{x},t)$ have the same energy E_n.

<u>Theorem</u>: If the energy spectrum is <u>not</u> degenerate, then $u_n(\vec{x})$ is real.

<u>Proof</u>:

$$\tilde{H}(\tilde{T}|n\rangle) = \tilde{T}\tilde{H}|n\rangle = E_n(\tilde{T}|n\rangle)$$

then $|n\rangle = \tilde{T}|n\rangle$ are the same state.

When the angular part of the wavefunction is expressed in Spherical harmonics,

$$Y_l^m(\theta,\varphi) \xrightarrow{\tilde{T}} Y_l^{m*}(\theta,\varphi) = (-1)^m Y_l^{-m}(\theta,\varphi) \Rightarrow \tilde{T}|l,m\rangle = (-1)^m|l,-m\rangle$$

In the momentum space

$$\tilde{T}|\alpha\rangle = \tilde{T}\int d\vec{p}'\,|\vec{p}'\rangle\langle\vec{p}'|\alpha\rangle = \int d\vec{p}'\,|-\vec{p}'\rangle\langle\vec{p}'|\alpha\rangle^* \qquad \vec{p}'' \to -\vec{p}'$$

$$\tilde{T}|\alpha\rangle = \int d\vec{p}''\,|\vec{p}''\rangle\langle-\vec{p}''|\alpha\rangle^*$$

Therefore,

$$\langle\vec{p}'|\tilde{T}|\alpha\rangle = \varphi_\alpha^*(-\vec{p}') = \tilde{T}\phi_\alpha(\vec{p}')$$

<u>2-14-22</u>

Particle with spin $(s = 1/2)$. In general,

$$T\vec{S}T^{-1} = -\vec{S} \qquad T \,\&\, \vec{S} \text{ Anti-Commute}$$

then for the z component

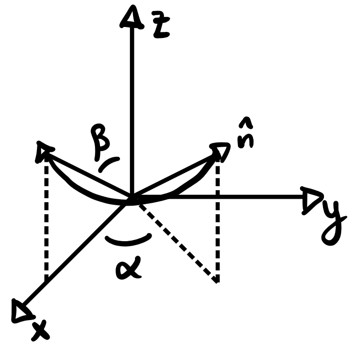
$$\tilde{S}_z(\tilde{T}|\pm\rangle) = -\tilde{T}(\tilde{S}_z|\pm\rangle) = \mp\frac{\hbar}{2}(\tilde{T}|\pm\rangle)$$

where $\tilde{T}|\pm\rangle$ is an eigenstate of $\tilde{S}_z$ with eigenvalue $\mp\hbar/2$. Conclusion is that

$$\tilde{T}|\pm\rangle = \eta|\mp\rangle \quad \text{const. a.f.b phase}$$

where η is a phase, $|\eta| = 1$.

In general, for arbitrary projection $\tilde{S}\cdot\hat{n}$, one can write the corresponding eigenket / eigenstates $|\hat{n},\pm\rangle$ explicitly in terms of $\tilde{S}_z$



Rotation β along $\hat{y}$ and α along $\hat{z}$

Peforming two rotations with Euler angles β & α

$$|\hat{n},\pm\rangle = e^{-i/\hbar\,\alpha\tilde{S}_z}e^{-i/\hbar\,\beta\tilde{S}_y}|+\rangle$$

where we know that

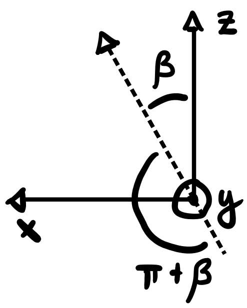
$$\tilde{T}e^{-i/\hbar\,\alpha\tilde{S}_z}\tilde{T}^{-1} = e^{i/\hbar\,\alpha(-\tilde{S}_z)} = e^{-i/\hbar\,\alpha(\tilde{S}_z)}$$

$\tilde{T}$ changes sign of $\tilde{S}_z$ but because of $i \Rightarrow$ nothing changed.

we use:

$$\tilde{T}|\hat{n},\pm\rangle = \eta|\hat{n},-\rangle = (\tilde{T}e^{-i/\hbar\,\alpha\tilde{S}_z}\tilde{T}^{-1})(\tilde{T}e^{-i/\hbar\,\beta\tilde{S}_y}\tilde{T}^{-1}\tilde{T})|+\rangle = e^{-i/\hbar\,\alpha\tilde{S}_z}e^{-i/\hbar\,\beta\tilde{S}_y}\tilde{T}|+\rangle$$

At the same time



$$|\hat{n},-\rangle = e^{-i\alpha\tilde{S}_z/\hbar}e^{-i\beta\tilde{S}_y(\pi+\beta)/\hbar}|+\rangle \Rightarrow \tilde{T} = \tilde{u}\tilde{k}$$

$$\tilde{T}|\hat{n}\rangle = \tilde{u}\tilde{k}|\hat{n}\rangle = e^{-i\alpha\tilde{S}_z/\hbar}e^{-i\beta\tilde{S}_y/\hbar}\tilde{u}\tilde{k}|+\rangle \Rightarrow \tilde{k} \text{ does nothing to it}$$

$$= e^{-i\alpha\tilde{S}_z/\hbar}e^{-i\beta\tilde{S}_y/\hbar}\tilde{u}|+\rangle = e^{-i\alpha\tilde{S}_z/\hbar}e^{-i(\pi+\beta)\tilde{S}_y/\hbar}\eta|+\rangle \quad \therefore$$

$$e^{-i\alpha\tilde{S}_z/\hbar}e^{-i\beta\tilde{S}_y/\hbar} = \eta e^{-i\alpha S_z/\hbar}e^{-i(\pi+\beta)\tilde{S}_y/\hbar}|+\rangle \qquad (*)$$

we can take $(*)$ and further we have

$$\tilde{u} = \eta e^{-i\pi\tilde{S}_y/\hbar} = \eta e^{-i\pi/2\,\sigma_y} = \eta[\cos(\pi/2) - i\sigma_y\sin(\pi/2)] = -i\eta\sigma_y$$

Or equivalently we can say

$$\tilde{u} = -i\eta\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \eta\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$$

From the above we can deduce and say

$\tilde{u}$ is symmetric $\Rightarrow \tilde{T}^2 = \mathbb{1}$, $\tilde{u}$ is Anti-symmetric $\Rightarrow \tilde{T}^2 = -\mathbb{1}$, $K^2 = \mathbb{1}$

When $\tilde{u}$ is Anti-Symmetric we can say

$$\tilde{T} = \tilde{u}\tilde{K} = -i\eta\sigma_y\tilde{K}$$

Using the rotation operator

$$\tilde{D}_y(\pi) = e^{-i\pi/2\,\sigma_y} = -i\sigma_y$$

$$\tilde{D}_y(\pi)|+\rangle = -i\sigma_y|+\rangle = -i(i|-\rangle) = |-\rangle$$

$$\tilde{D}_y(\pi)|-\rangle = -i\sigma_y|-\rangle = -i(-i|+\rangle) = -|+\rangle$$

Operating $\tilde{D}_y(\pi)$ on arbitrary ket

$$|\alpha\rangle = c_1|+\rangle + c_2|-\rangle$$

$$\tilde{T}|\alpha\rangle = \eta(c_1^*|-\rangle - c_2^*|+\rangle)$$

$$\Rightarrow \quad \tilde{T}^2|\alpha\rangle = \eta^*\eta(-c_1|+\rangle - c_2|-\rangle) = -|\alpha\rangle$$

Hence, $\tilde{T}^2 = -\mathbb{1}$ as found before. For spinless particles $\tilde{T} = \tilde{K}$ $\therefore$ $\tilde{T}^2 = \mathbb{1}$. One can generalize the previous results for arbitrary momentum $\vec{S} \to \vec{J}$ where $\tilde{T}\vec{J}\tilde{T}^{-1} = -\vec{J}$. In general we can say

$$\tilde{T} = \eta e^{-i\pi/2\,\vec{J}_y} \cdot \tilde{K}$$

Rotations leave the quantum number j of $|j,m\rangle$ state unchanged. For an arbitrary ket $|\alpha\rangle$

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

$$\tilde{T}|\alpha\rangle = \sum_m \tilde{T}(|j,m\rangle)\langle j,m|\alpha\rangle^*$$

$$= \sum_m (\eta e^{-i\pi\vec{J}_y/\hbar}|j,m\rangle)\langle j,m|\alpha\rangle^*$$

$$\tilde{T}^2|\alpha\rangle = \sum_m \eta^*\eta e^{-i\pi\vec{J}_y/\hbar} e^{-i\pi\vec{J}_y/\hbar} |j,m\rangle$$

$$= \sum_m e^{-2\pi i\vec{J}_y/\hbar} |j,m\rangle\langle j,m|\alpha\rangle$$

$$= \tilde{D}_y^{(j)}(2\pi)\sum_m |j,m\rangle\langle j,m|\alpha\rangle$$

$$= \tilde{D}_y^{(j)}(2\pi)|\alpha\rangle$$

Therefore, for any $|\alpha\rangle$,

$$\tilde{T}^2 = \tilde{D}_y^{(j)}(2\pi) = (-1)^{2j}$$

Although $\tilde{T}$ commutes with the Hamiltonian

$$[\tilde{T}, \tilde{\mathcal{H}}] = 0 \quad \therefore \quad \tilde{T}\tilde{\mathcal{H}}\tilde{T}^{-1} = \tilde{\mathcal{H}}$$

$\tilde{T}$ does not commute with the the Time evolution operator

$$\tilde{T} e^{-i\mathcal{H}t/\hbar} = e^{i\mathcal{H}t/\hbar} \tilde{T}$$

There are no quantum numbers associated with time reversal symmetry operator which are conserved.

Hence, $\tilde{T}$ symmetry does not imply in any additional conservation laws (besides energy)

Suppose that

$$\tilde{T}|\alpha'\rangle = \alpha'|\alpha'\rangle \, \ldots\ldots\ldots (I)$$

Time evolved ket is

$$|\alpha', 0; t\rangle = e^{-i\mathcal{H}t/\hbar}|\alpha'\rangle$$

I can say

$$\tilde{T}|\alpha', 0; t\rangle = \tilde{T} e^{-i\mathcal{H}t/\hbar}|\alpha'\rangle = e^{i\mathcal{H}t/\hbar}\tilde{T}|\alpha'\rangle = e^{i\mathcal{H}t/\hbar}\alpha'|\alpha'\rangle = (\alpha')|\alpha, 0; -t\rangle$$

time evolved ket in the opposite direction.

$\Rightarrow$ If $|\alpha'\rangle$ is an eigenket of $\tilde{T}$ at $t=0$, this is not satisfied at $t>0$.

However, the $\tilde{T}$ symmetry implies in extra degeneracies. If

$$\tilde{\mathcal{H}}|n\rangle = E_n|n\rangle$$

Then

$$\tilde{\mathcal{H}}(\tilde{T}|n\rangle) = \tilde{T}(\tilde{\mathcal{H}}|n\rangle) = E_n(\tilde{T}|n\rangle)$$

If $|n\rangle$ is an eigenstate of $\tilde{\mathcal{H}}$ then $\tilde{T}|n\rangle$ is also an eigenstate with the same energy. The question is whether $\tilde{T}|n\rangle$ and $|n\rangle$ are <u>linearly independent</u>.

<u>Theorem</u>: $\tilde{T}|n\rangle$ and $|n\rangle$ are linearly independent when $\tilde{T}^2 = -\mathbb{I}$

<u>Proof</u>: If $|\alpha\rangle$ is an arbitrary state, $|\beta\rangle \equiv \tilde{T}|\alpha\rangle$, Hence

$$|\alpha\rangle \xrightarrow{T} \tilde{T}|\alpha\rangle = |\tilde{\alpha}\rangle = |\beta\rangle, \quad |\beta\rangle \xrightarrow{T} \tilde{T}|\beta\rangle = |\tilde{\beta}\rangle = \tilde{T}^2|\alpha\rangle = -|\alpha\rangle$$

Therefore we can say,

$$\langle\tilde{\beta}|\tilde{\alpha}\rangle = \langle\alpha|\beta\rangle = -\langle\alpha|\beta\rangle$$

$\Rightarrow \langle\alpha|\beta\rangle = \langle\beta|\alpha\rangle = 0$. Hence, when $\tilde{T}^2 = \mathbb{I}$, $\tilde{T}|\alpha\rangle$ and $|\alpha\rangle$ are orthogonal $\Rightarrow$ degeneracy due to time reversal

Kramer's Theorem

The energy levels of a system of electrons with an odd number of energy levels must be at least doubly degenerate, regardless the symmetry of the system (In the absence of magnetic field).

Proof: The total spin $\vec{S} = \sum_i S_i$ is a half integer for an odd number of particles since $\hat{T}^2 = (-1)^{2j} = -1$ for half integer j.

For every eigenstate α there should be an orthogonal degenerate eigenket $T|\alpha\rangle$

$\Rightarrow$ Kramer's degeneracy