Two-Level Systems, Part II

This is a good time to introduce the parity operator Π.

$$x \xrightarrow[\Pi]{} -x \qquad y \xrightarrow[\Pi]{} -y \qquad z \rightarrow -z$$

(Classically)

$$\vec{p} = m\vec{v} = m\frac{d\vec{x}}{dt} \xrightarrow[\Pi]{} -\vec{p}$$

(In QM)

$$\langle x | \tilde{p} = -i\hbar \frac{d}{dx} \langle x | \xrightarrow[\Pi]{} +i\hbar\frac{d}{dx}\langle x|$$

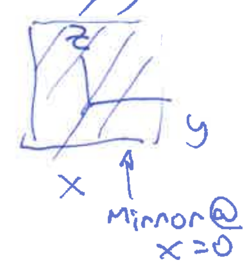
$$x^2 \xrightarrow{\Pi} x^2 \qquad p^2 \xrightarrow{\Pi} p^2$$

$$\vec{p} \xrightarrow[\Pi]{} -\vec{p} \quad \text{(radial vector)}$$

$$\vec{L} = m\vec{r}\times\vec{v} \xrightarrow[\Pi]{} m(-\vec{r})\times(-\vec{v}) = \vec{L} \quad \text{(axial vector)}$$

- Often we call Π-symmetry mirror symmetry, but there is a slight difference.

(Object @ $x = +1$ appears @ $x = -1$ when looking in mirror)



$$x \xrightarrow[M_x]{} -x \qquad y \xrightarrow[M_x]{} y \qquad z \xrightarrow[M_x]{} z$$

$$\Rightarrow \Pi = R_x(180^\circ)\, M_x$$

$$x \xrightarrow[R_x(180^\circ)]{} x \qquad y \xrightarrow[R(180^\circ)]{} -y \qquad z \xrightarrow[R_x(180^\circ)]{} -z$$

$\boxed{\mathrm{T}}$

What does Π do to $\psi(x)$?

$\Pi|x\rangle = |-x\rangle$ recall $\psi(x) = \langle x|\psi\rangle$

$$\Pi|\psi\rangle = \Pi\int_{-\infty}^{\infty}|x\rangle\langle x|\psi\rangle\,dx$$

$$= \int_{-\infty}^{\infty}|-x\rangle\langle x|\psi\rangle\,dx$$

$x' = -x$

$dx = -dx'$ but just keep as integral over dx

$$= \int_{+\infty}^{-\infty}|x'\rangle\langle -x'|\psi\rangle\,dx'$$

$$\Rightarrow \boxed{\langle x|\Pi|\psi\rangle} = \int_{-\infty}^{\infty}\underbrace{\langle x|x'\rangle}_{\delta(x-x')}\underbrace{\langle -x'|\psi\rangle}_{\psi(-x')}\,dx'$$

$$= \psi(-x)$$

$$\Updownarrow$$

$$\psi(x) \underset{\Pi}{\longleftrightarrow} \psi(-x)$$

Perhaps just overly formal way of saying (Reflection about origin)

A few other properties of Π.

- Unitary: $\underline{\Pi^{+} = \Pi^{-1}}$ (we know this from $\Pi|x\rangle = |-x\rangle$) $\Leftrightarrow \underline{\Pi\Pi^{+} = \mathbb{1}}$
- $\Pi^2|x\rangle = |-(-x)\rangle = |x\rangle \Rightarrow \underline{\Pi^2 = \mathbb{1}}$

From above two properties,

$\Rightarrow$ Hermitian $\underline{\Pi = \Pi^{+}}$

- Not continuously generated

Eigenvalues of Π are ± 1, since $\Pi^2 = \mathbb{1}$

Symmetries

Is Π a symmetry ?

- In general, a symmetry means that the transforming operator $\mathcal{U}$ has the following properties:

$$\langle \mathcal{U}\psi | H | \mathcal{U}\chi \rangle = \langle \psi | H | \chi \rangle$$

- If it leaves all matrix elements of H unchanged, since H governs time dynamics, this transform $\mathcal{U}$ leaves equations of motion unchanged $\Leftrightarrow$ symmetry

- $\langle \mathcal{U}\psi | H | \mathcal{U}\chi \rangle = \langle \psi | \mathcal{U}^{+} H \mathcal{U} | \chi \rangle$

(Thinking of transforming states) (thinking of transforming operator)

$\Rightarrow$ $\mathcal{U}$ is a symmetry of H if

$$\underbrace{\mathcal{U}^{+} H \mathcal{U}}_{\text{transformed } H} = H \, ,$$

so e.g. $\Pi^{+} \underset{\sim}{x} \Pi = -\underset{\sim}{x}$

$\Pi^{+} \underset{\sim}{p} \Pi = -\underset{\sim}{p}$

- For ammonia, what about $\Pi_\bullet$?

~~(All atoms reflected about origin. As far as z_N is concerned, reflection of Hs not important.) (Just a rotation of triangle)~~

- What is $\Pi_\bullet^+ H \Pi_\bullet$?

location of N relative to H plane.

$$V(z_N) \underset{\Pi_\bullet}{\longleftrightarrow} V(-z_N) = V(z_N)$$

(since symmetric potential)

($\Pi_\bullet$ replaces z with −z)

$$\frac{\tilde{p}^2}{2m} \underset{\Pi_\bullet}{\longleftrightarrow} \frac{(-\tilde{p})^2}{2m} = \frac{\tilde{p}^2}{2m}$$

$$\Downarrow$$

$$H \underset{\Pi_\bullet}{\longleftrightarrow} H$$

Apart from weak force, of course any molecule looks OK as viewed in mirror. But what we are doing here is reflecting only the N & not the Hs & asking if eqns of motion change.

or in terms of operator transformation

$$\Pi_\bullet^+ H \Pi_\bullet = H \iff [\Pi_\bullet, H] = 0$$

$$\Rightarrow \Pi\Pi^+ H \Pi = \Pi H \Rightarrow H\Pi = \Pi H$$

- ⇒ Yes, $\Pi_\bullet$ is a symmetry for ammonia

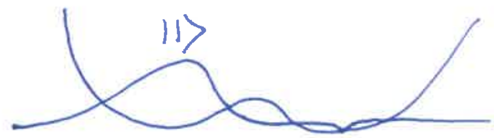
Equivalent to transforming coordinates of particle in an external potential which we refuse to transform

$\boxed{Q}$ Can $\Pi_\bullet$ carry an eigenstate of H to some different state?

$\boxed{A}$ Only if the state in question is degenerate in energy with other states ~~$[\Pi_\bullet, H] = 0$~~

- How does Π act on our various choices for basis states?

$$\Pi|1\rangle = |2\rangle$$



$$\Pi|2\rangle = |1\rangle$$

$$\Pi|+\rangle = \Pi\left(\tfrac{1}{\sqrt{2}}|1\rangle + \tfrac{1}{\sqrt{2}}|2\rangle\right) = +|+\rangle$$

$$\Pi|-\rangle = \Pi\left(\tfrac{1}{\sqrt{2}}|1\rangle - \tfrac{1}{\sqrt{2}}|2\rangle\right) = \tfrac{1}{\sqrt{2}}|2\rangle - \tfrac{1}{\sqrt{2}}|1\rangle = -|-\rangle$$

- Our Hamiltonian in the $|1\rangle, |2\rangle$ basis is

$$H = \begin{pmatrix} E_0 & -\Delta \\ -\Delta & E_0 \end{pmatrix}, \text{ where } \Delta > 0$$

- Let's see what happens when we take $\Delta \to 0$

$$E_+ = E_0 - \Delta \to E_0$$
$$E_- = E_0 + \Delta \to E_0$$
$\Rightarrow$ Degeneracy

- $|+\rangle$ & $|-\rangle$ are eigenstates of H, and so are $\underset{= \frac{1}{\sqrt{2}}(|+\rangle + |-\rangle)}{|1\rangle}$ & $\underset{= \frac{1}{\sqrt{2}}(|+\rangle - |-\rangle)}{|2\rangle}$. In general, $H(\alpha|+\rangle + \beta|-\rangle) = E_0(\alpha|+\rangle + \beta|-\rangle)$

So, let's see how Π acts on eigenstates of H.

$$\Pi |+\rangle = +|+\rangle \qquad \Pi |-\rangle = -|-\rangle$$

These are not changed by Π.

However

$$\Pi |1\rangle = |2\rangle \qquad \Pi |2\rangle = |1\rangle$$

These eigenstates of H are changed by Π

- Working in the $|+\rangle, |-\rangle$ basis, both operators are diagonal. We say that choice of basis "simultaneously diagonalizes both operators.
- When we turn on $\Delta > 0$, then the degeneracy is "lifted". There is only one state ($|+\rangle$ or $|-\rangle$) of each energy value ~~and that is given~~
- Summary: since $[\Pi, H] = 0$, Π can connect states only if they have same energy. If we chose a basis which simultaneously diagonalizes Π & H, then Π leaves the basis states alone. (And same idea for action of H)

In the $|1\rangle, |2\rangle$ basis

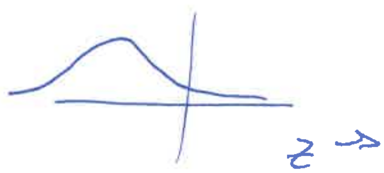
$$H = \begin{pmatrix} E_0 & -\Delta \\ -\Delta^* & E_0 \end{pmatrix}$$

~~We showed last class that Δ real works. But We~~

How do we know that Δ must be real?

This is what it means to put those elements in the matrix:

$$-\Delta = \langle 1 | H | 2 \rangle$$

We chose $|1\rangle =$ 

, a real function. & same for $|2\rangle$

$$H = \underbrace{-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}}_{\text{real}} + \underbrace{V(x)}_{\text{real}}$$

$\Rightarrow -\Delta$ is real

In $|1\rangle, |2\rangle$ basis

$$H = \begin{pmatrix} E_0 & -\Delta \\ -\Delta & E_0 \end{pmatrix}, \quad \Pi = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

In $|+\rangle, |-\rangle$ basis

$$H = \begin{pmatrix} E_0 - \Delta & 0 \\ 0 & E_0 + \Delta \end{pmatrix}, \quad \Pi = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$