Symmetries in quantum mechanics

Motivation through an example

Consider the H_2^+ molecule

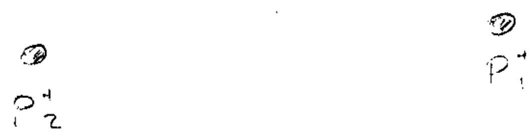
the base states are $|e_1\rangle$ = electron is orbiting around roton 1, and similarly for $|e_2\rangle$. The Hamiltonian of the lectron is

$$\hat{H} = \begin{bmatrix} E_0 & -A \\ -A & E_0 \end{bmatrix} \tag{1}$$

here E_0 is the energy of the electron when it is orbiting round a specific proton (this is the ground state of he hydrogen atom, $E_0 = -13.6\ eV$), the constant A epresents the amplitude for the electron to jump from one proton to the other.

Note that this problem has a symmetry: namely, hat if we reflect the system through a plane passing etween the two protons, the electron would never know.

Reflected state



This symmetry is visible in $\hat{H}$ because the diagonal terms are equal [the off-diagonal terms can't be touched because $\hat{H}$ must be Hermitian].

In order to describe this symmetry mathematically we define an operator $\hat{P}$ called a reflection operator, defined such that

$$\begin{aligned} \hat{P}\,|e_1\rangle &= |e_2\rangle \\ \hat{P}\,|e_2\rangle &= |e_1\rangle \end{aligned} \qquad (2)$$

Since we know how $\hat{P}$ acts on the base states, it is easy to compute its matrix elements

$$\langle e_1|\hat{P}|e_1\rangle = 0 \qquad \langle e_1|\hat{P}|e_2\rangle = 1$$

$$\langle e_2|\hat{P}|e_1\rangle = 1 \qquad \langle e_2|\hat{P}|e_2\rangle = 0$$

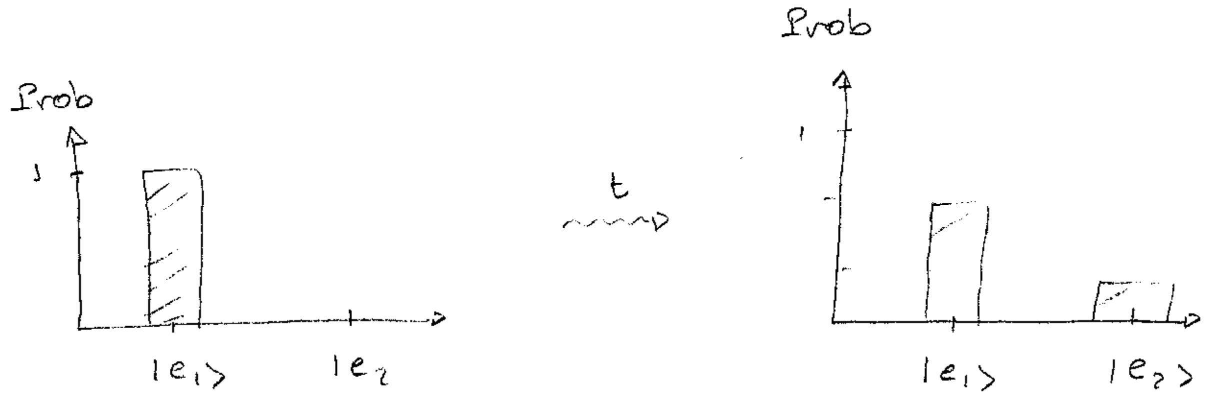
Thus

$$\hat{P} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} = \hat{\sigma}_x \qquad (3)$$

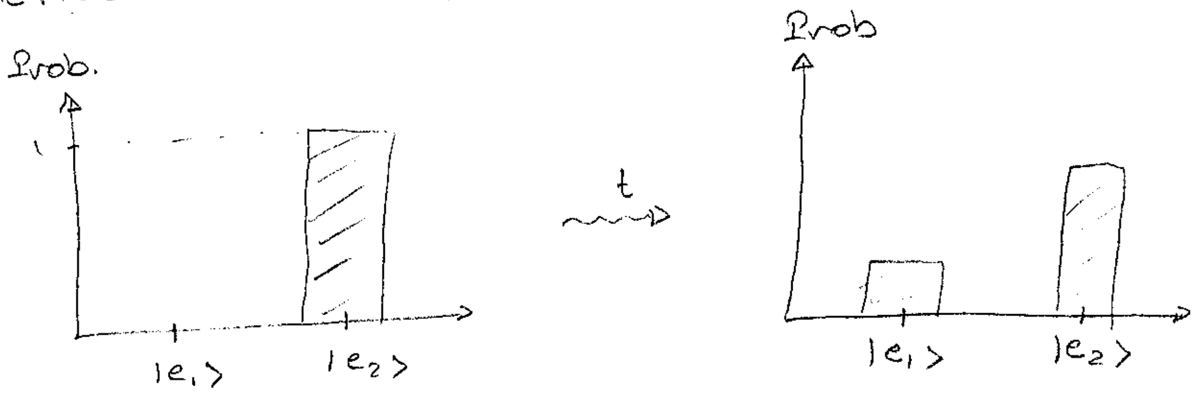
Its eigenvalues are ± 1.

the symmetry of the H_2^+ molecule must reflect on its ime evolution. Suppose we start at $t=0$ with the system in $|\alpha(0)\rangle = |e_1\rangle$. and suppose that at time t the state is

$$|\alpha(t)\rangle = \hat{U}(t)|e_1\rangle = a|e_1\rangle + b|e_2\rangle \qquad (4)$$



now what happens if $|\alpha(0)\rangle = |e_2\rangle$. well, the system is ymmetrical so we expect:



that is, we expect exactly the mirrored situation

$$|\beta(t)\rangle = \hat{U}(t)|e_2\rangle = b|e_1\rangle + a|e_2\rangle \qquad (5)$$

thus, because of symmetry, if we know the evolution f one state, we can predict the evolution of the other

From (4) and (5) we see that

$$|\beta(t)\rangle = \hat{P}\,|\alpha(t)\rangle$$

just like $\quad |e_2\rangle = \hat{P}\,|e_1\rangle$

this means that it doesn't matter if you perform a reflection at $t=0$ or at some other t.

$$|\beta(t)\rangle = \hat{U}\,|e_2\rangle = \hat{U}\hat{P}\,|e_1\rangle$$
$$= \hat{P}\,|\alpha(t)\rangle = \hat{P}\hat{U}\,|e_1\rangle$$

Hence we conclude that

$$[\hat{P}, \hat{U}] = 0 \qquad (6)$$

Since $\hat{U} = e^{-i\hat{H}t/\hbar}$ this also implies that

$$\boxed{[\hat{P}, \hat{H}] = 0} \qquad (7)$$

this is the mathematical statement of a symmetry. A system is invariant under a certain symmetry if the operator implementing this symmetry commutes with H.

You can check that (7) is true for $\hat{H}$ and $\hat{P}$ given in (1) and (3)

General Theory

It is quite easy to generalize what we just said to arbitrary systems. For a given symmetry, we define an operator $\hat{Q}$ which implements this symmetry. This operator must be unitary to conserve probability:

$$\hat{Q}\hat{Q}^{+} = \hat{Q}^{+}\hat{Q} = 1 \qquad (8)$$

If a system is invariant by this symmetry, then $[\hat{Q}, \hat{U}] = 0$ or, what is equivalent

$$\boxed{[\hat{Q}, \hat{H}] = 0} \qquad (9)$$

Essentially, this means that "Applying $\hat{Q}$ then evolving in time" is the same as "evolving in time then applying $\hat{Q}$".

Any unitary operator may be written as

$$\hat{Q} = e^{-i\lambda\hat{G}/\hbar} \qquad (10)$$

for some parameter λ and some Hermitian operator $\hat{G}$. This $\hat{G}$ is called the generator of the symmetry $\hat{Q}$ and can usually be associated with a physical observable

For small λ, $e^{-i\lambda\hat{G}/\hbar} \approx 1 - i\frac{\lambda}{\hbar}\hat{G}$ so Eq. (9) implies

$$\boxed{[\hat{G}, \hat{H}] = 0} \qquad (11)$$

By the way, since $Q^{+}Q = 1$, Eq. (9) is also sometimes written as

$$\hat{Q}\hat{H} = \hat{H}\hat{Q}$$

or

$$\boxed{\hat{Q}^{+}\hat{H}\hat{Q} = \hat{H}} \qquad (12)$$

This is a structure we have already seen before.

Since $[\hat{G}, \hat{H}] = 0$, it follows that $[\hat{G}, \hat{U}] = 0$. Thus, if $|\alpha(t)\rangle = \hat{U}(t)\,|\alpha(0)\rangle$, we get

$$\langle\hat{G}\rangle_t = \langle\alpha(t)|\hat{G}|\alpha(t)\rangle = \langle\alpha(0)|\hat{U}^{+}\hat{G}\hat{U}|\alpha(0)\rangle$$

$$= \langle\alpha(0)|\hat{G}\hat{U}^{+}\hat{U}|\alpha(0)\rangle$$

$$= \langle\alpha(0)|\hat{G}|\alpha(0)\rangle$$

that is

$$\boxed{\langle\hat{G}\rangle_t = \langle\hat{G}\rangle_0} \qquad (13)$$

the quantity $\hat{G}$ is <u>conserved</u>. This is the link first established by Nöether

$$\boxed{\text{Symmetry} \Leftrightarrow \text{Conservation law}}$$

Degeneracies

Let

$$\hat{H}|n\rangle = E_n|n\rangle \tag{14}$$

and suppose $\hat{H}$ is invariant by a certain symmetry $\hat{Q}$. Then

$$\hat{H}\hat{Q}|n\rangle = \hat{Q}\hat{H}|n\rangle = E_n\hat{Q}|n\rangle$$

thus $\hat{Q}|n\rangle$ is also an eigenvector of $\hat{H}$ with the same eigenvalue E_n.

It may happen that $\hat{Q}|n\rangle \propto |n\rangle$. But it is also possible that this is not true. In this case we see that the level E_n will be degenerate. So a symmetry may imply a degeneracy.

Let us consider specifically the case of rotations.

$$\hat{D}(R) = e^{-i\theta\vec{n}\cdot\vec{J}} \tag{15}$$

If a system is invariant under rotations, then

$$[\hat{D}(R), \hat{H}] = 0 \tag{16}$$

This implies that

$$[\vec{J}, \hat{H}] = 0 \qquad [\hat{J}^2, \hat{H}] = 0 \tag{17}$$

Thus, $\hat{H}$, $\hat{J}^2$ and $\hat{J}_z$ may be simultaneously diagonalized:

$$\hat{H} | n, j, m \rangle = E_n | n, j, m \rangle \tag{18a}$$

$$\hat{J}^2 | n, j, m \rangle = j(j+1) | n, j, m \rangle \tag{18b}$$

$$\hat{J}_z | n, j, m \rangle = m | n, j, m \rangle \tag{18c}$$

Since $\hat{D}(R) = e^{-i\theta \vec{n} \cdot \vec{J}}$, rotations only change the values of m, not j:

$$\hat{D}(R) | n, j, m \rangle = \sum_{m'=-j}^{j} D_{mm'} | n, j, m' \rangle \tag{19}$$

Thus, if a Hamiltonian commutes with $\hat{J}^2$ and $\hat{J}_z$, the degeneracy of each energy E_n will be at least $2j+1$, since this is the total number of m values for a given j. Of course, the degeneracy may be even higher than this.

Parity (Space Inversion)

In this section $\mathbb{r} = \vec{r}$
$\mathbb{p} = \vec{p}$
$\vdots$

Parity is the symmetry which takes

$$\mathbb{r} \rightarrow -\mathbb{r}. \qquad (20)$$

It is also called a space inversion. The parity operator $\hat{\pi}$ is defined as

$$\boxed{\hat{\pi}^{+} \, \hat{\mathbb{r}} \, \hat{\pi} = -\hat{\mathbb{r}}} \qquad (21)$$

Let $|\mathbb{r}\rangle = |x, y, z\rangle$ be the position ket, defined as

$$\hat{\mathbb{r}} \, |\mathbb{r}\rangle = \mathbb{r} \, |\mathbb{r}\rangle \qquad (22)$$

From (21) and since $\pi^{+} \pi = 1$, we also have

$$\hat{\mathbb{r}} \, \hat{\pi} = - \hat{\pi} \, \hat{\mathbb{r}} \qquad (23)$$

So

$$\hat{\mathbb{r}} \, \hat{\pi} \, |\mathbb{r}\rangle = - \hat{\pi} \, \hat{\mathbb{r}} \, |\mathbb{r}\rangle = - \hat{\pi} \, \mathbb{r} \, |\mathbb{r}\rangle = - \mathbb{r} \left(\hat{\pi} \, |\mathbb{r}\rangle \right)$$

This means that $\hat{\pi} |\mathbb{r}\rangle$ is an eigenvector of $\hat{\mathbb{r}}$ with eigenvalue $-\mathbb{r}$. Hence we must have

$$\boxed{\hat{\pi} \, |\mathbb{r}\rangle = |-\mathbb{r}\rangle} \qquad (24)$$

Applying the parity operator twice we get

$$\hat{\pi}^2 |\mathbb{r}\rangle = \hat{\pi} |-\mathbb{r}\rangle = |\mathbb{r}\rangle$$

thus

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

this means that $\hat{\pi}$ is not only unitary, but also Hermitian

$$\hat{\pi}^{+} = \hat{\pi} \qquad (25)$$

we expect similar properties for $\hat{\mathbb{p}}$:

$$\hat{\pi}^{+} \hat{\mathbb{p}}\, \hat{\pi} = -\hat{\mathbb{p}} \qquad (26)$$

what about angular momentum? well

$$\hat{\mathbb{L}} = \hat{\mathbb{r}} \times \hat{\mathbb{p}}$$

so if both $\mathbb{r}$ and $\hat{\mathbb{p}}$ change sign, nothing will happen with $\hat{\mathbb{L}}$

$$\boxed{\hat{\pi}^{+} \hat{\mathbb{L}}\, \hat{\pi} = \hat{\mathbb{L}}} \qquad (27$$

So $\hat{\mathbb{r}}$ and $\hat{\mathbb{p}}$ change sign under inversion. We say they are odd under parity, or that they are polar vectors. $\hat{\mathbb{L}}$, on the other hand, does not change sign, so it is even under parity, or we call it an axial vector.

What about dot products, such as $\hat{\mathbb{r}} \cdot \hat{\mathbb{p}}$ or $\mathbb{r} \cdot \hat{\mathbb{L}}$? We know that these are all invariant under rotations. But note that

$$\hat{\pi}^{\dagger} (\hat{\mathbb{r}} \cdot \hat{\mathbb{p}}) \hat{\pi} = (\hat{\mathbb{r}} \cdot \hat{\mathbb{p}}) \qquad (28)$$

since both $\hat{\mathbb{r}}$ and $\hat{\mathbb{p}}$ change sign. However

$$\hat{\pi}^{\dagger} (\hat{\mathbb{r}} \cdot \hat{\mathbb{L}}) \hat{\pi} = - (\hat{\mathbb{r}} \cdot \hat{\mathbb{L}}) \qquad (29)$$

The first type we call scalars and the second type we call pseudo-scalars. Note that everything I said is also true for classical vectors.

Before 1950 people believed that parity was conserved for all physical systems. In 1956 Lee and Yang proposed that parity conservation should be violated for weak interactions (which are usually involved in β decays). The reason is that the weak interaction contains a term $\vec{S} \cdot \vec{p}$ which, according to (29), is not invariant under parity. This was confirmed experimentally a year later by Wu and collaborators.

thus, electromagnetic, gravitational and nuclear interaction,

$$[\hat{\pi}, \hat{H}] = 0 \tag{30}$$

For the weak interaction

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