Lecture 9 The symmetry principle (Ⅲ)

Modified symmetry principle —

If the cause has a certain symmetry, but the results are not unique, then the set of the results must exhibit such a symmetry.

- Degeneracies of atomic orbitals
- Quantum mechanics is built on complex number field.
- gauge transformation
- spontaneous symmetry breaking — More is different!

§: When the results are not unique, how to use the symmetry principle?

① Newton's equation $\ddot{x} = -g$ — time translation invariant

$$\dot{x} = -gt + v_0 \rightarrow x = -\frac{1}{2}gt^2 + v_0 t + x_0$$

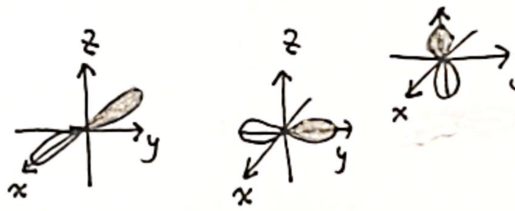
For a particular solution, $x(t)$ is not invariant under $t \rightarrow t - t_0$,

time-translation invariance: if $x(t)$ is a solution, then $x(t-t_0)$ is also a solution: → Shift the initial time.

time-reversal sym: if $x(t)$ is a solution, then $x(-t)$ is also a solution.

② Atomic orbital (Rotational symmetry + isotropic potential

- s-orbital (non-degenerate)
- p-orbital, (3-fold) P_x, P_y, P_z
- d-orbital (5-fold) $d_{x^2-y^2}$ $d_{r^2-3z^2}$ d_{xy} d_{yz} d_{xz}



3d rotations: 3×3 orthogonal matrices $O^T O = 1$, $\det O = 1$.

group G: $O_1 \in G$, $O_2 \in G$, then $O = O_1 O_2 \in G$.

if $O \in G$, there exist O^{-1}, $OO^{-1} = O^{-1}O = E$.

the existance of the identity E.

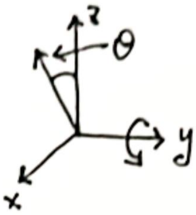
$$O_z(\theta) = \begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad O_x(\theta) = \begin{pmatrix} 1 & & \\ & \cos\theta & -\sin\theta \\ & \sin\theta & \cos\theta \end{pmatrix}, \quad O_y(\theta) = \begin{pmatrix} \cos\theta & 0 & \sin\theta \\ 0 & 1 & 0 \\ -\sin\theta & 0 & \cos\theta \end{pmatrix}$$

③

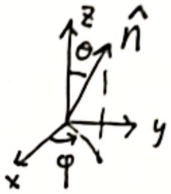
$|P_z\rangle \begin{pmatrix}0\\0\\1\end{pmatrix}$, $|P_x\rangle \begin{pmatrix}1\\0\\0\end{pmatrix}$, $|P_y\rangle \begin{pmatrix}0\\1\\0\end{pmatrix}$. Assume P_z is a solution of atomic orbital, but P_z itself does not exist sphericc sym.

Hence, the spherical symmetry should manifest in the set of solutions.

Apply $O_y |P_z\rangle = \begin{pmatrix}\cos\theta & & \sin\theta\\ & 1 & \\ -\sin\theta & & \cos\theta\end{pmatrix}\begin{pmatrix}0\\0\\1\end{pmatrix} = \begin{pmatrix}\sin\theta\\0\\\cos\theta\end{pmatrix}$



Hence, $\sin\theta|P_x\rangle + \cos\theta|P_z\rangle$ is also a solution.



More generally, any $\hat{n}\cdot|\vec{P}\rangle = n_x P_x + n_y P_y + n_z P_z$ can be rotated from $|P_z\rangle$.

Then we arrive at a linear space of superpositions of $|P_x\rangle, |P_y\rangle, |P_z\rangle$.

They span a multi-dimensional space — representation of SO_3 group.

(irreducible. Rep: means that the space cannot be smaller, otherwise. a state after rotation could be outise that space).

In fact, the linear space for Quantum mechanics is built based on Complex number field, not on real numbers. There also exists $(|P_x\rangle \pm i|P_y\rangle)/\sqrt{2}$. Such a state cannot be obtained from rotating $|P_z\rangle$.

a state of

Later, we see $O_z(\theta)\frac{1}{\sqrt{2}}\begin{pmatrix}1\\\pm i\\0\end{pmatrix} = e^{\pm i\theta}\begin{pmatrix}1\\\pm i\\0\end{pmatrix}/\sqrt{2}$, $O_z(\theta)\begin{pmatrix}0\\0\\1\end{pmatrix} = \begin{pmatrix}0\\0\\1\end{pmatrix}$.

eigenstates

eigenvalues

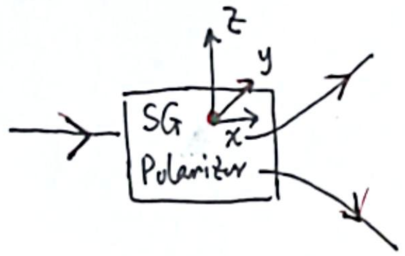
The degeneracy among $|P_x\rangle, |P_y\rangle, |P_z\rangle$ can be reached simply by SO(3) rotation. Nevertheless, the degeneracy among $\frac{|P_x\rangle \pm i|P_y\rangle}{\sqrt{2}}$, $|P_z\rangle$ is due to the linear superposition, and the fact that QM is built based on the complex number field.

③ Why should QM be based on complex number not on real number?

Stern-Gerlach experiment: Silver beam splits into 2 branches.

Polarizer along z: $\sigma_z = \begin{pmatrix} 1 & \\ & -1 \end{pmatrix} \rightarrow$ spin $|\uparrow\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$, spin $|\downarrow\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$.

According to the spherical symmetry, we should be able to get splitting along x, and y-axis.



If we only allow real number, then only $\sigma_z = \begin{pmatrix} 1 & \\ & -1 \end{pmatrix}$ and $\sigma_x = \begin{pmatrix} & 1 \\ 1 & \end{pmatrix}$ exist. spin $|+x\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$

spin $|-x\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}$.

But how to arrive at splitting along y-axis?

we need $\sigma_y = \begin{pmatrix} & -i \\ i & \end{pmatrix} \Rightarrow$ spin $|+y\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ i \end{pmatrix}$

$|-y\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -i \end{pmatrix}$

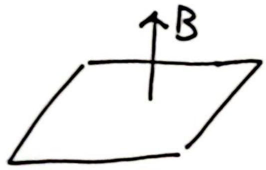
(If only real number are allowed, then the isotropy of space will be broken!)

· Gauge transformation

Even though there exists a symmetry, the Hamiltonian itself may not exhibit such a symmetry explicitly. Then there should exist a set of equivalent Hamiltonians...

For example, how to express Hamiltonian for a uniform B-field

$$\nabla \times \vec{A} = B\hat{z}$$



One choice is that $A_x = By$, $A_y = 0$, then

$$H = \frac{(P_x - \frac{e}{c}A_x)^2}{2m} + \frac{(P_y - \frac{e}{c}A_y)^2}{2m} = \frac{(P_x - \frac{e}{c}By)^2}{2m} + \frac{P_y^2}{2m}$$

H itself is not translationally invariant!

If we translate $\vec{A}(r) \to \vec{A}'(r) = \vec{A}(\vec{r} + \delta\vec{r})$, then $\nabla \times \vec{A}'(r) = \nabla \times \vec{A}(r)$,

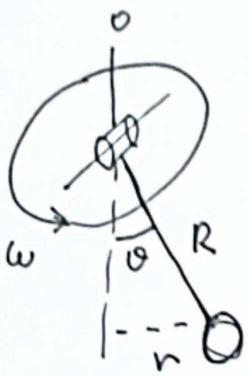
hence $\vec{A}'(r)$ and $\vec{A}(r)$ are equally good. We express

$$\begin{cases} \vec{A}'(r) = \vec{A}(r) + \nabla\varphi(r) \\ \psi'(r) = e^{i\phi(r)}\psi(r) \end{cases} \Rightarrow \begin{aligned} &(P_x - \tfrac{e}{c}A'(x))\psi'(x) \\ &= (P_x - \tfrac{e}{c}A_x - \tfrac{e}{c}\nabla\varphi)\psi(r)e^{i\phi(r)} \\ &= e^{i\phi(r)}(P_x - \tfrac{e}{c}A_x + \hbar\nabla\phi - \tfrac{e}{c}\nabla\varphi)\psi(r) \end{aligned}$$

set $\phi = \frac{e}{\hbar c}\varphi(r)$

$$\Rightarrow \begin{cases} H\psi(r) = E\psi(r) \\ H'\psi'(r) = E\psi'(r) \end{cases}$$

§ spontaneous symmetry breaking



$$\mathcal{U}(\theta) = -\frac{1}{2} m \omega^2 r^2 + mgR(1-\cos\theta)$$

$$r^2 = R^2 \sin^2\theta = \frac{(1-\cos 2\theta)}{2} R^2$$

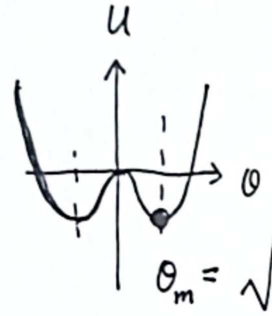
$$\mathcal{U}(\theta) = -\tfrac{1}{4} m \omega^2 R^2 (1-\cos 2\theta) + mgR(1-\cos\theta)$$

$$1-\cos\theta = \frac{\theta^2}{2!} - \frac{\theta^4}{4!}$$

$$1-\cos 2\theta = \frac{(2\theta)^2}{2!} - \frac{(2\theta)^4}{4!} = 2\theta^2 - \frac{4}{3}\theta^4$$

$$\Rightarrow \mathcal{U}(\theta) \simeq \frac{mR^2}{2}\left[(\omega_*^2 - \omega^2)\theta^2 + (\omega^2 - \frac{\omega_*^2}{4})\theta^4\right]$$

with $\omega_* = \sqrt{g/R}$



$$\theta_m = \sqrt{\frac{2(\omega^2-\omega_*^2)}{4\omega^2-\omega_*^2}}$$

two minimal

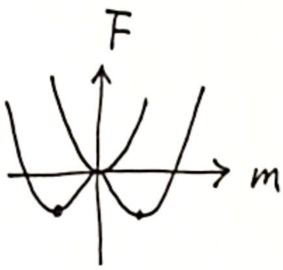
→ Mechnically the pendulum is trapped at one of them.

Landau theory of phase transitions:

order parameter - say, magnetization for a magnetic system $m(r)$

time-reversal symmetry $m(r)$ and $-m(r)$ are equivalent.

Energy (free energy)



$$F[m] = \alpha(T)\, m^2 + \frac{\beta}{4} m^4$$

$\alpha(T) < 0$ at $T < T_c$

$\alpha(T) > 0$ at $T > T_c$

At $T > 0T_c$, $\nwarrow \nearrow \swarrow \downarrow \uparrow \nearrow \searrow \nearrow$

$T < T_c$ $\uparrow\uparrow\uparrow\nwarrow\nearrow\uparrow\uparrow$

or $\downarrow\searrow\swarrow\downarrow\downarrow\downarrow\swarrow$

tunneling barrier ~~is~~ goes to infinity, and ergodicity is broken!