Summary of lecture one

•) Ehrenfest theorem

$$\frac{d}{dt}\langle\hat{F}\rangle = -\frac{i}{\hbar}\langle[\hat{F},\hat{H}]\rangle + \left\langle\frac{\partial\hat{F}}{\partial t}\right\rangle$$

$\hat{F}$ – observable operator

Conservation law in QM: $\boxed{\frac{d}{dt}\langle\hat{F}\rangle = 0} \rightarrow \boxed{\langle\hat{F}\rangle = \text{const.}}$

It happens when $\frac{\partial\hat{F}}{\partial t} = 0$ (no explicit time dependence)

and if

$$\boxed{[\hat{F},\hat{H}] = 0}$$

$\hat{F}$ and $\hat{H}$ have the same set of eigenstates.
In this basis both operators are diagonal.

•) Symmetry transformation

$$\Psi(\vec{r},t) \xrightarrow[\vec{r}\to\vec{r}_T = \hat{G}\vec{r}]{} \Psi_T(\vec{r},t) = \hat{U}\,\Psi(\vec{r},t)$$

$\hat{U}$ – symmetry operator

such that

$$|\Psi_T(\vec{r},t)|^2 = (\hat{U}\Psi(\vec{r},t))^+(\hat{U}\Psi(\vec{r},t)) =$$

$$= \Psi^*(\vec{r},t)\underbrace{\hat{U}^+\hat{U}}_{\mathbb{1}}\Psi(\vec{r},t) = |\Psi(\vec{r},t)|^2$$

conservation of probability density

$$\Rightarrow \boxed{\hat{U}^+\hat{U} = \mathbb{1}} \longleftrightarrow \boxed{\hat{U}^+ = \hat{U}^{-1}}$$

Symmetry operator is unitary

$\Psi(\vec{r},t)$ and $\Psi_T(\vec{r},t)$ should obey the same Schrödinger equation

$$\boxed{\hat{H}\,\Psi_T(\vec{r},t) = i\hbar\frac{\partial}{\partial t}\Psi_T(\vec{r},t)}$$

$$\underbrace{\hat{H}\,\hat{U}\,\Psi(\vec{r},t)} = i\hbar\frac{\partial}{\partial t}\hat{U}\,\Psi(\vec{r},t) =$$

$$= i\hbar\left(\frac{\partial\hat{U}}{\partial t}\right)\Psi(\vec{r},t) + \underbrace{i\hbar\,\hat{U}\,\frac{\partial\Psi(\vec{r},t)}{\partial t}}_{\underbrace{\hat{U}\hat{H}\,\Psi(\vec{r},t)}}$$

since

$$i\hbar\frac{\partial\Psi}{\partial t} = \hat{H}\,\Psi$$

Therefore,

$$[\hat{H},\hat{U}]\,\Psi(\vec{r},t) = i\hbar\left(\frac{\partial\hat{U}}{\partial t}\right)\Psi(\vec{r},t) \quad \forall\,\Psi(\vec{r},t)$$

$$\Rightarrow \qquad [\hat{H},\hat{U}] = i\hbar\left(\frac{\partial\hat{U}}{\partial t}\right)$$

In particular, if symmetry transformation does not depend explicitly on time

$$\boxed{[\hat{H},\hat{U}] = 0}$$

$\hat{U}$ - is conserved in time, but $\hat{U}$ is not observable (not Hermitian)

However, if we write

$$\boxed{\hat{U} = e^{ia\hat{F}}} \quad \text{with} \quad \underbrace{\hat{F}^{+} = \hat{F}}_{\hookrightarrow \text{ observable}}, \quad a \in \mathbb{R}$$

$$\hat{U}^{+} = e^{-ia\hat{F}} \quad \Rightarrow \quad \hat{U}^{+}\hat{U} = \mathbb{1}$$

$\hat{F}$ – generator of the symmetry transformation

Theorem:

$$[\hat{U}, \hat{H}] = 0 \quad \Rightarrow \quad \boxed{[\hat{F}, \hat{H}] = 0} \Rightarrow \boxed{\hat{F} \text{ – conserved observable}}$$

proof: $[\hat{U}, \hat{H}] = [e^{ia\hat{F}}, \hat{H}] = \sum_{n=0}^{\infty} \frac{(ia)^n}{n!} [\hat{F}^n, \hat{H}] =$

$$= \sum_{n=0}^{\infty} \frac{(ia)^n}{n!} \Big(\hat{F}^{n-1} \underbrace{[\hat{F}, \hat{H}]}_{= 0} + [\hat{F}^{n-1}, \hat{H}] \hat{F} \Big) = \dots = 0$$

by induction

□

•) Infinitesimal symmetry transformations

$$\hat{U}(a) |\psi\rangle = |\psi\rangle + a \frac{1}{i\hbar} \hat{F} |\psi\rangle + O(a^2)$$

where $\hat{F} |\psi\rangle = \lim_{a \to 0} \frac{i\hbar}{a} (\hat{U}(a) - 1)$

since $\hat{U}^{+}\hat{U} = \mathbb{1}$ and $\hat{U}(a) = \mathbb{1} + \frac{a}{i\hbar}\hat{F} + O(a^2)$

we get $\hat{F}^{+} = \hat{F}$

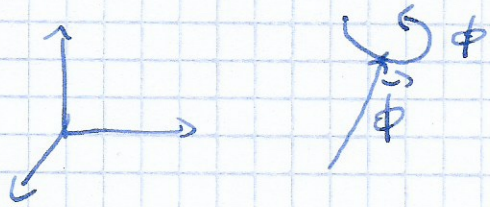
and

$$\boxed{\hat{U}(a) = e^{i\frac{a}{\hbar}\hat{F}}}$$

Lecture two

Rotations

Consider a rotation in space by an infinitesimal angle $\delta\vec{\Phi}$, around the axis defined by $\delta\vec{\Phi}$



$|\delta\bar{\Phi}| \ll 1$

this gives $\bar{r} \to \bar{r}_T = \bar{r} + \delta\bar{\Phi} \times \bar{r}$

symmetry transformation:

$$\psi_T(\bar{r}_T) = \psi(\bar{r}) \Leftrightarrow \psi_T(\bar{r}) = \psi(\bar{r} - \delta\bar{\Phi} \times \bar{r})$$

$$\psi_T(\bar{r}) \simeq \psi(\bar{r}) - (\delta\bar{\Phi} \times \bar{r}) \cdot \bar{\nabla}\psi(\bar{r}) + O(\delta\Phi^2) =$$

$$= \psi(\bar{r}) - \delta\bar{\Phi} \cdot (\bar{r} \times \bar{\nabla})\psi(\bar{r}) + \dots =$$

$$= \left(1 - \frac{i}{\hbar}\delta\bar{\Phi} \cdot (\bar{r} \times \hat{\bar{p}}) + \dots\right)\psi(\bar{r}) =$$

$$= \left(1 - \frac{i}{\hbar}\delta\bar{\Phi} \cdot \hat{\bar{L}} + \dots\right)\psi(\bar{r}) =$$

$$= e^{-\frac{i}{\hbar}\delta\bar{\Phi} \cdot \hat{\bar{L}}}\psi(\bar{r})$$

we get

$$\boxed{\hat{U}_R(\bar{\Phi}) = e^{-\frac{i}{\hbar}\bar{\Phi} \cdot \hat{\bar{L}}}}$$

$\hat{\bar{L}}$ – operator of angular momentum.

If $\hat{H}$ is invariant under rotation

$$[\hat{U}_R(\bar{\Phi}), \hat{H}] = 0$$

then $\boxed{[\hat{\bar{L}}, \hat{H}] = 0}$

13

conservation of angular momentum law

homogeneity of space $\longrightarrow$ momentum conservation

homogeneity of time $\longrightarrow$ energy conservation

isotropy of space $\longrightarrow$ angular momentum conservation

§3. Symmetries and degeneracy

If $\hat{H}|n\rangle = E_n|n\rangle$ and $\hat{H}|\tilde{n}\rangle = E_{\tilde{n}}|\tilde{n}\rangle$ and $|n\rangle$ and $|\tilde{n}\rangle$ are linearly independent we say that $E_n = E_{\tilde{n}}$ is <u>degenerate</u>.

Let $\hat{U}$ - is a symmetry operator

<u>Fact</u>: $\hat{U}|n\rangle$ is also energy eigenstate with the same E_n.

<u>proof</u>

$$\hat{H}\underbrace{\hat{U}|n\rangle}_{|n\rangle_T} \overset{[\hat{H},\hat{U}]=0}{=} \hat{U}\hat{H}|n\rangle = \hat{U}E_n|n\rangle = E_n\underbrace{\hat{U}|n\rangle}_{|n\rangle_T}$$

In the case where $|n\rangle_T$ is not linearly dependent on $|n\rangle$ the energy spectrum is degenerate.

$\square$

Degeneracy is a consequence of symmetry (*)

(*) not include accidential degeneracy.

§4. Parity (inversion) symmetry

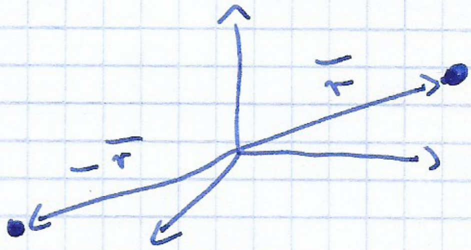
$\boxed{\text{discrete symmetries}}$

- parity $\quad \bar r \to -\bar r \quad$ P
- time reversal $\quad t \to -t \quad$ T
- charge $\quad \rho \to -\rho \quad$ C

Consider parity transformation

$$\bar r \to \bar r_T = -\bar r$$

$$\begin{pmatrix} x \\ y \\ z \end{pmatrix} \to \begin{pmatrix} x_T \\ y_T \\ z_T \end{pmatrix} = \begin{pmatrix} -x \\ -y \\ -z \end{pmatrix}$$



we use notation $\boxed{\hat U = \hat \Pi}$

If $\hat\Pi$ is symmetry operation $\boxed{[\hat H, \hat \Pi] = 0}$

Fact: $|\psi\rangle$ and $\hat\Pi|\psi\rangle$ have the same eigenenergy

proof:

$$\hat H |\psi\rangle = E|\psi\rangle \quad / \hat\Pi$$

$$\hat\Pi \hat H|\psi\rangle = \hat H \underbrace{\hat\Pi|\psi\rangle}_{|\psi\rangle_T} = E \underbrace{\hat\Pi|\psi\rangle}_{|\psi\rangle_T}$$

$\square$

Eigenvalues of $\hat\Pi$?

$$\hat\Pi|\psi\rangle = \pi|\psi\rangle \quad / \hat\Pi^2$$

$$\hat\Pi^2|\psi\rangle = \hat\Pi\pi|\psi\rangle = \pi\hat\Pi|\psi\rangle = \pi^2|\psi\rangle$$

but $\hat\Pi^2 = \mathbb{1} \Rightarrow \pi^2 = 1 \Rightarrow \boxed{\pi = \pm 1}$

$$\boxed{\hat{\Pi}\,\psi(r) = \begin{cases} \psi(\bar{r}) & \text{- even function} \\ -\psi(\bar{r}) & \text{- odd function} \end{cases}}$$

Remember: for vectors

$$\bar{A} \xrightarrow{\hat{\Pi}} \bar{A}_T = -\bar{A} \quad \text{- polar vectors}$$

$$\bar{A} \xrightarrow{\hat{\Pi}} \bar{A}_T = \bar{A} \quad \text{- axial vectors}$$

(pseudovectors)

Examples $\bar{r}$, $\bar{p}$, $\bar{E}$ – polar vectors

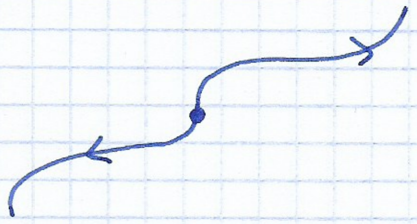
$\bar{L} = \bar{r} \times \bar{p}$, $\bar{M} = \bar{r} \times \bar{F}$, $\bar{B}$ – axial vectors

torque

§5. Time reversal symmetry (TRS)

$$\boxed{t \to t_T = -t}$$

In classical mechanics equation of motion is TRS. It is impossible to distinguish forward or backward time moving



$$\bar{r} \to \bar{r}_T = \bar{r}$$

$$\bar{p} \to \bar{p}_T = -\bar{p} \qquad \bar{p} = m\frac{d\bar{r}}{dt}$$

$$\dot{\bar{r}}_T(t) = \frac{d\bar{r}_T(t)}{dt} = \frac{d\bar{r}(-t)}{dt} = -\frac{d\bar{r}(-t)}{d(-t)} =$$

$$= -\dot{\bar{r}}(-t)$$

$$\bar{F} \to \bar{F}_T = \bar{F}$$

$$\bar{a}_T(t) = \ddot{\bar{r}}_T(t) = \ddot{\bar{r}}(-t) =$$

$$= \bar{a}(-t)$$

$$\bar{E} \to \bar{E}_T = \bar{E} \qquad \bar{F} = q\bar{E}$$

$$\bar{B} \to \bar{B}_T = -\bar{B} \qquad \bar{F} = q\bar{v} \times \bar{B}$$

How about TRS in quantum mechanics?

$$-\frac{\hbar^2}{2m}\nabla^2\Psi(\vec{r},t)+V(\vec{r})\Psi(\vec{r},t)=i\hbar\frac{\partial\Psi(\vec{r},t)}{\partial t}$$

$$\Updownarrow \qquad t \Rightarrow t_T=-t$$

$$-\frac{\hbar^2}{2m}\nabla^2\Psi(\vec{r},t)+V(\vec{r})\Psi(\vec{r},-t)=-i\hbar\frac{\partial\Psi(\vec{r},-t)}{\partial t}$$

Formally, this is the same equation if we take the <u>complex conjugation</u>

$$-\frac{\hbar^2}{2m}\nabla^2\Psi^*(\vec{r},t)+V(\vec{r})\Psi^*(r,-t)=i\hbar\frac{\partial\Psi^*(\vec{r},-t)}{\partial t}$$

Therefore, if TRS is demanded we find that

$$\Psi(\vec{r},t)\longrightarrow\Psi^*(\vec{r},-t)$$

Let $\hat{u}=\hat{\Theta}$ for TR symmetry operator

$$\boxed{\hat{\Theta}\,\Psi(\vec{r},t)=\Psi^*(\vec{r},-t)}$$

<u>Fact</u>: $\hat{\Theta}$ is <u>antilinear</u> (antiunitary) operator.
(<u>impossible</u> to formulate a unique eigenvalue problem).

<u>proof</u>:

$$\hat{\Theta}\left(c_1\Psi_1(t)+c_2\Psi_2(t)\right)=$$
$$=c_1^*\Psi_1^*(-t)+c_2^*\Psi_2^*(-t)=$$
$$=c_1^*\left(\hat{\Theta}\Psi_1(t)\right)+c_2^*\left(\hat{\Theta}\Psi_2(t)\right)\qquad\square$$

<u>Note</u>: $\langle\hat{\Theta}\phi|\hat{\Theta}\Psi\rangle=\langle\Psi|\phi\rangle=\langle\phi|\Psi\rangle^*$

only $|\langle\Psi|\phi\rangle|$ is conserved!