⇒ lecture 5-6 * Formalism of quantum mechanics* L.A.O

– Postulate 0 –

Let f be a physical quantity

"If in the system prepared in the state $\psi_1(q)$ the measurement of f gives ALWAYS f_1, and in the system prepared in $\psi_2(q)$ the measurement of f ALWAYS gives f_2, then any linear combination

$$\psi(q) = c_1 \psi_1(q) + c_2 \psi_2(q)$$

represents a state for which the measurement of f gives EITHER f_1 OR f_2."

– This is called:

Principle of superposition of the states

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* Operators *

— Postulate I —

f is a physical quantity

The value that can assume are either discrete $f_1, f_2, \to f_n$

or continuous $f(k)$. Consider discrete first

Let $\Psi_n(q)$ the wave function of the system when f has

the value f. Then there exist an operator $\hat{f}$ associated

to f such that:

$$\hat{f}\Psi_n(q) = f_n \Psi_n(q)$$

if $\lambda \in \mathbb{C}$ we can always write.

$$\lambda(\hat{f}\Psi_n(q)) = \lambda(f_n \Psi_n(q))$$

$$\Leftrightarrow \quad \hat{f}\tilde{\Psi}_n(q) = \tilde{\Psi}_n(q) \qquad \text{where } \tilde{\Psi}_n = \lambda \Psi_n$$

$\Rightarrow$ We can always chose λ such that:

$$\int |\Psi_n|^2 dq = 1$$

— Postulate II —

If the system is prepared in the state represented by $\Psi(q)$

then a measurement of f yields the value f_n and

leave the system in the state Ψ_n.

$$\Psi(q) \xrightarrow[f=f_n]{\text{measurement of } f} \Psi_n(q)$$

This implies that there is a non-zero probability to find the system prepared in the state Ψ, in the state Ψ_n

This automatically means that $\psi(q)$ can be written as a linear combination of ψ_n:

$$\psi = \sum_n a_n \psi_n$$

and when a measurement of f is made and f_m found, then

$$a_n \to 0 \text{ unless } n=k$$

If such lin. comb. is possible, the system of

$$\{\psi_1, \psi_2, \dots, \psi_n, \dots\} \text{ is said COMPLETE}$$

From $\psi = \sum_n a_n \psi_n$ we can find the probability to obtain f_m from a measurement of f.

— Postulate III —

If a system is in the state $\Psi(q,t)$, the average value of f at time t is:

$$\langle f \rangle_\psi = \int \psi^* (\hat{f} \psi)\, dq$$

$\langle f \rangle_\psi$ = expectation value

By def, if $\psi = \psi_n$ then

$$\langle f \rangle_{\psi_n} = \int \psi_n^* \underbrace{(\hat{f} \psi_n)}_{= f_n \psi_n} dq$$

$$= f_n \int \psi_n^* \psi_n \, dq = f_n$$

However, from the def of probability

$$\langle f \rangle_\psi = \sum_n f_n P(f_n)$$

where $P(f_n)$ = probability to obtain f_n from a measurement of f in the system prepared in ψ

By comparison

$$\langle f \rangle_\psi = \sum_n f_n P(f_n) = \int \psi^* (\hat{f} \psi)\, dq$$

use $\psi = \sum_m a_m \psi_m$ to rewrite:

$$\sum_n f_n P(f_n) = \sum_{k,l} a_k^* a_l \int \psi_k^* (\hat{f} \psi_l)\, dq$$

$$= \sum_{k,l} a_k^* a_l f_l \int \psi_k^* \psi_l \, dq$$

$$\equiv \sum_l f_l \left[\sum_k a_k^* a_l \int \psi_k^* \psi_l \, dq \right]$$

Therefore, we would identify:

$$P(f_n) = \sum_k a_k^* a_n \int \psi_k^* \psi_n \, dq \geq 0$$

For ARBITRARY ψ, this is possible only if:

$$\int \psi_k^* \psi_n \, dq = \delta_{kn}$$

or $\lambda \delta_{kn}$, λ get fixed by normalization $\Rightarrow \lambda > 0$

ORTHOGONality

$$\Rightarrow P(f_n) = \sum_k a_k^* a_n \delta_{kn} = |a_n|^2 \geq 0$$

So:

$$\boxed{\langle f \rangle_\psi = \sum_n f_n |a_n|^2}$$

· From

$$\int \psi^* \psi = 1$$

it follows

$$\sum_{n,m} a_n^* a_m \underbrace{\int \psi_n^* \psi_m \, dq}_{= \delta_{nm}} = 1$$

$$\Leftrightarrow \qquad \sum_n |a_n|^2 = 1 \quad \Leftrightarrow \text{ sum of probability } = 1 \ \checkmark$$

- How to find a_n?

From $\psi = \sum_n a_n \psi_n \xrightarrow{\text{Take the conj}} \psi^* = \sum_n a_n^* \psi_n^*$

then $\int |\psi|^2 dq = \sum_n a_n^* \int \psi \psi_n^* dq$

on the other hand $\int |\psi|^2 dq = \sum_n a_n^* a_n = 1 \Rightarrow$

$$\Rightarrow \boxed{a_n = \int \psi_n^* \psi \, dq}$$

if this is a scalar product, then

$$a_n = \langle \psi_n | \psi \rangle$$

- The completeness relation can be written as

$\psi(q) = \sum_n a_n \psi_n(q)$ but $a_n = \int \psi_n^*(q') \psi(q') dq' \Rightarrow$

$$\Rightarrow \psi(q) = \sum_n \int \psi_n^*(q') \psi(q') dq' \, \psi_n(q) = \int dq' \left[\sum_n \psi_n(q) \psi_n^*(q') \right] \psi(q') dq'$$

However, by def: $\psi(q) = \int \delta(q-q') \psi(q') dq' \quad \forall \psi \Rightarrow$

$$\Rightarrow \boxed{\sum_n \psi_n(q) \psi_n^*(q') = \delta(q-q')} \leftarrow \text{closure}$$

Notice, this can be written as:

$$\sum_n |\psi_n\rangle\langle\psi_n| = \hat{I}$$

Then

$$|\psi\rangle = \hat{I}|\psi\rangle$$

$$= \sum_n |\psi_n\rangle\langle\psi_n|\psi\rangle = \sum_n a_n |\psi_n\rangle$$

$$a_n = \langle\psi_n|\psi\rangle = \int \psi_n^*(q)\,\psi(q)\,dq$$

— CONSEQUENCES OF THE POSTULATES —

— An operator $\hat{f}$ has always a linear integral representation —

let

$$\hat{f}\psi = \sum_n a_n \hat{f}\psi_n$$

$$= \sum_n a_n f_n \psi_n$$

but $a_n = \int \psi_n^* \psi\, dq \Rightarrow \sum_n a_n f_n \psi_n(q) = \sum_n \int \psi_n^*(q')\psi(q')\,dq' f_n \psi_n(q)$

$$= \int \left[\sum_n f_n \psi_n^*(q')\psi_n(q)\right]\psi(q')\,dq'$$

$$\Leftrightarrow \quad (\hat{f}\psi)(q) = \int K(q,q')\,\psi(q')\,dq'$$

where

$$\boxed{K(q,q') = \sum_n f_n \psi_n^*(q')\psi_n(q)}$$

↑
Kernel of the operator

$$\boxed{K(q,q') = \sum_n f_n \psi_n(q)\,\psi_n^*(q')}$$

- Hermitian operators -

For a physical quantity it must be

$$\langle f \rangle_\psi \in \mathbb{R} \quad \forall \psi$$

So $\langle f \rangle_\psi = \int \psi^* (\hat{f} \psi) dq = (\langle f \rangle_\psi)^* = \int \psi (\hat{f} \psi)^* dq$

$$\equiv \int \psi (\hat{f}^* \psi^*) dq \qquad 1$$

def of conjugate operator

Def of conj. op:
if $(\hat{f}\psi) = \varphi$ then $\hat{f}^* : (\hat{f}^* \psi^*) = \varphi^*$

Now, the TRANPOSE of an operator $\hat{f}^T$ is defined as:

$$\hat{f}^T \equiv \int \phi(q) (\hat{f} \psi)(q) dq \equiv \int \psi(q) (\hat{f}^T \phi)(q) dq$$

$\forall \psi, \phi$

If in this def I take $\phi = \psi^* \Rightarrow$

$$\Rightarrow \langle f \rangle_\psi = \int \psi^* (\hat{f} \psi) dq = \int \psi (\hat{f}^T \psi^*) dq \qquad 2$$

Comparison of 1 and 2 show that it must be

$$\int \psi (\hat{f}^T \psi^*) dq = \int \psi (\hat{f}^* \psi^*) dq \Rightarrow$$

$$\Rightarrow \boxed{\hat{f}^T = \hat{f}^*} \quad \text{for an observable}$$

Taking the conjugate of both

$$(\hat{f}^T)^* = \hat{f}$$

<u>Def</u>: $$\hat{f}^{+} \equiv (\hat{f}^{T})^{*} = (\hat{f}^{*})^{T}$$

on if $\hat{f} = \hat{f}^{+} \Leftrightarrow \hat{f}$ is Hermitean

– Example –

From $$(\hat{f}\psi)(q) = \int K(q,q')\,\psi(q')\,dq'$$

it follows

$$\langle f\rangle_{\psi} = \int \psi^{*}(\hat{f}\psi)\,dq$$

$$= \int \psi^{*}(q)\,K(q,q')\,\psi(q')\,dq\,dq' = (\langle f\rangle_{\psi})^{*}$$

$$= \int \psi(q)\,K^{*}(q,q')\,\psi^{*}(q')\,dq\,dq' \qquad \text{swap } q \to q'$$

$$= \int \psi(q')\,K^{*}(q',q)\,\psi^{*}(q)\,dq\,dq'$$

$$= \int \psi^{*}(q)\,K^{*}(q',q)\,\psi(q')\,dq\,dq'$$

they are equal iff:

$$K(q,q') = K^{*}(q',q)$$

If $$K(q,q') = \sum_n f_n \psi_n^{*}(q')\,\psi_n(q) \Rightarrow K^{*}(q',q) = \sum_n f_n^{*}\,\psi_n(q)\,\psi_n^{*}(q')$$

$$\Rightarrow \boxed{f_n = f_n^{*}} \Rightarrow$$

$\Rightarrow$ The eigenvalues of an Hermitean operator are <u>real</u>!

- The eigen function of an Hermitian operator corresponding to different eigenvalues are orthogonal.

- Dim:

Let $\hat{f}\psi_n = f_n \psi_n$ and $\hat{f}\psi_m = f_m \psi_m \Rightarrow \hat{f}^* \psi_m^* = f_m \psi_m^*$

Then $\psi_m^* \hat{f} \psi_n = f_n \psi_m^* \psi_n$ subtract:

$\psi_n \hat{f}^* \psi_m^* = f_m \psi_n \psi_m^*$

$$\psi_m^* \hat{f} \psi_n - \psi_n \hat{f}^* \psi_m^* = (f_n - f_m)\psi_m^* \psi_n$$

Integrate both sides:

$$\int [\psi_m^* (\hat{f}\psi_n) - \underbrace{\psi_n(\hat{f}^* \psi_m^*)}] dq = (f_n - f_m)\int \psi_m^* \psi_n dq$$

$$= \int \psi_n (\hat{f}^T \psi_m^*) dq = \int \psi_m^* (\hat{f}\psi_n) dq \quad \text{by def}$$

Therefore

$$(f_n - f_m)\int \psi_n \psi_m^* dq = 0$$

if $f_n - f_m \neq 0 \Rightarrow \boxed{\int \psi_m^* \psi_n dq = 0}$

- If two operators $\hat{f}$ and $\hat{g}$ corresponding to the physical quantities f and g have the same eigenfunctions, then they commute: $[\hat{f}, \hat{g}] = 0$ -

Proof: $\hat{f}\psi_n = f_n \psi_n \qquad \hat{g}\psi_n = g_n \psi_n$

let $\psi = \sum_n a_n \psi_n$

then
$$
\begin{aligned}
(\hat{f}\hat{g})\psi &= \hat{f}(\hat{g}\psi) \\
&= \hat{f} \sum_n a_n (\hat{g}\psi_n) \\
&= \hat{f} \sum_n a_n g_n \psi_n \\
&= \sum_n a_n g_n (\hat{f}\psi_n) = \sum_n a_n g_n f_n \psi_n
\end{aligned}
$$

Similarly $(\hat{g}\hat{f})\psi = \sum_n a_n g_n f_n \psi_n \Rightarrow$

$$\Rightarrow (\hat{f}\hat{g} - \hat{g}\hat{f})\psi = 0 \;\; \forall \psi \Rightarrow [\hat{f}, \hat{g}] = 0$$

- The converse is also true - Later demonstration

- Function of operators -

let $\hat{f}\psi_n = f_n \psi_n$

Then, formally, $\varphi(\hat{f}) = \varphi(0) + \varphi'(0)\hat{f} + \frac{\varphi''(0)}{2!}\hat{f}^2 + \dots$

$$\Rightarrow \varphi(\hat{f})\psi_n = \left[\varphi(0) + \varphi'(0) f_n + \varphi''(0)\frac{f_n^2}{2!} + \dots\right]\psi_n = \varphi(f_n)\psi_n$$

Then

$$\varphi(\hat{f})\psi = \sum_n a_n \varphi(\hat{f})\psi_n$$

$$= \sum_n a_n \varphi(f_n)\psi_n(q) \qquad a_n = \int \psi_n^* \psi \, dq'$$

$$= \int \Big[\sum_n \varphi(f_n)\psi_n^*(q')\psi_n(q) \Big] \psi(q')\, dq'$$

$$\equiv \int K_\varphi(q,q')\psi(q')\, dq'$$

where

$$\boxed{K_\varphi(q,q') = \sum_n \varphi(f_n)\psi_n(q)\psi_n^*(q')}$$

↑ Note that this definition does not require actual power expansion

— Product of operators —

Remember def

$$\int u(\hat{f}v)\,dq = \int v(\hat{f}^T u)\,dq$$

Then I can write:

$$\int \psi(\hat{f}\hat{g})\phi\, dq = \int \underbrace{\psi}_{\equiv u}\big(\hat{f}\,\underbrace{(\hat{g}\phi)}_{\equiv v}\big) \overset{\text{Transpose}}{=} \int (\hat{g}\phi)(\hat{f}^T\psi)\,dq$$

However

$$\int (\hat{g}\phi)(\hat{f}^T\psi)\,dq = \int \underbrace{(\hat{f}^T\psi)}_{u}(\hat{g}\underbrace{\phi}_{v})\,dq = \int \phi(\hat{g}^T\hat{f}^T\psi)$$

That is:

$$\boxed{\int \psi(\hat{f}\hat{g}\phi)\,dq = \int \phi(\hat{g}^T\hat{f}^T\psi)}$$

If I def:

$$\hat{f}\hat{g} \equiv \hat{h}$$

Then

$$\hat{h}^T = (\hat{f}\hat{g})^T = \hat{g}^T\hat{f}^T$$

If I take the conj:

$$(\hat{f}\hat{g})^\dagger = \hat{g}^\dagger\hat{f}^\dagger$$

Therefore

$$(\hat{f}\hat{g})^\dagger = \hat{f}\hat{g} \quad \text{only if } [\hat{f},\hat{g}]=0$$

- In general:

$$\hat{f}\hat{g} = \underbrace{\frac{1}{2}(\hat{f}\hat{g}+\hat{g}\hat{f})}_{\text{Hermitian}} + \underbrace{\frac{1}{2}(\hat{f}\hat{g}-\hat{g}\hat{f})}_{\text{Anti-hermitian}}$$