Lecture 2

The Formulation of the theory

	Classical Mech.	Quantum Mech.
1) STATE	$(x,p) \in \mathbb{R}^{2d}$	$\psi(x) \in L^2(\mathbb{R}^d)$, $\lVert\psi\rVert_2 = 1$ "$\psi_t(x)$"
2) EVOLUTION	$t \to (x_t, p_t)$ sol. of Ham. eq.	$t \to \psi(t,x)$ sol of Schrö. eq.
3) OBSERVABLES possible outcomes	$f : (x,p) \to \mathbb{R}$ range of f	self-adjoint oper. on $\mathcal{H}$ $\sigma(A)$
4) PREDICTIONS	$f(x_t, p_t)$ with prob. 1 (DETERMINISTIC)	$\mathbb{P}(Q \in I; \psi_t)$ $= \langle \psi_t, E_A(I)\psi_t \rangle$ (PROBABILISTIC)

POSITION

$|\psi(x,t)|^2 =$ prob. density

Hence

$$\langle x_k \rangle (t) = \int_{\mathbb{R}^d} x_k \, |\psi(x,t)|^2 \, dx \qquad k = 1, \dots, d$$

$$= \langle \psi_t , \hat{x}_k \psi_t \rangle$$

$\langle \cdot , \cdot \rangle$ scal. prod.* in $L^2(\mathbb{R}^d)$

(also $(\cdot,\cdot)$)

Position operator

$$\hat{x}_k : \psi(x) \longrightarrow x_k \psi(x)$$

$\langle \psi_t | \hat{x}_k \psi_t \rangle$

see next page

* sc. p. antilinear in the 1st arg. $(af, g) = \bar{a}\,(f,g)$

Physics Book Notations

$|\cdot\rangle$ = ket , $\langle\cdot|$ = bra

scal prod. $\langle\cdot|\cdot\rangle$

Project onto $|\varphi\rangle$

$$P = |\varphi\rangle\langle\varphi|$$

$$P|\psi\rangle = |\varphi\rangle\underbrace{\langle\varphi|\psi\rangle}$$

$$\boxed{P\psi = \langle\varphi,\psi\rangle\,\varphi}$$ we use

or equivalently $(\varphi,\psi)\,\varphi$

MULTIPLICATION OPERATOR

Take $\varphi \in L^\infty(\mathbb{R}^d)$

$$\langle \varphi \rangle(t) = \int \varphi(x)\, |\psi(x,t)|^2\, dx$$

$$= \langle \psi_t, \hat{M}_\varphi\, \psi_t \rangle$$

$$\hat{M}_\varphi : \quad \psi(x) \longrightarrow \varphi(x)\psi(x)$$

MOMENTUM OPER.

LS

A nat. def. $\langle P_k \rangle (t) = \frac{d}{dt} m \langle x_k \rangle (t)$

by def. of $\langle x_k \rangle (t)$

$$= m \int dx \, x_k \frac{\partial}{\partial t} |\psi_t(x)|^2$$

Local conservation law

$$\frac{\partial}{\partial t} |\psi_t(x)|^2 + \operatorname{div} J = 0$$

$$J = \frac{i\hbar}{2m} (\psi \nabla \bar{\psi} - \bar{\psi} \nabla \psi)$$

int. by parts

$$= -\frac{i\hbar}{2} \int dx \, x_k \operatorname{div} J = m \int dx \, J_k$$

$$= i\hbar \int dx \left(\psi_t \frac{\partial}{\partial x_k} \bar{\psi}_t - \bar{\psi}_t \frac{\partial}{\partial x_k} \psi_t \right)$$

for ψ fast decay

$$= -i\hbar \int dx \, \bar{\psi}_t(x) \frac{\partial}{\partial x_k} \psi_t(x)$$

$$= \langle \psi_t, \frac{\hbar}{i} \frac{\partial}{\partial x_k} \psi_t \rangle$$

L6

$$\hat{x}_k : \quad \psi(x) \longrightarrow x_k\, \psi(x) \qquad (1)$$

$$\hat{p}_k : \quad \psi(x) \longrightarrow \frac{\hbar}{i} \frac{\partial}{\partial x_k} \psi(x) \qquad (2)$$

1st quantization procedure

"$p_k \to \hat{p}_k$"

$x_k \to \hat{x}_k$

ENERGY OP.

$$H(x,p) = p^2/2m + V(x)$$

(1) & (2)

$$\longrightarrow \boxed{\hat{H} = -\frac{\hbar^2}{2m}\Delta + V(x)}$$

$$\langle E \rangle(t) = \langle \psi_t , \hat{H} \psi_t \rangle$$

Time dep. Schrö'd eq.

$$i \frac{\partial}{\partial t} \psi(x,t) = \hat{H} \psi(x,t)$$

Few examples $\hat{x}_k$, $\hat{p}_k$, $\hat{H}$, $\hat{M}_\varphi$

LINEAR & symmetric

NICE! eigenvalues of symm. operators are real

For $\mathcal{H} = L^2(\mathbb{R}^d)$, $\varphi \in L^\infty(\mathbb{R}^d)$, M_φ : $(M_\varphi f)(x) = \varphi(x) f(x)$

M_φ IS BOUNDED

$$\| M_\varphi f \| \leq \| \varphi \|_{L^\infty} \| f \|$$

$$\| M_\varphi \| = \sup_{\substack{f \in L^2(\mathbb{R}^d) \\ f \neq 0}} \frac{\| M_\varphi f \|}{\| f \|} = \| \varphi \|_{L^\infty} < \infty$$

A bounded op. $(A, D(A))$ $D(A) \subset \mathcal{H}$ can be extended to the whole $\mathcal{H}$ in a unique way

$D(A)$ dense in $\mathcal{H}$

$\Rightarrow$

$D(A) = \mathcal{H}$

<u>Claim</u> $\mathcal{H} = L^2(\mathbb{R})$, $(Q_0 f)(x) = x f(x)$, $D(Q_0) = \mathcal{S}(\mathbb{R})$

$\Longrightarrow$ $(Q_0, D(Q_0))$ is <u>unbounded</u>

<u>Proof</u> $\exists\, f_n \in \mathcal{S}(\mathbb{R}) : \|f_n\|_2 = 1$ s.t. $\|Q_0 f_n\| \xrightarrow[n \to +\infty]{} \infty$

<u>Pick</u> $f_n(x) = \frac{1}{\pi^{1/4}} e^{-\frac{(x-n)^2}{2}}$, $\|f_n\|_2^2 = \frac{1}{\sqrt{\pi}} \int dx\, e^{-\frac{(x-n)^2}{2}} = 1$

$$\|Q_0 f_n\|^2 = \frac{1}{\sqrt{\pi}} \int dx\, x^2\, e^{-(x-n)^2} \underset{z = x-n}{=} \frac{1}{\sqrt{\pi}} \int dz\, (z+n)^2 e^{-z^2} \xrightarrow[n \to +\infty]{} +\infty$$

MOM. OPERATOR

$(P_0 f)(x) = -i f'(x)$ $\mathcal{H} = L^2(\mathbb{R})$

$(P_0, D(P_0) = \mathcal{S}(\mathbb{R}))$ is unbounded

Proof

$$f_n(x) = (\mathcal{F}^{-1} \tilde{f}_n)(x)$$

$$\tilde{f}_n(k) = \frac{1}{\pi^{1/4}} e^{-\frac{(k-n)^2}{2}}$$

For unbounded op. $(A, D(A))$

Observ. in QM will be described by self-adjoint operators

$\underline{A = A^*}$ & $D(A) = D(A^*)$

POSITION OP.

$$(Q_k \psi)(x) = x_k \psi(x)$$

Proof: TUTORIAL class

Monday 15-17

$$D(Q_k) = \left\{ \psi \in L^2(\mathbb{R}^d) \;\middle|\; \int dx \, |x_k \psi(x)|^2 < \infty \right\}$$

if A s.a.

$\sigma(A) \subseteq \mathbb{R}$

MOM. OPERATOR

$$(P_k \psi)(x) = \frac{\hbar}{i} \frac{\partial \psi}{\partial x_k}(x)$$

$$D(P_k) = \left\{ \psi \in L^2(\mathbb{R}^d) \;\middle|\; \int dp \, |p_k \tilde{\psi}(p)|^2 < \infty \right\}$$

COMMUTATION RELATIONS

$$[\hat{x}_k, \hat{p}_\ell]\psi = \hat{x}_k \hat{p}_\ell \psi - \hat{p}_\ell \hat{x}_k \psi$$

$$= x_k \frac{\hbar}{i} \frac{\partial}{\partial x_\ell} \psi - \frac{\hbar}{i} \frac{\partial}{\partial x_\ell} (x_k \psi) = -\frac{\hbar}{i} \delta_{k,\ell} \psi$$

$$[\hat{x}_k, \hat{p}_\ell]\psi = i\hbar \delta_{k,\ell} \mathbb{1} \psi$$

Physical meaning ?

$$\Delta x_k(t) \, \Delta p_\ell(t) \geq \frac{\hbar}{2} \delta_{k,\ell}$$

HEISENBER PRINCIPLE (1927)

→ It is essentially impossible to follow trajectories !

<u>Prop.</u> Let A, B, C be linear, symm. op. on $\mathcal{H}$. Let $\psi \in \mathcal{H}$ s.t.

$$[A,B]\psi = iC\psi$$

Denote $\Delta A^2 = \langle \psi, (A - \langle A\rangle)^2 \psi\rangle$ and ΔB^2 similarly. Then

$$\Delta A \cdot \Delta B \geq \frac{1}{2} |\langle C\rangle|$$

<u>Proof.</u> $\Delta A \cdot \Delta B = \|(A - \langle A\rangle)\psi\| \, \|(B - \langle B\rangle)\psi\| \overset{CS}{\geq} |\langle (A-\langle A\rangle)\psi, (B - \langle B\rangle)\psi\rangle|$

symm.

$$= |\langle \psi, \underbrace{(A - \langle A\rangle)(B - \langle B\rangle)}\psi\rangle|$$

$$\frac{1}{2}\left[(A-\langle A\rangle)(B-\langle B\rangle) + (B-\langle B\rangle)(A-\langle A\rangle)\right] + \frac{1}{2}\underbrace{[A,B]}^{iC}$$

$$:= F + \frac{i}{2} C \qquad F, C \text{ symmetric}$$

Hence $\Delta A \cdot \Delta B \geq |\langle F\rangle + i/2 \langle C\rangle|$

mean value of sym. operators is real

$$= \left(\langle F\rangle^2 + \frac{1}{4}\langle C\rangle^2\right)^{1/2} \geq \frac{1}{2}|\langle C\rangle| \qquad \blacksquare$$

the minimum uncertainty is reached when

$$\begin{cases} (B-\langle B\rangle)\psi = \lambda\,(A-\langle A\rangle)\psi & \lambda\in\mathbb{R} \\ \langle (A-\langle A\rangle)^2\rangle = 0 & \end{cases} \iff \langle F\rangle = 0$$

Ex $d=1$ $\boxed{\Delta x\,\Delta p = \hbar/2}$

$\beta>0$ $$\psi_\beta(x) = \left(\frac{\beta}{\pi\hbar}\right)^{1/4} e^{-\frac{\beta}{2\hbar}(x-x_0)^2 + \frac{i}{\hbar}p_0 x}$$

coherent state

$$\langle x\rangle = x_0$$

$$\langle p\rangle = p_0$$

Ex. Show that

$$(\Delta x)^2 = \frac{\hbar}{2\beta}\,, \quad (\Delta p)^2 = \frac{\hbar\beta}{2}$$

$\beta = \frac{\Delta p}{\Delta x}$

PREDICTIONS let ψ_t the state of the system at time t, L!S

$\psi_t \in L^2(\mathbb{R})$,

$(Q, D(Q))$ $\mathbb{P}(x \in I; \psi_t) = \int_I dx\, |\psi_t(x)|^2$

prob. of find. a particle in a point $= 0$

$(P, D(P))$ $\mathbb{P}(p \in I; \psi_t) = \int_I \frac{dp}{\hbar} |\tilde{\psi}_t(p/\hbar)|^2$

$(A, D(A))$ $\sigma(A) = \{ a_i \text{, non degenerate} \}$

$A\varphi_i = a_i \varphi_i$, $\{\varphi_i\}$ basis in $\mathcal{H}$

$\rightarrow$ $\mathbb{P}(a \in I; \psi_t) = \sum_{n: a_n \in I} |(\varphi_n, \psi_t)|^2$

prob. to find as an outcome of the measure the eigenv. corr. to φ_n

Note $\mathbb{P}(A = a_i; \varphi_i) = 1$

For a generic observable $\mathcal{Q}$ described by a self-adj. operator $\underline{A}$ we have

$$\mathcal{P}(\mathcal{Q} \in I \subseteq \mathbb{R}; \psi_t) = \langle \psi_t, E_A(I)\, \psi_t \rangle$$

where $\{E_A(\lambda)\}_{\lambda \in \mathbb{R}}$ the spectral family associated to the operator A

$f \in \mathcal{H}, \lambda \in \mathbb{R}$ $\longrightarrow$ next Monday 9-11

$\curvearrowright$ $F^f(\lambda) = \langle E(\lambda)f, f \rangle$

Distribution function

1) Physical consequences of the linearity of the space

$\psi_1, \psi_2 \in \mathcal{H}$

$\|\psi_1\|_2, \|\psi_2\|_2 = 1$

$\Rightarrow$ $\psi(x) = \dfrac{\psi_1(x) + \psi_2(x)}{\|\psi_1 + \psi_2\|_2^2}$

is also a possible state

purely quantum effect

$$|\psi(x)|^2 = c\left(|\psi_1(x)|^2 + |\psi_2(x)|^2 + 2\mathrm{Re}\,\overline{\psi_1(x)}\,\psi_2(x)\right)$$

→ INTERFERENCE TERM

the prob. distribution of $\psi_1 + \psi_2$ is **NOT** the sum of the prob. distributions of having the particle either in ψ_1 or in ψ_2

2) EFFECT of MEASURE (in the standard Copenhagen interpretation)

<u>Guiding idea</u> $\mathcal{A}$ repr. by $\hat{A}$ s.t. $\sigma(A) = \{a_i\}$

and ψ not eigenfunction of A

measure of A onto ψ $\xrightarrow[\text{with prob. } |\langle \varphi_0, \psi \rangle|^2]{}$ a_0 $\xrightarrow[\text{again after a "short time"}]{\varphi_0 \text{ measure } A}$ a_0 with prob. 1

INTERPRETATION the 1st measure has produced an istantaneous transition from ψ to φ_0 (COLLAPSE of the wave function)

STOCHASTIC + NON LINEAR

Measure –

INTERACTION $\boxed{\text{QUANTUM + CLASSICAL object}}$

SHRÖDINGER CAT PROBLEM: superposition states are transfered to the measurement device

$$\psi = \psi_1 + \psi_2 \qquad |\psi|^2 = \left(|\psi_1|^2 + |\psi_2|^2 \cancel{+ \cdots} \right)$$

microscopic stat

For all Practice Purposes (FAPP) Bell '63
the collapse of wave functio works

References

Contents of this class (in a more extended form) can be found in

Sections 3.4 & 3.5 }
Chapter 5 } Alessandro Teta's book

BACKUP

Def. The operator B defined on $D(B)$ is an extension of A defined on $D(A)$ if

$$D(B) \supseteq D(A)$$

and

$$Bf = Af \quad \forall f \in D(A)$$

Notation: $B \supseteq A$ or $B \supset A$ if $D(B) \neq D(A)$