Chapter 5 (3rd edition)

Chapter 6. The general Structure of Wave Mechanics

本章節將波動力學之整結構整理再重述一次

* Wave mechanics :

The state of a system $\Rightarrow \Psi(x,t)$

(波函數)

測量量以 operator 表示, $\hat{O}$. $\hat{O}$ = Hermitian, $\langle \hat{O} \rangle$ = real } 將會更進一步討論

$$\begin{cases} \hat{O}\,\psi_a = a\,\psi_a \\ a = \text{eigenvalue} \Leftarrow \begin{cases} \text{為精確測量所能測到之值} \\ \text{可為 discrete 或 continuous} \end{cases} \\ \psi_a = \text{eigenstate / eigenfunction} \end{cases}$$

orthonormal basis

$$\int \psi_n^*(x)\,\psi_m(x)\,dx = \delta_{n,m} \qquad a \Rightarrow a_n = \text{discrete},\ n=1,2,3.$$

$\{\psi_a\}$ forms

$$\int \psi_{a'}^*(x)\,\psi_a(x) = \delta(a'-a) \qquad a = \text{continuous spectrum}.$$

適當的 "measure"

因此, 任意 $\Psi(x,t) = \sum_n C_n\,\psi_n(x) + \int da\ C(a)\,\psi_a(x)$

discrete   continuous

expansion postulate

$$C_n = \int \psi_n^*(x)\,\Psi(x,t)\,dx \qquad C(a) = \int dx\ \psi_a^*(x)\,\Psi(x,t)$$

$$\int dx\, |\psi(x,t)|^2 = 1$$

$$\Leftrightarrow \quad \sum_n |C_n|^2 + \int da\, |C_a|^2 = 1$$

$\therefore$ $|C_n|^2$ 為找到/測到粒子/系統 $\left\{ a=a_n \right.$ 在 $\psi_{a_n}(x)$ 之机率

$|C_a|^2 da$ 為測到 $(a, a+da)$ 中之机率.

測量值在

→ 測量之後波函數 collapse 到 $\hat{O}$ 之 eigenstate

* Completeness relation

$$\psi(x) = \sum_a C_a \psi_a(x) \quad , \quad C_a = \int dx\, \psi_a^*(x)\, \psi(x)$$

$$1 = \sum_a |C_a|^2 = \sum_a \underbrace{\int dx\, \psi_a^*(x)\, \psi(x)}_{C_a}\ \underbrace{\int dy\, \psi_a(y)\, \psi^*(y)}_{C_a^*}$$

$$= \int dx \int dy\, \psi(x) \left(\sum_a \psi_a^*(x)\, \psi_a(y) \right) \psi^*(y)$$

$$= \int dx\, \psi(x)\, \psi^*(x)$$ 比較之

$\therefore$ $\underbrace{\sum_a \psi_a^*(x)\, \psi_a(y) = \delta(x-y)}_{\text{提供 } \delta(x) \text{ 之 representation}}$ ⇐ 此為 Completeness relation.

例 $\psi_a(x) = \dfrac{1}{\sqrt{2\pi}} e^{ikx}$

$$\underbrace{\int \frac{dk}{2\pi}}_{\sum_a} e^{ikx}\, e^{-iky} = \delta(x-y)$$

例：$\hat{H}$ = Hamiltonian Operator
掌管 $\psi(x,t)$ 之時間演化

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

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x},t).$$

二個皆需要

若 $V(x,t) = V(x)$, $\psi(x,t) = \sum_n C_n \psi_n(x) e^{-\frac{i}{\hbar}E_n t}$

$$+ \int dp\, C(p)\, \psi_p(x)\, e^{-\frac{i}{\hbar}\frac{p^2}{2m}t}$$

$$\int dx\, \psi_n^*(x)\, \psi_m(x) = \delta_{n,m}$$

$$\int dx\, \psi_p^*(x)\, \psi_q(x) = \delta(p-q)$$

$$\int dx\, \psi_n^*(x)\, \psi_p(x) = 0$$

* Hermitian operator

在量子物理中代表 observables 之 operators 皆為
所謂的 linear operators.

$$\hat{A}(\alpha\psi_1(x) + \beta\psi_2(x)) = \alpha\hat{A}\psi_1(x) + \beta\hat{A}\psi_2(x)$$

其作用為將 $\psi(x)$ 帶到另一個 state $\tilde{\psi}(x)$
(map)

$\tilde{\psi}(x) = \hat{A}\psi(x)$ 且滿足

例：$\hat{A} = \hat{p}$, $\hat{H}$, 或由 $\hat{A}$ 所組出之代數組合.
如 $\hat{A}^2$, $e^{\hat{A}} = \mathbb{I} + \hat{A} + \frac{\hat{A}^2}{2!} + \cdots$ 仍為 linear.

除了 linear 之外，成為 observable，也須為 Hermitian：

$$\langle \hat{A} \rangle = \int dx\, \psi^*(x) \hat{A} \psi(x) = \langle \hat{A} \rangle^* = \int dx\, \psi(x) (\hat{A} \psi(x))^*$$

for any $\psi(x)$! ← ①

特例：取 $\psi(x) \Rightarrow \hat{A}$ 的 eigenfunction ψ_a

$$\therefore \langle \hat{A} \rangle = a \int dx\, |\psi_a|^2 = a$$

$$\langle \hat{A} \rangle^* = a^*$$

$\therefore a = a^*$ ∴ 所有的 eigenvalues 皆為實數！

結合 Hermitian 與 linear 給出 Hermitian operator 之另一定義：

$$\int dx\, \phi^*(x) [\hat{A} \psi(x)] = \int dx\, (\hat{A}\phi)^* \psi(x)$$

証明：$\psi(x) = \sum_n \alpha_n \psi_n(x)$，$\hat{A}\psi(x) = \sum_n \alpha_n a_n \psi_n(x)$

$\phi(x) = \sum_n \beta_n \psi_n(x)$，$\hat{A}\phi(x) = \sum_n \beta_n a_n \psi_n(x)$

$$\int dx\, \phi^*(x) [\hat{A} \psi(x)] \underset{\text{linear}}{=} \sum_{m,n} \int dx\, \beta_m^* \psi_m^*(x)\, \alpha_n a_n \psi_n(x)$$

$$= \sum_n \beta_n^* \alpha_n a_n \quad \Leftarrow \int dx\, \psi_m^*(x) \psi_n(x) = \delta_{n,m}$$

$$\int dx\, (\hat{A}\phi)^* \psi(x) = \sum_{m,n} \int dx\, (\beta_m a_m \psi_m(x))^* \alpha_n \psi_n(x)$$

$$= \sum_{m,n} \int dx\, a_m \beta_m^* \psi_m^*(x) \psi_n(x) = \sum_n a_n \beta_n^* \alpha_n$$

$$\therefore \int dx\, \phi^*(x) [\hat{A} \psi(x)] = \int dx\, (\hat{A}\phi)^* \psi(x)$$

Hermitian Conjugate :

在 Hermitian Conjugate 中，我們得計算

$$\int dx \left(\hat{A}\phi(x)\right)^* \psi(x) \text{ 之量}$$

與 $\int dx\, \phi^*(x)\left(\hat{A}\psi(x)\right)$ 之形式 十分不同，

為了讓二者看起來一致，定義

← 例子，見 p.6-5-1

$$\int dx \left[\hat{A}\phi(x)\right]^* \psi(x) \equiv \int dx\, \phi^*(x)\left[\hat{A}^+\psi(x)\right]$$

Hermitian operator : $\hat{A}^+ = \hat{A}$　　　　Hermitian conjugate of $\hat{A}$

* 向量之類比與 Dirac notation

(i) $\vec{A} = A_1\hat{e}_1 + A_2\hat{e}_2 + \cdots + A_n\hat{e}_n$

$\Leftrightarrow \psi(x) = \sum_k a_k \psi_k(x)$

$A_k \leftrightarrow a_k$

$\hat{e}_k \leftrightarrow \psi_k(x)$

(ii) 相加 $(\vec{A}+\vec{B})_i = A_i + B_i$

$\phi(x) + \psi(x) \equiv (\phi+\psi)(x)$

注意：$n=3$ 為一般所知之3維情形，

$\hat{e}_1 = \hat{x}$，$\hat{e}_2 = \hat{y}$，$\hat{e}_3 = \hat{z}$

$\hat{e}_1, \hat{e}_2, \hat{e}_3$ 為三個線性獨立向量.

(iii) 正規化：$\hat{e}_n \cdot \hat{e}_m = \delta_{n,m}$

$$\hat{e}_n = \begin{pmatrix} \xi_{n1} \\ \vdots \\ \xi_{nn} \end{pmatrix}$$

此處 ξ_{n1} 為在 $\hat{x}$ 軸之投影，ξ_{n2} 為在 $\hat{y}$ - - - ，ξ_{n3} ⇒ 在 $\hat{z}$ 軸之投影

$$\sum_i \xi_{ni}\, \xi_{mi} = \delta_{n,m}$$

$$\Leftrightarrow \int dx\, \psi_n^*(x)\, \psi_m(x) = \delta_{n,m}$$

$x \Leftrightarrow$ component index i

差別 x = continuous

∞ dimension

例：　$\hat{A}=\frac{\hbar}{i}\frac{d}{dx}$　求 $\hat{A}^{+}=?$

$$\int dx\,(\hat{A}\phi(x))^{*}\psi(x)$$

$$=\int dx\,\frac{\hbar}{-i}\frac{d\phi^{*}}{dx}\psi(x)=\int_{-\infty}^{\infty}dx\,\frac{-\hbar}{i}\left[\frac{d}{dx}(\phi^{*}\psi(x))-\phi^{*}\frac{d\psi}{dx}\right]$$

$$=-\frac{\hbar}{i}\underbrace{\phi^{*}(x)\psi(x)\Big|_{x=-\infty}^{x=\infty}}_{=0}+\int_{-\infty}^{\infty}dx\,\phi^{*}(x)\left(\frac{\hbar}{i}\frac{d\psi}{dx}\right)$$

$$\equiv\int_{-\infty}^{\infty}dx\,\phi^{*}\hat{A}^{+}\psi$$

$$\therefore\ \hat{A}^{+}=\frac{\hbar}{i}\frac{d}{dx}$$

注意，設 $\hat{B}=\frac{d}{dx}$，　$\hat{B}^{+}=-\frac{d}{dx}$　(見以下之例)

例：　$\hat{A}=\alpha\hat{B}$，　則 $\hat{A}^{+}=\alpha^{*}\hat{B}^{+}$

依據定義，for any ϕ 與 ψ

$$\int(\hat{B}\phi(x))^{*}\psi(x)\,dx\equiv\int\phi(x)\hat{B}^{+}\psi\quad-(i)$$

$$\int(\hat{A}\phi(x))^{*}\psi(x)\,dx\equiv\int\phi(x)\hat{A}^{+}\psi\quad-(ii)$$

現在 $\hat{A}=\alpha\hat{B}$

$$\int(\hat{A}\phi(x))^{*}\psi(x)\,dx$$

$$=\alpha^{*}\int(\hat{B}\phi(x))^{*}\psi(x)\,dx$$

$$\overset{(i)}{=}\alpha^{*}\int\phi(x)\hat{B}^{+}\psi(x)\,dx$$

$$=\int\phi(x)\,\alpha^{*}\hat{B}^{+}\psi(x)\,dx\overset{(ii)}{=}\int dx\,\phi(x)\hat{A}^{+}\psi$$

$$\therefore\ \hat{A}^{+}=\alpha^{*}\hat{B}^{+}$$

$$A_n = \hat{e}_n \cdot \vec{A} = \sum_i \xi_{ni} A_i$$

$$\Leftrightarrow \quad C_n = \int dx\ \psi_n^*(x)\,\psi(x)$$

(iv) 内積

$$\int dx\ \phi^*(x)\,\psi(x) \Leftrightarrow \underbrace{\vec{A}\cdot\vec{B} = \sum_i A_i B_i}$$

矩陣表示 $= (A_1, \ldots, A_N)\begin{pmatrix} B_1 \\ \vdots \\ B_N \end{pmatrix}$

$= \vec{A}^T \vec{B}$

總而言之，$\psi(x)$ 相當於向量分量 A_i

一般$\boxed{\text{整個向量}}$記為 $\vec{A}$

$\Leftrightarrow$ 整個 State $\Rightarrow |\psi\rangle$，其中 $| \,\rangle \equiv$ ket 相當於向量 $\vec{A}$ 上方之 $\rightharpoonup$
而 ψ 相當於 A.

在内積中，$(\vec{A}^T)_i$，則相當於 $\phi^*(x)$

$\therefore$ $\phi^*(x)$ 為 $\langle\phi|$ 之分量　　　$\langle\phi| \Leftrightarrow \vec{A}^T$

$\langle\, | \equiv$ bra.

ket 和 bra 為所謂的 Dirac notations!

以此 notation 表示 $\int dx\, \phi^*(x)\,\psi(x) = \langle\phi|\psi\rangle$.

(V) linear operators as matrices

首先 $\psi(x)=\sum_n a_n\psi_n(x)$ 可記為 $|\psi\rangle=\sum_n a_n|n\rangle$

$(\Leftrightarrow\ \vec{A}=\sum_n A_n\hat{e}_n)$

$\psi'(x)=\hat{O}\,\psi(x)=\sum_n a_n(\hat{O}\,\psi_n(x))$ (linear)

即 $|\psi'\rangle=\sum_n a_n\underbrace{\hat{O}|n\rangle}$
某-state，又記作 $|\hat{O}n\rangle$

所以，要知道 $\hat{O}$ 之作用，只要知道 $\hat{O}\,\psi_n(x)$ 即可！

但 $\hat{O}\,\psi_n(x)$ 可以以 $\{\psi_m\}$ 展開

$$\hat{O}\,\psi_n(x)=\sum_m \underbrace{O_{mn}}\ \psi_m(x)$$

其

$$O_{mn}=\int dx\ \psi_m^*(x)\left[\hat{O}\,\psi_n(x)\right]$$

所以，一旦知道 O_{mn} 則 $\hat{O}$ 之作用即知！

$$\hat{O}\,\psi(x)=\sum_n a_n(\hat{O}\,\psi_n(x))$$

$$=\sum_{m,n}\underbrace{a_n O_{mn}}\ \psi_m(x)=\sum_m b_m\psi_m(x)$$

因此，$|\psi\rangle \Leftrightarrow \begin{pmatrix}a_1\\a_2\\\vdots\\\vdots\end{pmatrix}$.
$\Rightarrow$ 以 ψ_n 為底

$\hat{O}\,\psi(x)\Leftrightarrow\hat{O}|\psi\rangle$

$$\begin{pmatrix}b_1\\b_2\\\vdots\\\vdots\end{pmatrix}=\begin{pmatrix}O_{11}&O_{12}&O_{13}&\cdots\\O_{21}&O_{22}&O_{23}&\cdots\\O_{31}&&\cdots&\end{pmatrix}\begin{pmatrix}a_1\\a_2\\a_3\\\vdots\end{pmatrix}$$

因此，任意 linear operator $\hat{A}$ 即相當於

一個 matrix
$$\underbrace{\begin{pmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & \\ A_{31} & & \cdots \\ & & \end{pmatrix}}_{\text{以 } \{\psi_n(x)\} \text{ 為底}}$$

例： $\int dx\, \phi^*(x)[\hat{A}\,\psi(x)]$

$$= (\beta_1^*, \beta_2^*, \ldots) \begin{pmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & \cdots \\ A_{31} & A_{32} & \cdots \end{pmatrix} \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \vdots \end{pmatrix} \quad \text{—②}$$

其中 $\psi(x) = \sum_n \alpha_n \psi_n(x)$, $\phi(x) = \sum_n \beta_n \psi_n(x)$

例： $\int dx\, (\hat{A}\phi(x))^* \psi(x) = \int dx\, \psi(x) (\hat{A}\phi(x))^*$

$$= (\alpha_1, \alpha_2, \ldots, \alpha_n, \ldots) \begin{pmatrix} A_{11}^* & A_{12}^* & A_{13}^* \\ A_{21}^* & A_{22}^* & \vdots \\ A_{31}^* & \cdots & \vdots \end{pmatrix} \begin{pmatrix} \beta_1^* \\ \beta_2^* \\ \vdots \end{pmatrix}$$

$$= (\beta_1^*, \beta_2^*, \ldots) \begin{pmatrix} A_{11}^* & A_{21}^* & A_{31}^* \cdots \\ A_{12}^* & A_{22}^* & \\ A_{13}^* & \cdots & \end{pmatrix} \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \vdots \end{pmatrix} \quad \text{—③}$$

矩陣乘法規則

例: $\int dx\, \phi^*(x) [A^+ \psi(x)]$ $\qquad A^+ \equiv B$

$$= (\beta_1^*, \beta_2^*, \ldots) \begin{pmatrix} B_{11} & B_{12} & B_{13} & \ldots \\ B_{21} & B_{22} & B_{23} & \ldots \\ B_{31} & B_{32} & \ldots & \end{pmatrix} \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \vdots \\ \vdots \end{pmatrix} \quad — ④$$

比較 ③ = ④

可知 A^+ = A矩陣作 transpose + Complex Conjugate

A的 Hermitian Conjugate

比較 ① = ② . Hermitian operator

則 $$\begin{pmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & \\ A_{31} & \ldots & \end{pmatrix} = \begin{pmatrix} A_{11}^* & A_{21}^* & A_{31}^* \\ A_{12}^* & A_{22}^* & \\ A_{13}^* & \ldots & \end{pmatrix}$$

$$\boxed{A_{ij} = A_{ji}^*}$$

由以上可知,向量子力學與線性代數密切相關了!

* Degeneracy & simultaneous observables.

Theorem:

若 $[\hat{A}, \hat{B}] = 0 \Leftrightarrow$ 可以找到共同之 eigenfunction $\{\psi_{ab}(x)\}$ 基底

使得 $\hat{A}\psi_{ab}(x) = a\,\psi_{ab}(x)$

$\hat{B}\psi_{ab}(x) = b\,\psi_{ab}(x)$

(參考書本 p.122-124 之証明)

參考

"⇒" 若 $\hat{A}\,\psi_{ab}(x) = a\,\psi_{ab}(x)$

$\hat{B}\,\psi_{ab}(x) = b\,\psi_{ab}(x)$

$\Rightarrow [\hat{A},\hat{B}]\,\psi_{ab} = (ab-ba)\,\psi_{ab} = 0$

$\because$ Any $\psi(x) = \sum C_{ab}\,\psi_{ab}(x)$

$\therefore [\hat{A},\hat{B}]\,\psi(x) = \sum_{ab} C_{ab}\,[\hat{A},\hat{B}]\,\psi_{ab}(x) = 0$ for any ψ

$\therefore [\hat{A},\hat{B}] = 0$

反之 若 $[\hat{A},\hat{B}]=0$. 考慮某一 $\hat{B}$ 之 eigenstate ψ_b

即 $\hat{B}\,\psi_b(x) = b\,\psi_b(x)$

$\because [\hat{A},\hat{B}]\,\psi_b = 0 \quad \therefore \hat{A}\,(\underbrace{\hat{B}\psi_b}_{b}) - \hat{B}\,\hat{A}\psi_b = 0$

$\therefore \hat{B}(\hat{A}\psi_b) = b(\hat{A}\psi_b)$ —(1) $\therefore \hat{A}\psi_b$ 也是 $\hat{B}$ 之 eigenstate

若 b is non-degenerate, 則 $\hat{A}\psi_b \propto \psi_b$. 令 $\hat{A}\psi_b = a\,\psi_b$

此時, a 為 b 之函數, 我們找到了 $\hat{A},\hat{B}$ 之共同 eigenstate.
(即為 ψ_b)

若 b 是 degenerate, 以 degeneracy = 2 為例,

即 对一個 b, 有 二個 eigenstate ϕ_b^1, ϕ_b^2

$\hat{B}\phi_b^1(x) = b\,\phi_b^1(x)$

$\hat{B}\phi_b^2(x) = b\,\phi_b^2(x)$

且 $\underbrace{\phi_b^1 \text{ 和 } \phi_b^2}_{\text{independent}}$ 不成正比

則只能推論 $\hat{A}\phi_b^1 = b_{11}\,\phi_b^1 + b_{12}\,\phi_b^2$
由(1)式 (取 $\psi_b = \phi_b^1$)
及 $\psi_b = \phi_b^2$ $\hat{A}\,\phi_b^2 = b_{21}\,\phi_b^1 + b_{22}\,\phi_b^2$

由於任意 ϕ_b^1 及 ϕ_b^2 之線性組合仍是 $\hat{B}$ 之 eigenstate：

$$\hat{B}(\alpha\phi_b^1+\beta\phi_b^2) = b(\alpha\phi_b^1+\beta\phi_b^2)$$

我們令 $\psi_b = \alpha\phi_b^1+\beta\phi_b^2$ 代入 上式中之 $\hat{A}\psi_b$

使 $\underbrace{\hat{A}\psi_b = \alpha\hat{A}\phi_b^1+\beta\hat{A}\phi_b^2}$ & $\psi_b = \lambda\psi_b$

$$\alpha(b_{11}\phi_b^1+b_{12}\phi_b^2) + \beta(b_{21}\phi_b^1+b_{22}\phi_b^2) = \lambda(\alpha\phi_b^1+\beta\phi_b^2)$$

$\therefore$ $\alpha b_{11}+\beta b_{21} = \lambda\alpha$, $\alpha b_{12}+\beta b_{22} = \lambda\beta$ 即 $\begin{pmatrix} b_{11} & b_{21} \\ b_{12} & b_{22}\end{pmatrix}\begin{pmatrix}\alpha\\ \beta\end{pmatrix} = \lambda\begin{pmatrix}\alpha\\ \beta\end{pmatrix}$

$\therefore$ 找 $\begin{pmatrix} b_{11} & b_{21} \\ b_{12} & b_{22}\end{pmatrix}$ 之 eigenvector $\begin{pmatrix}\alpha\\ \beta\end{pmatrix}$ 即可找到 ψ_b

為 $\hat{A}$ 之 eigenstate（注意，此時 λ 可以有 2 個解 λ_a^1, λ_a^2）

故可以找到 $\hat{A}$ 與 $\hat{B}$ 之共同 eigenstate (simultaneous eigenstate)

結論

(i) 由於測量是測到 eigenvalues，測量後為 observable operator 之 eigenstate，則 $[\hat{A},\hat{B}]=0$

表示 $\hat{A}$ 與 $\hat{B}$ 可以同時被測量。 可以有共同之 eigenstates 所以

(ii) 若 $\hat{B}$ 是 degenerate，其 degeneracy 可由另一個

operator $\hat{A}$，$[\hat{A},\hat{B}]=0$ 來被進一步區分出來

（如以上之例 $\lambda_a^1 \neq \lambda_a^2$）

若 $\hat{A}$ 與 $\hat{B}$ 之共同 eigenstate 中仍有 degeneracy，表示

有另一 operator $\hat{C}$，$[\hat{A},\hat{B}]=[\hat{B},\hat{C}]=[\hat{C},\hat{A}]=0$，$\hat{C}$ 可

進一步區分這些 degeneracy

如此下去，我們可以找到一組 observables $\hat{A}, \hat{B}, \hat{C}, \ldots, \hat{M}$

$$[\hat{A}, \hat{B}] = 0, \quad [\hat{B}, \hat{C}] = 0, \quad [\hat{A}, \hat{M}] = \ldots$$

使得 state 由 $\underbrace{\quad}_{\hat{A}, \hat{B} \ldots \hat{M}}$ 唯一決定

此 set $\{\hat{A}, \hat{B}, \ldots, \hat{M}\} \Rightarrow$ Complete set of commuting observables.

* Uncertainty relations

Appendix B.

$$(\Delta A)^2 \equiv \langle (A - \langle A \rangle)^2 \rangle$$
$$= \langle A^2 - 2A\langle A \rangle + \langle A \rangle^2 \rangle$$
$$= \langle A^2 \rangle - \langle A \rangle^2$$

$$(\Delta A)^2 (\Delta B)^2 \geq \frac{1}{4} \langle i[A, B] \rangle^2$$

例. $\hat{A} = \hat{x}$, $\hat{B} = \hat{p}$, $[\hat{x}, \hat{p}] = i\hbar$

$$\Delta x^2 \Delta p^2 \geq \hbar^2/4$$

* 平均值的時間變化.

一個 operator 之平均 與時間有關：

$$\langle A \rangle_t = \int dx \; \psi^*(x,t) \, \hat{A} \, \psi(x,t)$$

有二個來源 $\begin{cases} \psi(x,t) \text{ depends on } t \\ \hat{A} \text{ 本身與 } t \text{ 有關, 如 } \hat{A} = \hat{x}\cos 2t \ldots \end{cases}$

$$\therefore \frac{d\langle \hat{A}\rangle_t}{dt} = \int \psi^*(x,t)\frac{d\hat{A}}{dt}\psi(x,t)\,dx \quad \rightarrow = \left\langle \frac{d\hat{A}}{dt}\right\rangle_t$$

$$+\int \psi^*(x,t)\boxed{\hat{A}}\frac{d\psi(x,t)}{dt}\,dx \quad \rightarrow \frac{1}{i\hbar}\boxed{\hat{H}}\psi(x,t)$$

$$+\int \frac{d\psi^*}{dt}\hat{A}\,\psi(x,t)\,dx$$

$$\downarrow$$

$$\left(\frac{1}{i\hbar}\hat{H}\psi(x,t)\right)^* = \frac{i}{\hbar}\hat{H}\psi^*$$

$$= \left\langle \frac{d\hat{A}}{dt}\right\rangle_t - \frac{i}{\hbar}\int \psi^*(x,t)\,\hat{A}\hat{H}\,\psi(x,t)\,dx$$

$$+\frac{i}{\hbar}\int \psi^*(x,t)\,\hat{H}\hat{A}\,\psi(x,t)\,dx$$

integration by part , $\hat{H} = \frac{-\hbar^2}{2m}\frac{d^2}{dx^2}+V$

$$\int\left(\frac{d^2}{dx^2}\psi^*\right)\underbrace{\phi(x)}_{=\hat{A}\psi(x,t)}dx = \int \psi^*(x)\frac{d^2}{dx^2}\phi(x)\,dx$$

$$\therefore \boxed{\frac{d\langle \hat{A}\rangle_t}{dt} = \left\langle\frac{d\hat{A}}{dt}\right\rangle_t + \frac{i}{\hbar}\langle[\hat{H},\hat{A}]\rangle} \quad \text{eq. of motion}$$

Ehrenfest theorem

$\langle[\hat{A},\hat{B}]\rangle$ = 純虛數 $A^+=A$, $B^+=B$

特例： $\frac{d\hat{A}}{dt}=0$ ($\hat{A}$ 沒有 explicit time dependence)

且 $[\hat{H},\hat{A}]=0$ 則 $\frac{d\langle \hat{A}\rangle_t}{dt}=0$

即 $\langle \hat{A}\rangle_t$ 與時間無關，$\hat{A}$ ⇒ constant of motion

即若 t=0 時 $\hat{A}\psi(x,0)=a\psi(x,0)$, $\psi(x,0)=\psi_a(x)$

t≠0 時 $\langle\hat{A}\rangle_t$ 亦 $=a$, ∴ $\hat{A}\psi(x,t)=a\psi(x,t)$ too!

事實上, ∵ $[\hat{H},\hat{A}]=0$, 可找到 $\psi(x,0)$ 為 $\hat{H}$, $\hat{A}$ 之共同 eigenstate, 因此, $\psi(x,t)=\psi(x,0)e^{-\frac{iE}{\hbar}t}$

$\hat{H}\psi(x,0)=E\psi(x,0)$

例: 取 $\hat{A}=\hat{x}$

$$\frac{d\langle x\rangle}{dt}=\frac{i}{\hbar}\langle[H,x]\rangle=\frac{i}{\hbar}\langle[\frac{p^2}{2m}+V(x),x]\rangle$$

$[V(x),x]=0$

有用的等式 $[\hat{A}\hat{B},\hat{C}]=\hat{A}[\hat{B},\hat{C}]+[\hat{A},\hat{C}]\hat{B}$

$$\therefore [\hat{p}^2,\hat{x}]=\hat{p}[\hat{p},\hat{x}]+[\hat{p},\hat{x}]\hat{p}=-2i\hbar\hat{p}$$

(見 Page 3-10-2)

$$\therefore \frac{d\langle\hat{x}\rangle}{dt}=\langle\frac{\hat{p}}{m}\rangle=\frac{\langle\hat{p}\rangle}{m} \quad —⑥$$

若取 $\hat{A}=\hat{p}$

$$\frac{d\langle\hat{p}\rangle}{dt}=\frac{i}{\hbar}\langle[\frac{p^2}{2m}+V(x),p]\rangle$$

$$=\frac{i}{\hbar}\langle[V(x),p]\rangle$$

NO.
DATE 6-15

對任意 $\psi(x)$, $[V(x),\hat{p}]\psi(x) = V(x)\frac{\hbar}{i}\frac{d}{dx}\psi(x) - \frac{\hbar}{i}\frac{d}{dx}(V(x)\psi(x))$

$$= -\frac{\hbar}{i}\frac{dV(x)}{dx}\psi(x) \qquad \therefore [V(x),\hat{p}] = i\hbar\frac{dV}{dx}$$

$$\therefore \frac{d\langle\hat{p}\rangle}{dt} = \left\langle -\frac{dV(x)}{dx}\right\rangle \quad \text{—⑦} \Rightarrow m\frac{d^2}{dt^2}\langle x\rangle = -\left\langle\frac{dV}{dx}\right\rangle$$

* Ex13 是一個好的練習，注意：Ex13 中要算的是

$\left\langle\frac{dx}{dt}\right\rangle = \frac{d\langle x\rangle}{dt}$, $\frac{d\langle p\rangle}{dt}$, $\frac{d\langle H\rangle}{dt}$.

* 古典的極限

⑥式和⑦式和古典運動方程式很相似

$$\frac{dx_{cl}}{dt} = \frac{p_{cl}}{m} \quad \text{---⑧}$$

$$m\frac{d^2x_{cl}}{dt^2} = \frac{dp_{cl}}{dt} = F = -\frac{dV(x_{cl})}{dx_{cl}} \quad \text{---⑨}$$

很明顯的，x_{cl} 似乎對應到 $\langle x\rangle$!

唯一不同的是：⑦式中 $\left\langle\frac{dV(x)}{dx}\right\rangle \neq \frac{d}{d\langle x\rangle}V(\langle x\rangle)$

若設 $F(x) \equiv -\frac{dV}{dx}$

則 $F(x) = F(\langle x\rangle) + (x-\langle x\rangle)F'(\langle x\rangle)$

以 $x=\langle x\rangle$ 展開 $\qquad + \frac{(x-\langle x\rangle)^2}{2}F''(\langle x\rangle) + \cdots$

$$\therefore \langle F(x)\rangle = F(\langle x\rangle) + \frac{1}{2}\langle(x-\langle x\rangle)^2\rangle F''(\langle x\rangle) + \cdots$$

$$= F(\langle x\rangle) + \frac{1}{2}\Delta x^2 F''(\langle x\rangle) + \cdots$$

Paper House

∴若 Δx 很小，則 $\langle F(x)\rangle \simeq F(\langle x\rangle)$，即 $\langle \frac{dV}{dx}\rangle \simeq \frac{dV(\langle x\rangle)}{d\langle x\rangle}$

則⑦式 $\Rightarrow m\frac{d^2\langle x\rangle}{dt^2} \simeq -\frac{dV(\langle x\rangle)}{d\langle x\rangle}$

此時，量子之表示式⑥與⑦ ≃ 古典的運動方程式

$(\langle x\rangle = x_{cl})$

∴古典的極限：Δx 很小，

但很小，是什麼意思呢？

⇒ 只指 $\Delta x \ll V(x)$ 的變化長度 (Characteristic length)

如圖所示