Chapter 2.

什麼是 $\Psi(x,t)$？(物質波)

更重要的是它遵守什麼方程式？

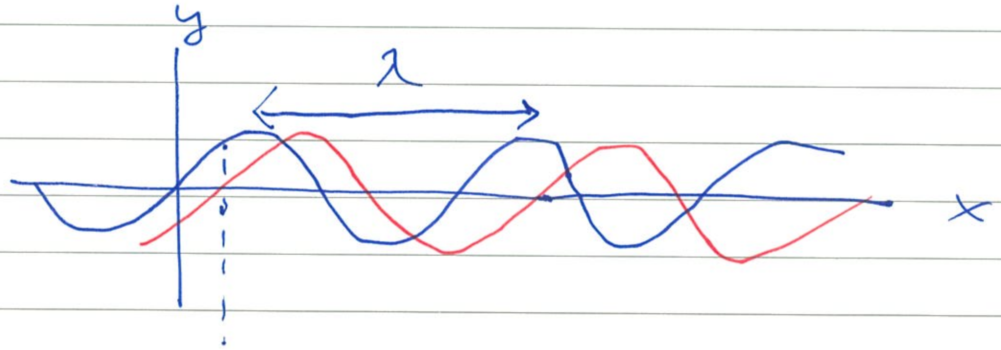
在這一章裏，我們將從波的一般談起，最後說服自己，這樣的方程式確實存在！(Schrödinger eq.)

* Basic Relations

$$\lambda = \frac{h}{p}, \quad p = \boxed{\hbar k}$$

$$E = h\nu = \frac{h}{2\pi} 2\pi\nu = \boxed{\hbar\omega}$$

Sinusoidal wave $\quad y = A\sin(kx - \omega t)$



固定 x ⇒ periodic in time $\quad T =$ 週期，$\nu = \frac{1}{T}$

$$k = \frac{2\pi}{\lambda} = \text{wave number}$$

即 2π 中有多少 λ.

$$\omega = \frac{2\pi}{T} = \text{angular frequency}$$

即 2π 中有多少 T

phase speed : valley 或其中固定 phase 走的速度

即 $kx-\omega t = \text{const}$. 走的速度

$\because k\frac{dx}{dt}-\omega=0 \quad \therefore v_p = \frac{\omega}{k} = \nu\lambda.$

particle speed : $\frac{dy}{dt}$.

$\downarrow$

$\sin(kx-\omega t)$

$=\sin k(x-v_pt)$

note that $\cos(kx-\omega t)$ is equally good

* Superposition

要得到干涉之效果，superposition 扮演了很重要的角色（記得双狭縫干涉，$\vec{E}=\vec{E_1}+\vec{E_2}$，$I\propto|\vec{E}|^2$）

何謂 superposition？

在微分方程式中，你們學到

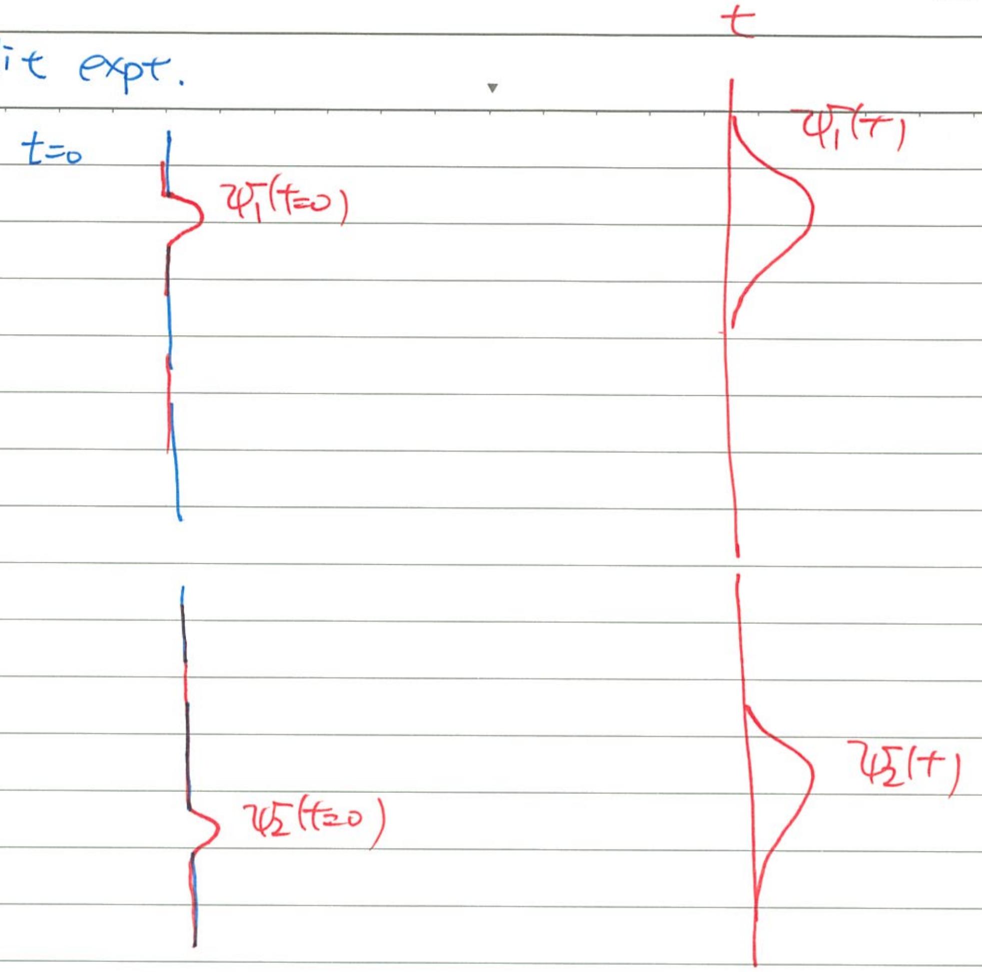
若 $\psi_1(x,t)$，$\psi_2(x,t)$ 是解

則 $\psi_1+\psi_2$ is also a solution.

Usually, this happens because the governing eq is <u>linear</u>.

這裏，我們也將假設這是对的，否則干涉的現象就不易產生.

two slit expt.



$$\psi(t=0) = \psi_1(t=0) + \psi_2(t=0)$$

$$\Rightarrow \psi(t) = \psi_1(t) + \psi_2(t)$$ Superposition !

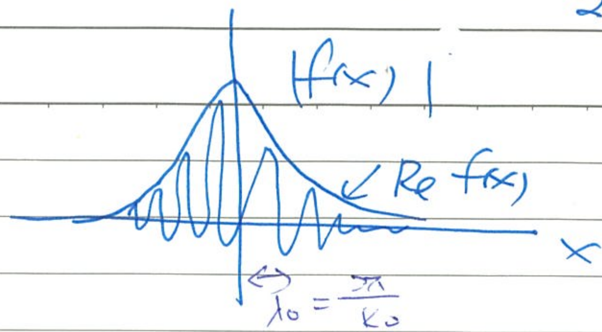
* . Wave packets

As we have seen, $\sin kx$ & $\cos kx$ describe sinusoidal equally good.

In fact, they can be combined as $e^{ikx} = \cos kx + i \sin kx$

This is the situation when the particle has definite momentum. $p = \hbar k$.

$\therefore |f(x)| = \sqrt{\frac{\pi}{\alpha}}\, e^{-x^2/4\alpha}$



所以，大家可以看到，適當的組合平面波 (e^{ikx}) 可得到一個所謂的 localized wave packet.

This gives us hints to compromise particle & wave duality: when the material behaves like particles, their wavepackets are more localized.

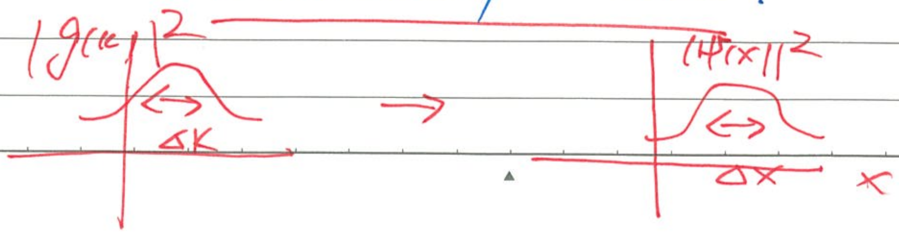
Note that (in the above example) Δx (以 $|f(x)|^2$ 定之) $= 2\sqrt{2\alpha}$

$$\therefore \Delta k \Delta x \simeq \frac{2}{\sqrt{2\alpha}} \cdot 2\sqrt{2\alpha} = 4 \sim O(1)$$

$\Delta x \Delta k \gtrsim O(1)$ in general

$\because p = \hbar k \quad \therefore \Delta p \Delta x \geq \hbar/2$ uncertainty principle

implication: impossible to make Δx & Δk simultaneously small!



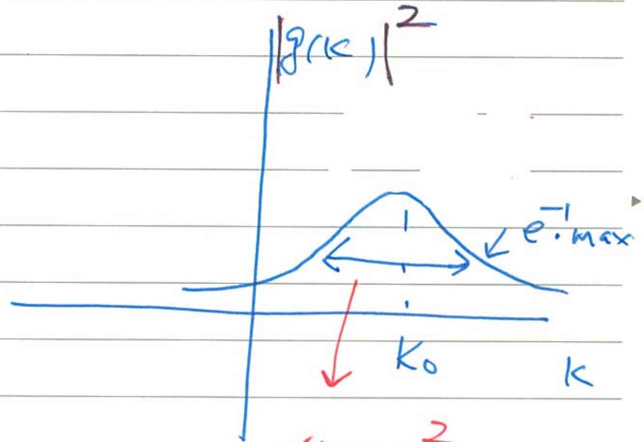
$\Delta k \Delta x \gtrsim O(1)$

The superposition principle allows us to form

$$f(x) = \int_{-\infty}^{\infty} dk\, \underbrace{g(k)}_{\text{描述 } e^{ikx} \text{ 之間的相對強度}}\, e^{ikx}$$

這樣的表示為所謂的 Fourier transformation
($g(k)$ 為 $f(x)$ 之 Fourier transformation
反之 $f(x)$ 為 $g(k)$ 之 inverse Fourier transformation)

例如 $g(k) = e^{-\alpha(k-k_0)^2}$



$\Delta k \simeq \frac{2}{\sqrt{2\alpha}}$

則 $f(x) = \int_{-\infty}^{\infty} dk\, e^{-\alpha(\underbrace{k-k_0}_{\bar{k}})^2} e^{ikx}$

$$= \int_{-\infty}^{\infty} d\bar{k}\, e^{-\alpha\bar{k}^2} e^{i(\bar{k}+k_0)x}$$

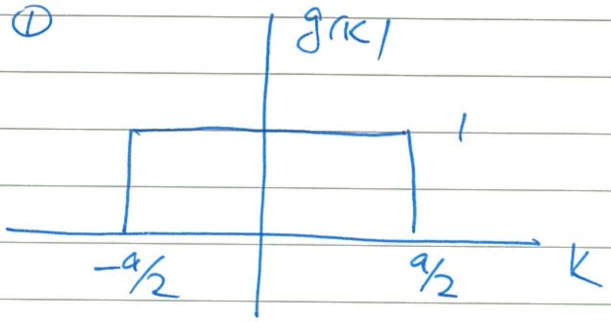
$$= \int_{-\infty}^{\infty} d\bar{k}\, \underbrace{e^{-\alpha\bar{k}^2} e^{i\bar{k}x}}_{\parallel}\, e^{ik_0x}$$

$$e^{-\alpha(\bar{k}-\frac{ix}{2\alpha})^2}\, e^{-\frac{x^2}{4\alpha}}$$

$\int_{-\infty}^{\infty} dy\, e^{-\alpha y^2} = \sqrt{\frac{\pi}{\alpha}}$ $\qquad \therefore = e^{-\frac{x^2}{4\alpha}} e^{ik_0x} \sqrt{\frac{\pi}{\alpha}}$

(Gaussian wave packet)

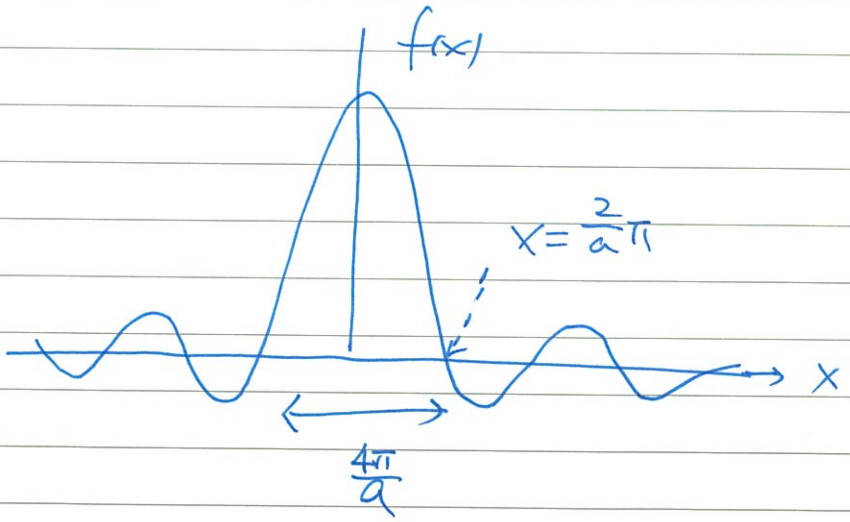
More example :

① 

$$f(x) = \int_{-a/2}^{a/2} e^{ikx}\, dk$$

$$= \frac{1}{ix} e^{ikx} \Big|_{k=-a/2}^{k=a/2} = \frac{1}{ix} 2i\sin x \cdot a/2$$

$$= \frac{2\sin\frac{a}{2}x}{x}$$



$$\Delta x \Delta k \sim a \cdot \frac{4\pi}{a} \gtrsim O(1)$$

② $\Delta k = 0$, $g(k) = \delta(k - k_0)$

$f(x) = e^{ik_0x}$, $\Delta x = \infty$.

* Inverse Fourier transformation

$$f(x) = \int_{-\infty}^{\infty} g(k) e^{ikx} dk$$

$$g(k) = \int_{-\infty}^{\infty} e^{-ikx} f(x) \frac{dx}{2\pi}$$

參考 Appendix A

⇒ 如此之類似对稱性說明了 $\Delta x \Delta k \geq 1$ 中 x 与 k 之对稱性

這裏用到 $\frac{1}{2\pi}\int_{-\infty}^{\infty} dk\, e^{ik(x-y)} = \delta(x-y)$

或是 $\frac{1}{2\pi}\int dx\, e^{ix(k-k')} = \delta(k-k')$

⟵ ①

more generally $f(x) = \int_{-\infty}^{\infty} g(k) e^{ikx} dk \cdot \alpha$

$g(k) = \int_{-\infty}^{\infty} f(x) e^{-ikx} dx\ \beta$

$\alpha\beta = \frac{1}{2\pi}$ ∴ 如果取 $\alpha = 1$, $\beta = \frac{1}{2\pi}$

Another common choice $\alpha = \frac{1}{\sqrt{2\pi}}$, ∴ $\beta = \frac{1}{\sqrt{2\pi}}$

↳ see over

Understanding ①: $\boxed{\text{Note that } \int_{-\infty}^{\infty} \delta(x-y) f(y)\, dy = f(x)}$

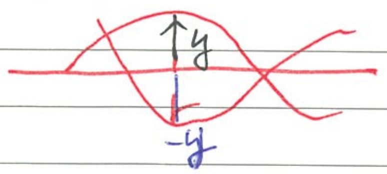
Obviously, 若 $x=y$ $\frac{1}{2\pi}\int_{-\infty}^{\infty} dk\, e^{ik(x-y)} = \infty$

反之若 $x \neq y$, 讓 $r = x-y$

則 $\int_{-\infty}^{\infty} dk\, e^{ikr}$ 為 所有不同波長之波在 r 處的和

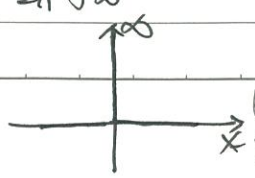
且所有波之比重都一樣! 因此, 如果某一個波貢獻 y

一定可以找到另一個波 ⇒ contribute $(-y)$



∴ $\int_{-\infty}^{\infty} dk\, e^{ikr} = 0$ ∴ $\frac{1}{2\pi}\int_{-\infty}^{\infty} dk\, e^{ik(x-y)}$

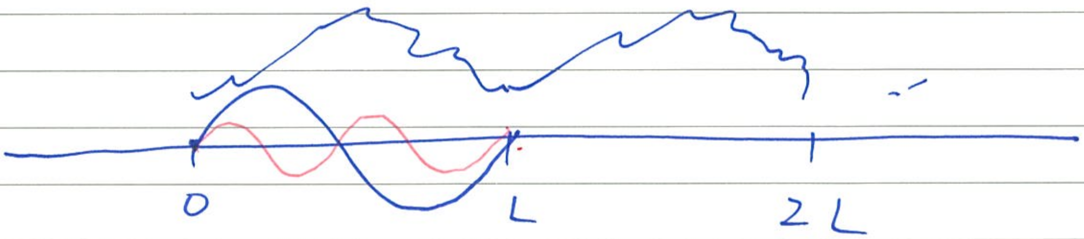
⇒



Appendix A Dirac delta function 與 Fourier Analysis

正如 Taylor expansion：以多項式來逼近一個函數，

在波的世界，我們以"平面波" e^{ikx} 之和 來逼近任一個波。



週期（空間中）為 L 之平面波（正弦波 sinusoidal）有許多種

$\sin\frac{2\pi x}{L}$ $\cos\frac{2\pi x}{L}$

$\sin\frac{4\pi x}{L}$ $\cos\frac{2\pi x}{L/2}$

$= \sin\frac{2\pi x}{L/2}$ ⋮

$\Rightarrow$ 整合於 $e^{i\frac{2\pi}{L}nx}$ → 以下平移座標 $-L/2$ $L/2$

$\therefore$ 一般波：$f(x+L)=f(x)$ （書本上以 $(-L,L)$ 為例）

$$f(x)=\sum_{n=-\infty}^{\infty} a_n e^{\frac{i2\pi n x}{L}} \quad \text{—— ①}$$

（注意若 $a_n=a_{-n}$ 時，reproduce $\cos\frac{2\pi nx}{L}$ 波）

$a_n=-a_{-n}$ 〃 $\sin\frac{2\pi nx}{L}$ 〃

給定 $f(x)$, $a_n = ?$

這可以利用

$$\frac{1}{L}\int_{-L/2}^{L/2} dx\, e^{i\frac{2\pi n}{L}x}\, e^{-i\frac{2\pi m}{L}x}$$

$$= \begin{cases} 1 & m=n \\ 0 & m\neq n \end{cases} \equiv \delta_{n,m}$$

① $\times \frac{1}{L} e^{-i\frac{2\pi m}{L}x}$ 再 $\int_{-L/2}^{L/2} dx$

$$\therefore\ a_m = \frac{1}{L}\int_{-L/2}^{L/2} dx\, f(x)\, e^{-i\frac{2\pi m}{L}x} \quad —②$$

Continuum limit:

以上的結果可以用在一個看似沒有週期的函數: 取 $L\to\infty$

此時 $\frac{2\pi n}{L} \equiv k_n \to 0$ $\because \Delta k = \frac{2\pi}{L}$, $\Delta k = 1$

$$\therefore ① \Rightarrow f(x) = \frac{L}{2\pi}\sum_n a_n e^{ik_n x}\Delta k$$

$$= \sum_n g(k_n)\, e^{ik_n x}\Delta k$$

$$\rightarrow \int_{-\infty}^{\infty} g(k)\, e^{ikx}\, dk$$

$$\boxed{g(k) = \frac{L}{2\pi} a_n}$$

$$② \Rightarrow g(k) = \frac{1}{2\pi}\int_{-\infty}^{\infty} f(x)\, e^{-ikx}\, dx$$

12 hours

Dirac delta function

$$\because f(x) = \int_{-\infty}^{\infty} g(k)\, e^{ikx}\, dk$$

$$g(k) = \frac{1}{2\pi}\int_{-\infty}^{\infty} f(y)\, e^{-iky}\, dy$$

$$\therefore f(x) = \int_{-\infty}^{\infty} f(y) \underbrace{\left[\int \frac{dk}{2\pi}\, e^{ik(x-y)}\right]}_{\text{此函數即為 Dirac delta function}} dy$$

$\boxed{\text{for any function } f(x)}$

$$\delta(x-y) = \int \frac{dk}{2\pi}\, e^{ik(x-y)}$$

$\Leftrightarrow$ orthogonal relation

$\hat{x}\cdot\hat{y} = 0,\quad \hat{x}\cdot\hat{z} = 0,\quad \hat{x}\cdot\hat{x} = 1$

$$\therefore f(x) = \int_{-\infty}^{\infty} \delta(x-y)\, f(y)\, dy$$

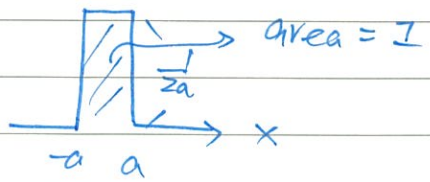
$\sum_k \frac{e^{ikx}}{2\pi}\cdot e^{-iky} \propto \delta_{x,y}.$

Other representations of $\delta(x-y)$:

(a) $\Delta(x,a) = 0 \qquad x < -a$

$\qquad = \frac{1}{2a} \qquad -a < x < a$

$\qquad = 0 \qquad x > a$



$$\lim_{a\to 0} \Delta(x,a) = \delta(x)$$

$$\lim_{a\to 0}\int dx\, f(x)\,\Delta(x,a) = f(0) \lim_{a\to 0}\int dx\, \Delta(x,a) = f(0)$$

any peaked function with width → 0 height → ∞

such that $\int \Delta(x,a)\,dx = 1$ can serve as

the Dirac delta function.

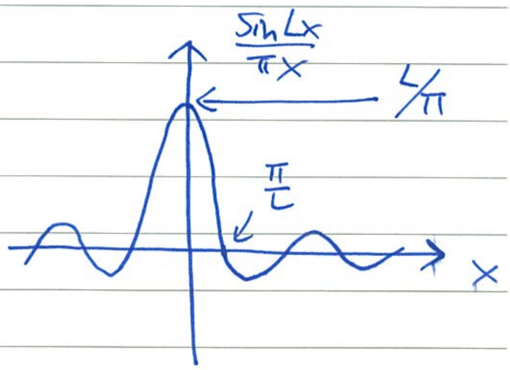
ex $\delta(x) = \lim_{a\to\infty} \frac{a}{\sqrt{\pi}} e^{-a^2x^2}$

$$\boxed{\int_{-\infty}^{\infty} \frac{a}{\sqrt{\pi}} e^{-a^2x^2} dx = \frac{a}{\sqrt{\pi}} \cdot \sqrt{\frac{\pi}{a^2}} = 1}$$

$\delta(x) = \lim_{a\to 0} \frac{1}{\pi} \frac{a}{x^2+a^2}$ $\qquad \int \frac{1}{\pi} \frac{a}{x^2+a^2} dx = 1$

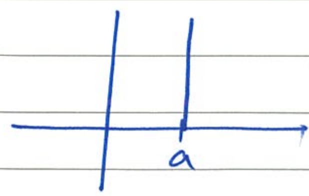
(b) $\delta(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk\, e^{ikx}$

$$= \frac{1}{2\pi} \lim_{L\to\infty} \underbrace{\int_{-L}^{L} dk\, e^{ikx}}_{\left.\frac{e^{ikx}}{ix}\right|_{k=-L}^{k=L}}$$



$$= \frac{1}{2\pi} \lim_{L\to\infty} \frac{1}{ix} \left(e^{ixL} - e^{-iLx}\right) = \lim_{L\to\infty} \frac{\sin Lx}{\pi x}$$

(c) $\int_{-\infty}^{x} dy\, \delta(y-a) = \begin{cases} 0 & x<a \\ 1 & x>a \end{cases}$



$= \theta(x-a) \qquad \therefore \frac{d}{dx}\theta(x-a) = \delta(x-a)$

* Propagation of wave packets

以上的考慮是靜止的情形。

當把時間 t 考慮進行，則有以下的情形，

① Any f(x,t) can be Fourier transformed for x & t separately:

$$f(x,t)=\int_{-\infty}^{\infty}\frac{dk}{2\pi}\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\, e^{i(kx-\omega t)}\, g(k,\omega)$$

時間之 convention 取 $e^{-i\omega t}$

$$g(k,\omega)=\int_{-\infty}^{\infty}dx\int_{-\infty}^{\infty}dt\, e^{-i(kx-\omega t)}\, f(x,t)$$

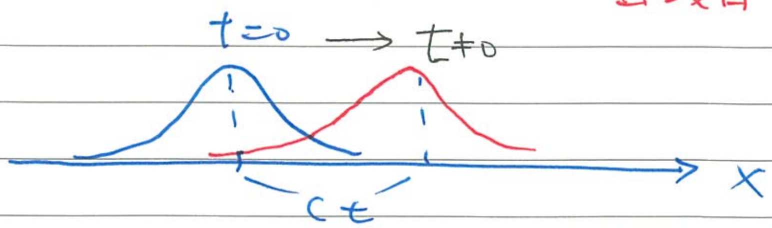
② 在① 之情形，x 與 t 是 2 獨立變數，可自由變化！但对於波來說就不是了！

若 $\omega=ck$，則每一個平面波為 $e^{i(kx-\omega t)}$
$=e^{ik(x-ct)}$

此時 $f(x,t)=\int_{-\infty}^{\infty}dk\, g(k)\, e^{ik(x-ct)}$ $\quad \boxed{g(k)e^{-ikct}=g(k,t)}$

$=f(x-ct)$

換句話說，波形 f 以速度 c 向右移動 (if c>0) 且沒有 distortion！



③ In general, $\underbrace{\omega = \omega(k)}$ 不一定 $= ck$!

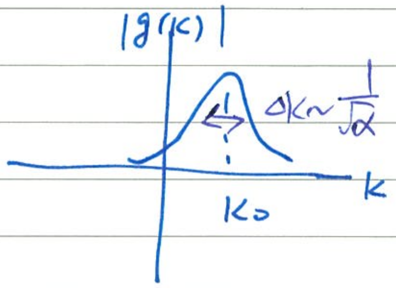
此時 dispersion relation ! (色散關係, 另不同的 k 可以走不同之速度)

$$\Downarrow$$

$$v_k = \frac{\omega(k)}{k}$$

$$f(x,t) = \int_{-\infty}^{\infty} dk\, g(k)\, e^{i(kx - \omega(k)t)}$$

若 $g(k)$ 集中在 $k = k_0$



$\Leftarrow$ 如 $g(k) = e^{-\alpha(k-k_0)^2}$

we can then expand

$$\omega(k) = \omega(k_0) + (k-k_0)\underbrace{\left.\frac{d\omega}{dk}\right|_{k=k_0}}_{\substack{\parallel \\ v_g}} + \frac{1}{2}(k-k_0)^2 \underbrace{\left(\frac{d^2\omega}{dk^2}\right)_{k_0}}_{\substack{\parallel \\ 2\beta}} + \cdots$$

若設 $k - k_0 = k'$

則 $f(x,t) \cong e^{i(k_0 x - \omega(k_0)t)}$

$$\int_{-\infty}^{\infty} dk' \underbrace{e^{-\alpha k'^2} e^{ik'(x - v_g t)} e^{-ik'^2 \beta t}}_{e^{-(\alpha + i\beta t)k'^2} e^{ik'(x - v_g t)}}$$

$$= e^{i(k_0 x - \omega(k_0)t)} \left(\frac{\pi}{\alpha + i\beta t}\right)^{\frac{1}{2}} e^{-\frac{(x - v_g t)^2}{4(\alpha + i\beta t)}}$$

(Gaussian packet)

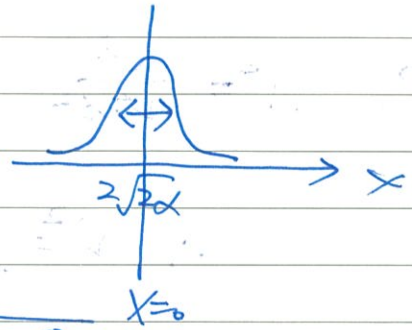
$$\therefore \quad |f(x,t)|^2 = \left(\frac{\pi^2}{\alpha^2+\beta^2t^2}\right)^{\frac{1}{2}} \underbrace{\left| e^{-\frac{(x-v_g t)^2}{4(\alpha^2+\beta^2t^2)}(\alpha-\beta i t)} \right|^2}$$

$$e^{A+iB} = e^{A}\, e^{iB}$$

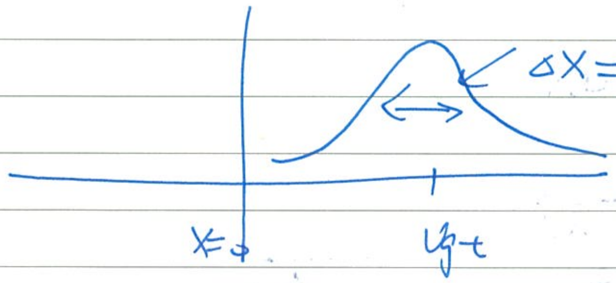
$$|e^{iB}| = 1$$

$$= \left(\frac{\pi^2}{\alpha^2+\beta^2t^2}\right)^{\frac{1}{2}} e^{-\frac{\alpha(x-v_g t)^2}{2(\alpha^2+\beta^2t^2)}}$$

$t=0.$ $\quad |f(x,0)|^2 = \frac{\pi}{\alpha}\, e^{-\frac{x^2}{2\alpha}}$



$t>0$



$$\Delta x = 2\sqrt{2\left(\alpha+\frac{\beta^2t^2}{\alpha}\right)}$$

additional growth

$\sim (\Delta k t)^2 \sim (\Delta p t)^2$

$\therefore$ It's spreading!

物理圖像：各k所走之速度不同！

類比
一個跑步
一個表演的
隊伍
在隊伍中移動的
wave

Note that wave packet's velocity

$= v_g = \left.\frac{d\omega}{dk}\right|_{k_0} =$ group velocity!

與 phase velocity $= \frac{\omega}{k}$ 不同

只有當 $\frac{\omega}{k} =$ 常數時，$v_g =$ phase velocity!

$\rightarrow$ $v_g = \frac{\Delta\omega}{\Delta k}$，$\left\{\begin{matrix}\omega \\ k\end{matrix}\right.$之差決定 v_g 有一點類似拍的現象

14 hour (+ HW I. 之檢討)

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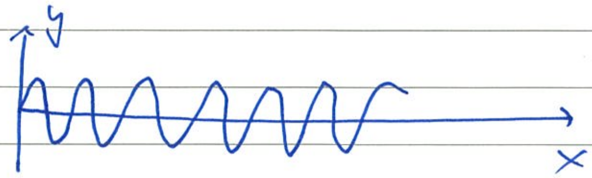
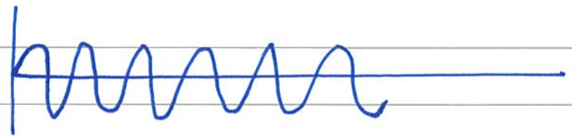
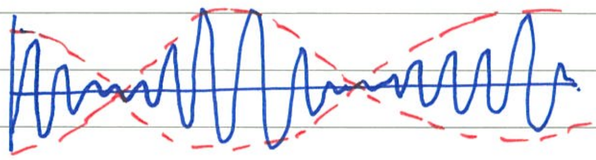
類似的現象 — 拍 (beat) ∵ 考慮二 ω 與 k 相近之波



$\omega_1 = \omega + \frac{1}{2}\delta\omega$ $\quad$ $k_1 = k + \frac{1}{2}\delta k$



$\omega_2 = \omega - \frac{1}{2}\delta\omega$ $\quad$ $k_2 = k - \frac{1}{2}\delta k$



$$y_1 = A\sin(k_1x - \omega_1t)$$

$$= A\sin\left[(kx-\omega t) + \frac{1}{2}(\delta k x - \delta\omega t)\right]$$

$$y_2 = A\sin(k_2x - \omega_2t)$$

$$= A\sin\left[(kx-\omega t) - \frac{1}{2}(\delta k x - \delta\omega t)\right]$$

$$y = y_1 + y_2$$

$$= 2A\sin(kx-\omega t)\cos\left[\frac{\delta k}{2}x - \frac{\delta\omega}{2}t\right]$$

$$= \underbrace{2A\cos\left[\frac{\delta k}{2}x - \frac{\delta\omega}{2}t\right]}_{\text{envelope}}\sin(kx-\omega t)$$

envelope (= 紅線部分之行進情形)

∴ $k_{beat} = \frac{\delta k}{2}$, $\omega_{beat} = \frac{\delta\omega}{2}$

$$\boxed{\begin{aligned} &\cancel{\frac{1}{\lambda_{beat}} = \frac{k_{beat}}{2\pi} = \frac{1}{4\pi}(k_1-k_2) = \frac{1}{2}\left(\frac{1}{\lambda_1}-\frac{1}{\lambda_2}\right)} \\ &\cancel{f_{beat} = 2\pi\,\omega_{beat} = \pi\,\delta\omega = \frac{1}{2}(f_1-f_2)} \end{aligned}}$$

波包之 Speed

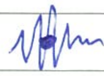
$$= \frac{\delta\omega/2}{\delta k/2} = \frac{\delta\omega}{\delta k} \; !$$

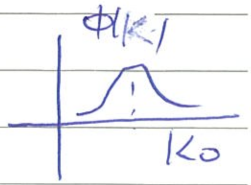
若 $\frac{\omega_1}{k_1} = \frac{\omega_2}{k_2}$

則 $\frac{\omega_1}{k_1} = \frac{\omega_2}{k_2} = \frac{\omega_1-\omega_2}{k_1-k_2} = \frac{\delta\omega}{\delta k}$

* Free particles & Schrödinger eq.

(i) De Broglie : free particles are wavepackets of matter waves





$$\therefore\ v_g = \frac{d\omega}{dk} \text{ should } = \left.\frac{p}{m}\right|_{k=k_0}$$

Now, if one assume $E = \hbar\omega$, $\therefore\ \omega = \frac{p^2}{2m\hbar}$

we get $v_g = \frac{1}{2m\hbar}\frac{dp^2}{dk} = \frac{p}{m\hbar}\frac{dp}{dk}$ 即只有 peak $p=k_0$ 滿足 $v_g = p/m$

Equating $\frac{p}{m\hbar}\frac{dp}{dk} = \frac{p}{m}$ $\therefore\ \frac{dp}{dk} = \hbar$

$\therefore\ p = \hbar k$ i.e. $\lambda = \frac{h}{p}$ $\because\ k_0$ is arbitrarily chosen, $\therefore\ p = \hbar k$ is generally correct.

(ii) A natural candidate to describe the matter wave of a free particle is: with time-dependence; (including the superposition principle)

上述 group velocity 合適用，且沒有高次項

$$\psi(x,t) \propto \int dk\ \tilde{\phi}(k)\ e^{i(kx-\omega t)}$$

$\hbar k = p$
$\hbar\omega = E$

$$\psi(x,t) = \int \frac{dp}{\sqrt{2\pi\hbar}}\ \phi(p)\ e^{i\left(\frac{px - E_p t}{\hbar}\right)}$$

$\Leftarrow$ 為了方便

inverse $\Leftrightarrow$ $\frac{\phi(p)}{\sqrt{2\pi\hbar}} e^{\frac{-iE_p t}{\hbar}} = \int \frac{dx}{2\pi}\ \psi(x,t)\ e^{\frac{-ipx}{\hbar}}$

$$\boxed{E_p = \hbar\omega = \frac{p^2}{2m}}$$ $\Leftarrow$ free particle

Each $e^{\frac{i}{\hbar}(px - E_p t)}$ is a plane wave describing the particle with p & energy E_p.

由於 $E_p = \frac{p^2}{2m}$，則 $\psi(x,t)$ 滿足

$$i\hbar \frac{d\psi}{dt} = \frac{1}{\sqrt{2\pi\hbar}} \int dp\, \phi(p) E_p\, e^{i\frac{1}{\hbar}(px - E_p t)}$$

$$= \frac{1}{\sqrt{2\pi\hbar}} \int dp\, \phi(p) \underbrace{\frac{p^2}{2m} e^{i\frac{1}{\hbar}(px - E_p t)}}_{\frac{1}{2m}(-\hbar^2)\frac{d^2}{dx^2}}$$

$$= -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi$$

此即為 free matter wave 所遵守之方程式，稱為 Schrödinger 方程式.

此方程式是由 Schrödinger 猜出來，以上並非其推導！但在猜的過程，$E = \frac{p^2}{2m}$ 具有 guide 之作用.

當 matter wave 不 free 時，$\because E = \frac{p^2}{2m} + V(x)$

可以考慮一特例：$p=0$，V=常數來說服自己

↳ 多維之推廣

a natural guess is then

$$i\hbar \frac{d\psi(x,t)}{dt} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x,t) + V(x,t)\psi(x,t)$$

此即為 Schrödinger eq.

似乎有這樣的對應 / 取代

古典中之 $p \to -i\hbar\frac{d}{dx}$

注意它滿足了 Superposition principle (by construction)

$E \to i\hbar\frac{d}{dt}$

在數學上 ⇒ linear.

* <u>The uncertainty relations.</u> complementary variables.

As we have seen, $\Delta x \Delta p \gtrsim \hbar$. (uncertainty relation) Heisenberg 提出

It indicates, when $\Delta p \Rightarrow 0$, $\Delta x = \infty$,

for example, the plane wave solution $\psi \propto e^{\frac{i}{\hbar}(px - Et)}$

$|\psi|^2 = \text{const.}$ ∴ particles can be found equally probably at each space point!

⇒此為粒子具波動性之極限.

On the other hand, if $\Delta x \to 0$, $\Delta p \to \infty$,

即如果粒子被localized，其動量就有許多可能。

這指出了我們不能同時指定精確的 x 與 p 給粒子！此與古典的情形完全不同！(那時, a particle is described by x & v!)

注意：由於 ħ 很小，所以對古典之particle 而言，uncertainty relation 並不是detectable!

如：a particle with $m = 0(gm)$

$v = 0(cm/sec)$, if $\Delta p \lesssim 10^{-2}$ (gm cm/sec)

$\Delta x \simeq 10^{-25}$cm! ($\hbar \sim 10^{-27}$ erg·sec)

幾乎是測不到! 波動性 (Δx為其波動性之範圍)

(∵m small)

但对於 microscopic object, Δp 很小, $\therefore \Delta x$ 可以到 $\mathring{A}$ 之範圍而被測到.

以下是一些所謂的 Gedanken expt. (假想但可實現的實驗) 用以說明測不準原理 :

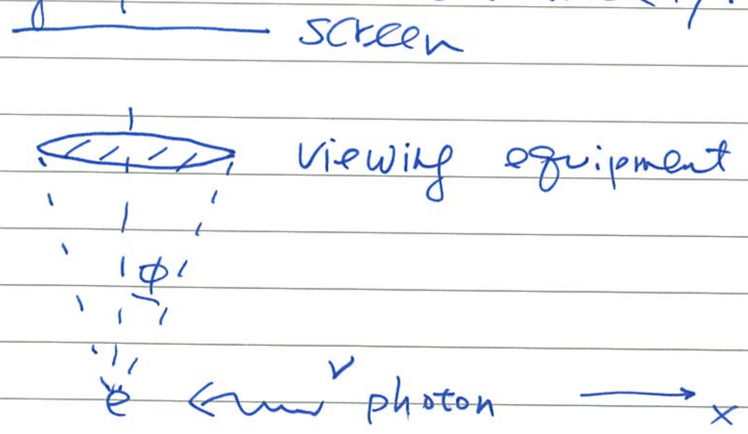
(a) The Heisenberg Microscope 新版 有新的例子, see page 32-33

假設我們要測量一個電子之位置, 如何測呢?

typical: look at it !

by looking at it, we use light to shine on the electron.

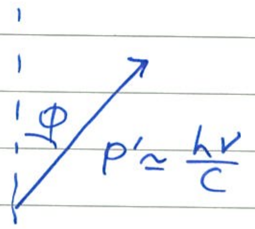
In order to disturb the electron as little as possible, we have to reduce the intensity of light. So, finally, the electron only interacts with one photon as shown in the following picture schematically:



To see where the electron is, we need to view it via the microscope.

Now, before collision, photon, $\boxed{p = \frac{h\nu}{c}}$

let's use γ-ray so that $E = h\nu$ is large.



∴ after collison $E' \simeq h\nu$

$\therefore p' \simeq \frac{h\nu}{c}$

$\therefore \boxed{\underbrace{\Delta p_x \text{ of electron}}_{} \simeq 2\frac{h\nu}{c}\sin\phi}$

uncertainty of electron's momentum after collision.

A fact from optics: microscope 所能定之位置有一定的 resolution limit:

$$\Delta x \gtrsim \frac{\lambda}{\sin\phi}$$ (即電子之位置之偵測有不準度!)

$\therefore \Delta p_x \Delta x \gtrsim h \sim \hbar$

Note that: 每一次做實驗, photon 之 recoil 的 momentum 方向都不同, 這是 Δp_x 之起源! 因此或許有人想去測 screen 之 momentum 以定出 photon 的 momentum 這時就必須將 screen 納入分析! 一旦定出其 momentum, 則 $\Delta x = \infty$, 此時就不知电子之位置了!

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Resolution of a microscope

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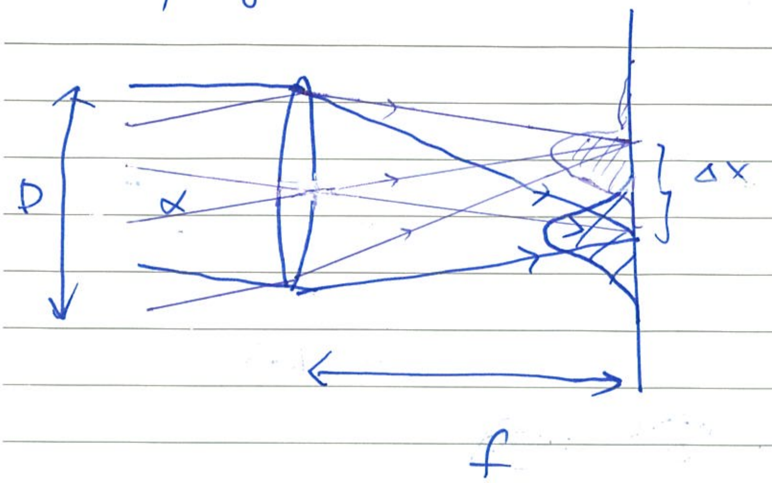
* Rayleigh criterion:

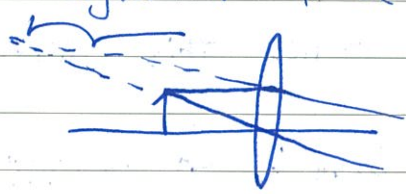


$\Delta x \gtrsim \alpha f$

$\alpha \gtrsim 1.22\frac{\lambda}{D}$ (min angle to be resolved)

($D\sin\alpha \sim \lambda$!)

A microscope essentially use a magnifier + a telescope:



magnifer

物品要放在 f 左右, 使出來之光 almost parallel

$d\theta$ = 平行光夾 α 角可被區分之 criterion is $\alpha \gtrsim 1.22\frac{\lambda}{D}$

but $\frac{\Delta x}{f} \sim \alpha$ $\therefore$ $\Delta x \gtrsim 1.22\lambda\frac{f}{D} \sim \frac{1.22\lambda}{2\sin\phi}$

$\sim \frac{\lambda}{\sin\phi}$

(仔細的計算: $\Delta x = \frac{1.22\lambda}{2\sin\phi \cdot n}$)

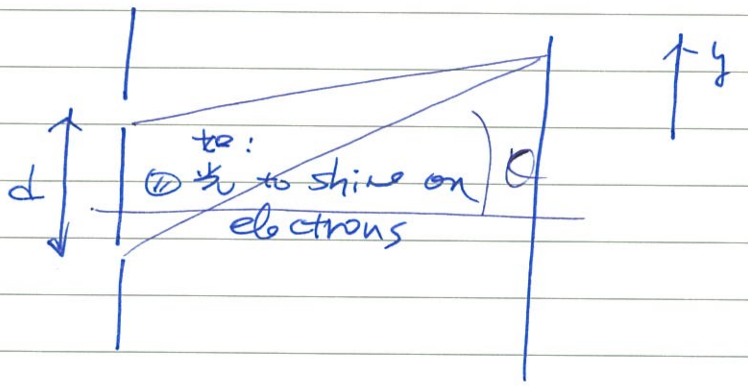
n ← microscope 所處在 liquid or air 之折射率

Monitor
(b) the two-slit expt.

如果我們要決定電子到底從那一個 slit 通過，
在 two-slit expt 中

則我們一定要能測量電子之 position y

such that $\Delta y < d/2$



此時，photon 會給 e 一個 $\Delta p_y \gtrsim \frac{2}{d} h$

因此，電子走的方向就有以下之不確定性

$$\frac{\Delta p_y}{p} \gtrsim \frac{2}{d}\frac{h}{p} \simeq \frac{2\lambda}{d}$$

而因為造成干涉條紋：為：$d\sin\theta = n\lambda$

∴ 相鄰條紋：$\Delta\sin\theta = \frac{\lambda}{d}$

因此，此方向不確定 > 條紋之間距

將條紋"洗掉"！ 形成

回到像粒子之行為

(c) Can we measure the orbits in the Bohr atom?

$$R_n = \frac{1}{4\pi}\frac{n^2 h^2}{Ze^2 m} = \frac{n^2 \hbar^2}{Ze^2 m} \qquad Z=1$$

$$= n^2\hbar \frac{\hbar c}{e^2}\frac{1}{mc}$$

$$= \frac{n^2\hbar}{\alpha mc}, \qquad v = \frac{2\pi e^2 Z}{nh} = c\cdot\frac{Z\alpha}{n}$$

To measure the orbit, $\Delta x \ll R_n - R_{n-1} \simeq \frac{2\hbar n}{\alpha mc}$

$\therefore \Delta p \gg \frac{mc\alpha}{2n}$

→ 不代表 Δ = 微分!

$\therefore \Delta E \sim \Delta \frac{p^2}{2m} \sim \frac{p}{m}\Delta p$ (order of magnitude analysis)

$$\gg \frac{mc\alpha}{2n}\cdot\frac{c\,\alpha}{n} = \frac{1}{2}\frac{mc^2\alpha^2}{n^2} = \frac{13.6\,eV}{n^2}$$

$\therefore \Delta E \gg 13.6\,eV$, 此時 electron 早已被電離出去

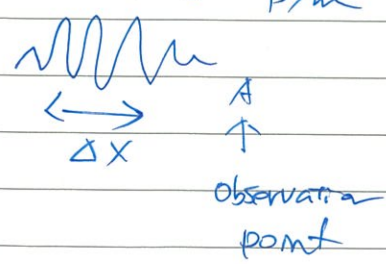
所以測不到 orbit.

(d) The energy-time uncertainty relation

If we rewrite $\Delta x \Delta p \geq \hbar$ as

$$\left(\frac{p}{m}\Delta p\right)\left(\Delta x \frac{m}{p}\right) \geq \hbar, \qquad \rightarrow v = p/m$$

we can $\boxed{\text{re-interprete}}$ it as



$$\Delta E \underbrace{\Delta t}_{\text{確定物質波通過A點之時間}} \geq \hbar$$

此時 $\Delta E \sim \Delta \frac{p^2}{2m}$，$\Delta t = \frac{\Delta x}{v}$ = uncertainty in its localizability in time.

此關係也可由 ω 與 t 互為 Fourier transformation 之事實（⟺ p 與 x 之關係）可得到！

不過在 non-relativistic Q.M. 中，$\Delta E \Delta t \geq \hbar$ 與 $\Delta p \Delta x \geq \hbar$ 之關係不同：

* $\Delta p \Delta x \geq \hbar$ 可以由 Q.M. 嚴格推出，但 $\Delta E \Delta t \geq \hbar$ 無法
（有測量之意義）（則）. . . . .

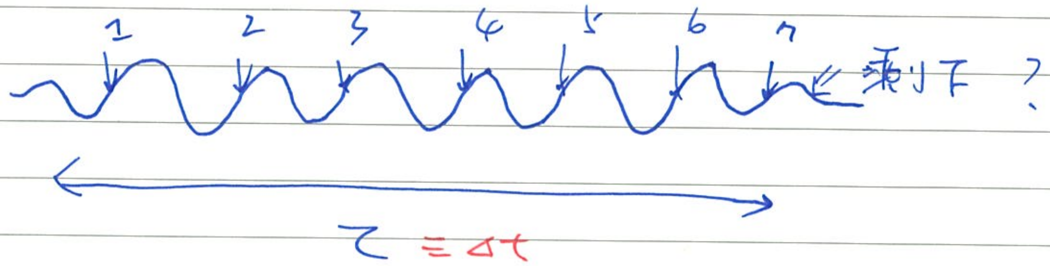
主要是因為 time 在 Q.M. 只是一個參數並沒有測量之意義！

但是 $\Delta E \Delta t \geq \hbar$ 對定性了解一些行為仍是有所幫助！

example：在談光譜時 $\frac{E-E'}{h} = \nu$，我們基本假設放出之光子的頻率正為 ν 可是這樣的波，是由 t=−∞ to t=∞ 振盪的

In reality, it has a finite decay time (從發光到結束), say, $\tau \sim 10^{-8}$ sec,

∴ The wave looks like



此時，$\nu = ?$

$\because \nu = \dfrac{\#\ \text{of cycles}}{\tau}$ ，而在此 # of cycles

因在二端之 amplitude decrease 之關係，可能會

少算 1 或多算 1 個

$\therefore \Delta N = \pm 1$ 真實的推導為 $\frac{1}{2}$

$\therefore \Delta \nu = \dfrac{1}{\tau}$ $\therefore \Delta t\, \Delta \nu \gtrsim 1$ $\therefore \Delta E\, \Delta t \gtrsim \hbar$

此為 $\Delta E\, \Delta t \gtrsim \hbar$ 之“寫實”意義.

Note that $\because \tau = 10^{-8}$ sec

$\therefore \Delta \nu \gtrsim \dfrac{1}{2\pi\tau} = 1.6 \times 10^{7}\ s^{-1}$

$\Delta E = \hbar \Delta \omega = h \Delta \nu = 6.6 \times 10^{-8}\ eV \ll 13.6\ eV.$

h: 4.14×10^{-15} eV·s

ΔE: $E_n - E_m$ 之不準度

*Order of magnitude Estimates

The uncertainty relation can be used to estimate useful quantities:

example. 1. Ground state energy of H-atom

approximate $p \sim \Delta p \quad r \sim \Delta r$

$$\Delta p \Delta r \sim \hbar . \quad \Delta p \sim \frac{\hbar}{r}$$

$$\therefore E = \frac{p^2}{2m} - \frac{e^2}{r} = \frac{\hbar^2}{2mr^2} - \frac{e^2}{r}$$

$\frac{dE}{dr} = 0$ 求 E 之 min

$$\Rightarrow -\frac{\hbar^2}{mr^3} + \frac{e^2}{r^2} = 0 \quad \therefore r = \frac{\hbar^2}{me^2} = \frac{\hbar}{mc}\frac{\hbar c}{e^2} = \frac{\hbar}{mc\alpha}$$

$$\therefore E_{min} = \frac{\hbar^2}{2m}\left(\frac{mc\alpha}{\hbar}\right)^2 - e^2\frac{mc\alpha}{\hbar}$$

$$= +\frac{mc^2}{2}\alpha^2 - mc^2\underbrace{\left(\frac{e^2}{\hbar c}\alpha\right)}_{=\alpha^2}$$

$= -\frac{1}{2}mc^2\alpha^2$ 與 exact 解一樣

這當然只是巧合，若 $\Delta p \Delta r$ 取得不是 $\hbar$ 而是 $\frac{\hbar}{2}$，則結果會不同！

不過重點是 Q.M. 與 classical 不同，$\frac{e^2}{r}$ 無法將電子無限的在 $r=0$ 綁住！∵ $r \to 0$, Δp↑（動能↑）

example 2. Binding energy for neucleons

电子的 binding energy $\sim O(eV)$

what about neucleon ?

$m \simeq 1.6 \times 10^{-24} gm$

$r \sim 10^{-13} cm$. $\Delta p \sim p \sim \hbar / r \sim \dfrac{10^{-27} erg\ sec}{10^{-13} cm}$

$\sim 10^{-14} gm\ cm/sec$

$\therefore \dfrac{p^2}{2m} \sim \dfrac{10^{-28}}{3.2 \times 10^{-24}} \sim 3 \times 10^{-5} ergs$

$1 eV = 1.6 \times 10^{-19} Joule \simeq 1.6 \times 10^{-12} ergs$

$\therefore \dfrac{p^2}{2m} \sim 2 \times 10^{7} eV = 20 MeV$

$\therefore$ binding energy $\gtrsim 20 MeV \sim O(MeV)$

rather than $O(eV)$! (Note : $MeV \neq meV$)

example 3. Pions

Yukawa 在 1953年提出 nuclear force 是由于二 neucleon 會放 pi-meson (pions) 再被其他 neucleon 吸收之故.

若設 $\mu =$ pion 之質量 $E \sim \mu c^2$

當放出 pion 時. neucleon 之 energy 有一不準度

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利用 測不準原理, Yukawa argued

只要這個過程發生在 Δt. 且 $\underbrace{\Delta t \Delta E \gtrsim \hbar}$ 即可!

若我們盯著 neucleon 看,对其作時間的頻譜分析,
則有 $\Delta\omega$, $\Delta E = \hbar \Delta\omega$
即其能量並不準.

$\because \Delta E \sim \mu c^2$

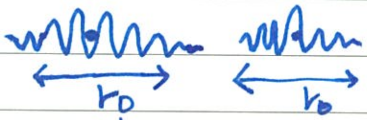
$\therefore \Delta t \sim \hbar / \mu c^2$

若此 particle 之速度 ~c)

則 $c\Delta t \sim \frac{\hbar}{\mu c}$ 為 neucleus force 之範圍!

$\because$ neucleus $\sim O(1.4 \times 10^{-13}\ \text{cm})$ 記 r_0 (~ size of neucleon)

$\therefore \frac{\hbar}{\mu c} \sim r_0 \qquad \mu c^2 \sim \frac{\hbar c}{r_0} \sim \frac{10^{-27} \times 3 \times 10^{10}}{1.4 \times 10^{-13}}\ \text{erg}$



$\sim 130\ \text{MeV}$

後來 pion 被發現了, $\mu c^2 \simeq 140\ \text{MeV}$!

Chapter 3.

由上一章的討論得知，物質波可由所謂的波函數 $\Psi(x,t)$ 來描述其在空間及時間上的行為

① $\Psi(x,t)$ 為 complex (in general)

② $\Psi(x,t)$ satisfies the Schrödinger eq. (猜出來的！)

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi(x,t) + \underbrace{V(x,t)}_{\text{位能}}\Psi(x,t) = i\hbar\frac{\partial\Psi(x,t)}{\partial t}$$

$\equiv \hat{H}\Psi(x,t)$

↳ Hamiltonian.

為 $E = \frac{p^2}{2m} + V$ 之反映

③ $|\Psi(x,t)|^2$ = probability density at (x,t)

$\int_{-\infty}^{\infty}|\Psi(x,t)|^2dx = 1$ (normalization, 正規化)

在這一章，我們將討論 Schrödinger 方程式及機率解釋之一些基本性質。

* Linearity

若 $\Psi_1(x,t)$ 是解，$\Psi_2(x,t)$ 是解，則 $\Psi(x,t) = \Psi_1(x,t) + \Psi_2(x,t)$ 也是解 (Superposition)

若 $\Psi(x,t)$ 是解，$c\Psi(x,t)$ 也是解！

* First order in time

∴ if $\underbrace{\Psi(x,0)}_{\text{initial state}}$ is known, $\Psi(x,t)$ is known :

initial state ⟺ classical $x(0)$, $v(0)$

$$\Psi(x,t+\Delta t)=\Psi(x,t)+\frac{\partial}{\partial t}\Psi(x,t)\,\Delta t$$

$$=\Psi(x,t)+\frac{-i}{\hbar}\hat{H}\,\Psi(x,t)\,\Delta t$$

example : free particle

$$i\hbar\frac{\partial}{\partial t}\Psi(x,t)=-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2}$$

$$\Psi(x,t)=\frac{1}{\sqrt{2\pi\hbar}}\int dp\,\boxed{\phi(p)}\,e^{\frac{i}{\hbar}\left(px-\frac{p^2}{2m}t\right)}$$

與t無關 才能滿足Schrödinger 方程式

initial state $\Psi(x,0)=\frac{1}{\sqrt{2\pi\hbar}}\int dp\,\phi(p)\,e^{\frac{i}{\hbar}px}$

$$\therefore\ \frac{1}{\sqrt{2\pi\hbar}}\phi(p)=\int\frac{dx}{2\pi}\,e^{-\frac{i}{\hbar}px}\,\Psi(x,0)$$

$\therefore$ 一旦 $\Psi(x,0)$ is Known, $\phi(p)$ is Known

$\Rightarrow$ $\Psi(x,t)$ is Known!

example : 之前作 $v_g=\frac{d\omega}{dk}$ 之例

Note that in general if $V\neq 0$, $\phi(p)$ will also depend on t i.e., $\phi(p)\Rightarrow\phi(p,t)$

這对應到古典的一個事實: Force=0 p是固定的

* The role of phases

in general $\Psi(x,t)=R(x,t)\,e^{\frac{i}{\hbar}S(x,t)}$

Real ! $\begin{cases} R(x,t)=|\Psi(x,t)| \text{ is the } \boxed{\text{amplitude}} \\ S(x,t)/\hbar \text{ is the phase of } \Psi(x,t) \end{cases}$

Since $|\psi(x,t)|^2 = R^2(x,t)$ gives the probability density, it would appear that $S(x,t)$ is unimportant.

This is not correct!

First, we note that $S(x,t)$ is defined up to $\boxed{2\pi \cdot \text{integer} \times \hbar}$!

Secondly, by supperposition, if ψ_1 & ψ_2 are solution, $\psi = \psi_1 + \psi_2 = R_1 e^{i\theta_1} + R_2 e^{i\theta_2}$ is also the solution.

超導為例

此時 $|\psi|^2 = R_1^2 + R_2^2 + \underbrace{2R_1R_2\cos(\theta_1 - \theta_2)}$

the relative phase $\theta_1 - \theta_2$ gives rise to interference in $|\psi|^2$

* Probability Current

We shall show that if at $t=0$

$$\int_{-\infty}^{\infty} P(x, t=0)\, dx = 1 \quad \text{is satisfied,}$$

at later time t, $\int_{-\infty}^{\infty} P(x,t)\, dx = 1$ is always satisfied!

This is guaranteed by the existence of probability current:

Let us calculate $\frac{dP(x,t)}{dt}$, $P(x,t) = |\psi(x,t)|^2$

$= \psi(x,t)\,\psi^*(x,t)$

$$\because \frac{dP(x,t)}{dt} = \frac{d\psi(x,t)}{dt}\psi^*(x,t) + \psi(x,t)\frac{d\psi^*(x,t)}{dt}$$

$$i\hbar \frac{d\psi(x,t)}{dt} = \frac{-\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V\psi \quad \text{——} \ (1)$$

$$-i\hbar \frac{d\psi^*}{dt} = \frac{-\hbar^2}{2m}\frac{d^2\psi^*}{dx^2} + V^*\psi^* \quad \text{—} \ (2)$$

若 $V^* = V$, $\psi^* \times (1) - \psi \times (2)$

see Ex 3.3 for the case when $V^* \neq V$

$$i\hbar\left[\psi^*\frac{d\psi}{dt} + \psi\frac{d\psi^*}{dt}\right]$$

$$= \frac{-\hbar^2}{2m}\left[\psi^*\frac{d^2\psi}{dx^2} - \psi\frac{d^2\psi^*}{dx^2}\right]$$

$$= \frac{-\hbar^2}{2m}\frac{d}{dx}\left[\psi^*\frac{d\psi}{dx} - \psi\frac{d\psi^*}{dx}\right]$$

$$\frac{dP(x,t)}{dt} = \psi^*\frac{d\psi}{dt} + \psi\frac{d\psi^*}{dt}$$

$$= \frac{i\hbar}{2m}\frac{d}{dx}\left[\psi^*\frac{d\psi}{dx} - \psi\frac{d\psi^*}{dx}\right] \equiv -\frac{d}{dx}j(x,t)$$

$$j(x,t) \equiv \frac{\hbar}{2mi}\left(\psi^*\frac{d\psi}{dx} - \psi\frac{d\psi^*}{dx}\right) = \text{probability current density}$$

$$= \frac{1}{2m}\left[\psi^*\hat{p}\psi + \psi(\hat{p}\psi)^*\right]$$

$$[P(x,t)] = \frac{\text{Probability}}{\text{length}}$$

$$[j(x,t)] = \frac{[P(x,t)]}{\text{time}} \times \text{length}$$

$$= P(x,t) \times \frac{\text{length}}{\text{time}} = [p(x,t)\, v]$$

$$\Leftarrow\quad j_e = \rho v$$

example. $\psi(x,t) = Ae^{i(kx-\omega t)}$ $\qquad Ae^{i\varphi}$

$$j = |A|^2 \frac{\hbar \nabla \varphi}{m}$$

$$j(x,t) = \frac{\hbar}{2mi}\left[A^* ik A - A(-ik)A^*\right]$$

$$= \frac{\hbar k}{m}|A|^2 = \frac{p}{m}|\psi(x,t)|^2 = v\, P(x,t)$$

$$\frac{\partial P(x,t)}{\partial t} + \frac{\partial}{\partial x} j(x,t) = 0$$

為所謂的 local conservation law for probability:

x_1 —— x_2

$\int_{x_1}^{x_2} P(x,t)\,dx$ = probability of finding the particle at (x_1, x_2)

$$\frac{d}{dt}\int_{x_1}^{x_2} p(x,t)\,dx = \int_{x_1}^{x_2} \frac{\partial P}{\partial t}\,dx$$

$$= \int_{x_1}^{x_2} -\frac{\partial}{\partial x} j(x,t)\,dx$$

$$= j(x_1,t) - j(x_2,t)$$

meaning

$j(x,t) = \frac{\text{probability}}{\text{time}}$ flow across. x point

$(\Rightarrow\ >0,\ \Leftarrow\ -)$

$\therefore\ j(x_1,t) - j(x_2,t) =$ 流入 (x_1,∞) 之机率 per time

$-$流入 (x_2,∞) .. ..

$=$ 流入 (x_1,x_2) 之机率 per time

$= \frac{d}{dt}\int_{x_1}^{x_2} p(x,t)\,dx$!

取 $x_2=\infty$, $x_1=-\infty$. $\because\ j(\infty,t)=0.\ j(-\infty,t)=0$

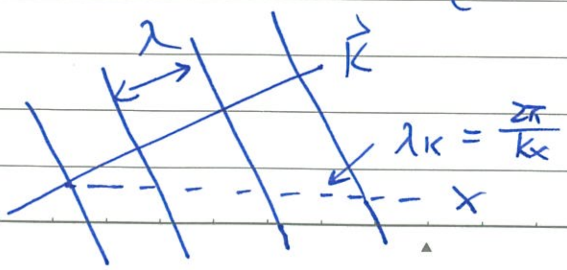
$\therefore\ \frac{d}{dt}\int_{-\infty}^{\infty} p(x,t)\,dx = 0$

$\therefore\ \int_{-\infty}^{\infty} p(x,t)\,dx = \int_{-\infty}^{\infty} p(x,0)\,dx = 1$

Generalized to 3D

3D plane waves e^{ikx}

$\Rightarrow\ e^{i\vec{k}\cdot\vec{r}}$



$$\therefore \Psi(\vec{r},t) = \left(\frac{1}{\sqrt{2\pi\hbar}}\right)^3 \int dp_x \int dp_y \int dp_z \, \Phi(\vec{p}) \, e^{\frac{i}{\hbar}(\vec{p}\cdot\vec{r} - \frac{p^2}{2m}t)}$$

describes the free particle!

$$i\hbar \frac{\partial}{\partial t} \Psi(\vec{r},t) = \left(\frac{1}{\sqrt{2\pi\hbar}}\right)^3 \int d^3\vec{p} \, \Phi(\vec{p}) \, \frac{1}{2m}(p_x^2+p_y^2+p_z^2) \, e^{\frac{i}{\hbar}(\vec{p}\cdot\vec{r} - \frac{p^2}{2m}t)}$$

$$= \frac{-\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) \Psi(x,t)$$

$\therefore$ Schröding equation in 3D

$$i\hbar \frac{\partial}{\partial t} \Psi(\underbrace{x, y, z}_{\vec{r}}, t) = \frac{-\hbar^2}{2m} \underbrace{\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)}_{\nabla^2} \Psi(x,y,z,t)$$

$$+ U(x,y,z,t)\, \Psi(x,y,z,t)$$

此時 $$\frac{\partial \rho(\vec{r},t)}{\partial t} + \vec{\nabla}\cdot\vec{j} = 0$$

$[\rho] = \frac{机率}{L^3}$

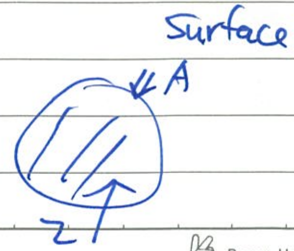
此時 $[j] = \frac{机率}{L^2 \cdot sec}$

$$\vec{j}(\vec{r},t) = \frac{\hbar}{2mi}\left(\Psi^* \vec{\nabla}\Psi - \Psi \vec{\nabla}\Psi^*\right)$$

$\because j \cdot area = \frac{机率}{sec}$

$$\vec{\nabla}\cdot\vec{j} = \frac{\partial j_x}{\partial x} + \frac{\partial j_y}{\partial y} + \frac{\partial j_z}{\partial z}$$

$$\frac{d}{dt}\int_\tau \rho(\vec{r},t)\, d^3r = \oint_A \vec{j}\cdot d\vec{s}$$



* Expectation values

(期望值)

例: 擲一個骰子之平均點數 $= \frac{1}{6}\times 1 + \frac{1}{6}\times 2 + \frac{1}{6}\times 3 + \cdots \frac{1}{6}\times 6$

$\parallel$

<點數> $= 3.5$

expt. 擲 10^4 次

1600 次 1 點

1700 次 2 點

⋮

$$\frac{1600\times 1 + 1700\times 2 + \cdots}{10^4}$$

$$= \frac{1600}{10^4}\times 1 + \frac{1700}{10^4}\times 2 + \cdots$$

$$\simeq \frac{1}{6}\times 1 + \frac{1}{6}\times 2 + \cdots$$

∴ Given a matter wave function $\psi(x,t)$

前提 $\int_{-\infty}^{\infty} |\psi(x,t)|^2 dx = 1$

$$\langle x \rangle = \int_{-\infty}^{\infty} \underbrace{dx\, |\psi(x,t)|^2}_{\substack{\text{probability of finding} \\ \text{the particle in } (x,\, x+dx)}} \cdot x$$

$$= \int_{-\infty}^{\infty} dx\, \psi^*(x,t) \times \psi(x,t)$$

(不一定發生在 $P(x,t)$ 之最大值)

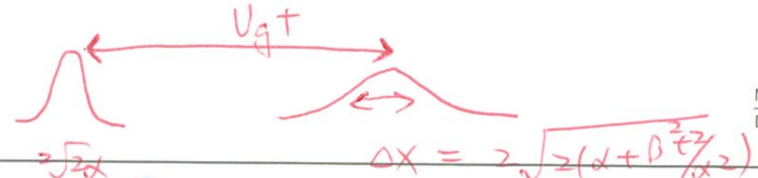
期望值是要針對某一wave function而言的!

同理

$$\langle f(x) \rangle = \int_{-\infty}^{\infty} dx\, \psi^*(x,t)\, f(x)\, \psi(x,t)$$

example. Gaussian wave packet

$$\psi(x,t) = e^{i(k_0 x - \omega(k_0)t)} \sqrt{\frac{\pi}{\alpha + i\beta t}}\; e^{-\frac{(x - v_g t)^2}{4(\alpha + i\beta t)}}$$



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NO. (HW.2)

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3-P.

先檢查 $\psi(x,t)$ 是否規一化 (normalized):

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

$$= \sqrt{\frac{\pi^2}{\alpha^2+\beta^2t^2}} \int_{-\infty}^{\infty} dx\, e^{-\frac{\alpha(x-v_gt)^2}{2(\alpha^2+\beta^2t^2)}}$$

$$= \sqrt{\frac{\pi^2}{\alpha^2+\beta^2t^2}} \underbrace{\int_{-\infty}^{\infty} dx'\, e^{-\frac{\alpha x'^2}{2(\alpha^2+\beta^2t^2)}}}_{\sqrt{\frac{\pi}{\frac{2(\alpha^2+\beta^2t^2)}{\alpha}}}}$$

$x' = x - v_g t$

$$= \sqrt{\frac{\alpha}{2}}\, \frac{\pi^{3/2}}{\alpha^2+\beta^2t^2} \quad \text{未規一化.}$$

此時 $$\langle f(x)\rangle = \frac{\int_{-\infty}^{\infty} dx\, \psi^*(x,t)\, f(x)\, \psi(x,t)}{\int_{-\infty}^{\infty} dx\, \psi^*(x,t)\, \psi(x,t)} \longleftarrow \boxed{\text{總數}}$$

$\because$ 規一化之波函數 $$\psi_N = \frac{\psi(x,t)}{\sqrt{\int_{-\infty}^{\infty} dx\, |\psi|^2}}$$

$$\therefore \langle x\rangle = \frac{\int_{-\infty}^{\infty} dx\, |\psi(x,t)|^2\, x}{\int_{-\infty}^{\infty} dx\, |\psi(x,t)|^2}$$

$$\because \int_{-\infty}^{\infty} dx\, |\psi(x,t)|^2 x = \int_{-\infty}^{\infty} dx \sqrt{\frac{\pi^2}{\alpha^2+\beta^2t^2}}\, e^{-\frac{\alpha(x-v_gt)^2}{2(\alpha^2+\beta^2t^2)}}\, x$$

$$= \int_{-\infty}^{\infty} dx' \sqrt{\frac{\pi^2}{\alpha^2+\beta^2t^2}}\, e^{-\frac{\alpha x'^2}{2(\alpha^2+\beta^2t^2)}} (\cancelto{0}{x'} + v_g t) = v_g t \int_{-\infty}^{\infty} |\psi|^2 dx$$

$x' = x - v_g t$

$\therefore \langle x\rangle = v_g t.$ (time-dependent!)

$\langle p \rangle = ?$

對量子力學而言，比較困難的是如何求 $\langle p \rangle$？

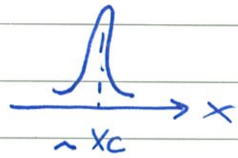
因為測不準原理告訴我們 $\Delta x \Delta p$ 之大

因此，給定 $\Psi(x,t)$，$dx|\Psi(x,t)|^2$ 給出找到質點在 $(x, x+dx)$ 之机率。這些都是和 x 有關的，那找到質點在 $(p, p+dp)$ 之机率為何？

Guidance: classical particle $\Leftrightarrow$ sharp wavepacket

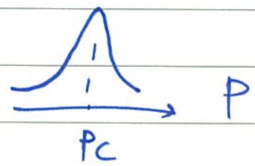
利用 correspondence principle

$$P_c = m\frac{dx_c}{dt}$$



$$x_c \simeq \langle x \rangle$$

$$p_c \simeq \langle p \rangle$$



∴ 期待：$\langle p \rangle = m\frac{d\langle x \rangle}{dt}$ to be correct!

（事實上，這是可以証明的！）

由此可得 $\langle p \rangle$！

$$\langle p \rangle = m\frac{d}{dt}\int_{-\infty}^{\infty} dx\, \Psi^*(x,t) \times \Psi(x,t)$$

$$= m\int_{-\infty}^{\infty} dx \left[\frac{d\Psi^*(x,t)}{dt} \times \Psi(x,t) + \Psi^*(x,t) \times \frac{d\Psi(x,t)}{dt}\right]$$

$\frac{dx}{dt}=0$ 以x為一變數！

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Basic properties of $\langle \ \rangle$

$$\langle \alpha x \rangle = \alpha \langle x \rangle \quad , \quad \langle \alpha f(x) \rangle = \alpha \langle f(x) \rangle$$

Constant

$$\langle X_1 + X_2 \rangle = \langle X_1 \rangle + \langle X_2 \rangle$$

$$\langle X^2 \rangle \neq \langle X \rangle \langle X \rangle$$

即 $\langle p \rangle = m \int_{-\infty}^{\infty} dx \times \underbrace{\frac{d}{dt} P(x,t)}_{= -\frac{d}{dx} j(x,t)}$

$$= -m \int_{-\infty}^{\infty} dx \; \cancel{\frac{d}{dx}[x j(x,t)]} - \underbrace{\frac{dx}{dx}}_{=1} j(x,t)$$

0 by integration by parts

$$= \int_{-\infty}^{\infty} dx \; \underbrace{m j(x,t)}$$

$[j] = v P(x,t)$ (意義很清楚!)

$$= \int_{-\infty}^{\infty} dx \; m \frac{\hbar}{2mi} \left(\psi^* \frac{d\psi}{dx} - \psi \frac{d\psi^*}{dx} \right)$$

第二項 $-\int_{-\infty}^{\infty} \psi \frac{d\psi^*}{dx} dx = -\int_{-\infty}^{\infty} dx \frac{d}{dx}(\psi\psi^*) - \psi^* \frac{d\psi}{dx}$

$$= \cancel{\psi\psi^*} \Big|_{x=-\infty}^{x=\infty} + \int dx \, \psi^* \frac{d\psi}{dx}$$

0

= 第一項

$$\therefore \langle p \rangle = \int_{-\infty}^{\infty} dx \; m \frac{\hbar}{2mi} \psi^*(x,t) \frac{d\psi(x,t)}{dx} \times 2$$

$$= \int_{-\infty}^{\infty} dx \; \psi^*(x,t) \frac{\hbar}{i} \frac{d\psi(x,t)}{dx} \quad \text{— ①}$$

∴ 和 $\langle x \rangle = \int_{-\infty}^{\infty} dx \; \psi^*(x,t) \times \psi(x,t)$ 不同處

即 $x \Rightarrow$ replaced by $\frac{\hbar}{i}\frac{d}{dx}$

∴ 似乎，p 在做平均時要以 $\boxed{\frac{\hbar}{i}\frac{d}{dx} = \hat{p}\ (\text{operator})}$ 來取代！(這件事也在猜 Schrödinger eq 發生過)

這樣合理嗎？

Let's look at eq. ① from another point of view:

$$\psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int dp\ \phi(p)\ e^{\frac{ipx}{\hbar}}, \quad \phi(p) = \int \frac{dx}{\sqrt{2\pi\hbar}}\ \psi(x) e^{-\frac{ipx}{\hbar}}$$

$$\therefore \langle p \rangle = \int dx\ \psi^*(x) \frac{\hbar}{i} \frac{d}{dx} \psi(x)$$

$$= \int dx\ \psi^*(x)\ \frac{\hbar}{i}\frac{d}{dx}\left(\int_{-\infty}^{\infty} \frac{dp}{\sqrt{2\pi\hbar}}\ \phi(p) e^{\frac{i}{\hbar}px} \right)$$

$$= \int dx\ \psi^*(x) \int \frac{dp}{\sqrt{2\pi\hbar}}\ p\,\phi(p)\ e^{\frac{i}{\hbar}px}$$

$$= \int dp\ p\,\phi(p) \underbrace{\int \frac{dx}{\sqrt{2\pi\hbar}}\ \psi^*(x)\ e^{\frac{i}{\hbar}px}}_{\phi^*(p)}$$

$$= \int dp\ \phi^*(p)\ p\,\phi(p)$$

$$= \int dp\ p\ |\phi(p)|^2 \iff \langle x \rangle = \int dx\ x |\psi(x)|^2$$

這建議了 $|\phi(p)|^2$ 與 $|\psi(x)|^2$ 一樣有機率密度之意義！

就是 $[|\phi(p)|^2] = \frac{\text{机率}}{dp} \Rightarrow |\phi(p)|^2 dp$

$= \text{在}(p, p+dp)$ 間出現之机率

$[|\psi(x)|^2] = \frac{\text{机率}}{dx}$, $|\psi(x)|^2 dx$

$= \text{在}(x, x+dx)$ . . . .

但這樣之解釋必須有：

$$\int_{-\infty}^{\infty} |\phi(p)|^2 dp = 1$$

$$\Leftrightarrow \int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1$$

這是由 Parseval's theorem 來保証的：

$$f(x) = \int_{-\infty}^{\infty} g(p) e^{i\frac{px}{\hbar}} dp\, \alpha \quad g(p) = \int_{-\infty}^{\infty} e^{-i\frac{px}{\hbar}} f(x)\, dx\, \beta$$

$$\int_{-\infty}^{\infty} |f(x)|^2 dx = \int_{-\infty}^{\infty} f^*(x)\, dx \int_{-\infty}^{\infty} g(p) e^{i\frac{px}{\hbar}} dp \cdot \alpha$$

$$= \int_{-\infty}^{\infty} g(p) \underbrace{\left[\int_{-\infty}^{\infty} f^*(x) e^{i\frac{px}{\hbar}} dx\right]}_{= g^*(p)/\beta} dp \cdot \alpha$$

$$= \frac{\alpha}{\beta} \int_{-\infty}^{\infty} |g(p)|^2 dp$$

$\alpha\beta = \frac{1}{2\pi\hbar}$, $\boxed{\text{若 } \alpha = \beta = \frac{1}{\sqrt{2\pi\hbar}}}$ $\int_{-\infty}^{\infty} |f(x)|^2 dx = \int_{-\infty}^{\infty} |g(p)|^2 dp$!

(這和 Chapter 2 之作業 Ex2.1 有關)

一旦建立了 $dp\,|\phi(p)|^2$ = 找到質点之動量在 $(p, p+dp)$ 之机率

則对任意 p 之函数 $f(p)$

$$\langle f(p)\rangle = \int_{-\infty}^{\infty} dp\ f(p)\ |\phi(p,t)|^2$$

$$= \int_{-\infty}^{\infty} dp\ \phi(p,t)\, f(p)\ \underbrace{\int \frac{dx}{\sqrt{2\pi\hbar}}\ \psi^*(x,t)\ e^{\frac{i}{\hbar}px}}_{\phi^*(p,t)}$$

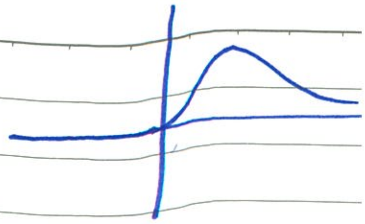
$$= \int dx\ \psi^*(x,t) \int_{-\infty}^{\infty} \frac{dp}{\sqrt{2\pi\hbar}}\ \underbrace{f(p)\ e^{\frac{i}{\hbar}px}}_{\substack{\shortparallel \\ f(\frac{\hbar}{i}\frac{\partial}{\partial x})\, e^{\frac{i}{\hbar}px}}}\ \phi(p,t)$$

$$= \int dx\ \psi^*(x,t)\ f(\tfrac{\hbar}{i}\tfrac{\partial}{\partial x}) \underbrace{\int_{-\infty}^{\infty} \frac{dp}{\sqrt{2\pi\hbar}}\ \phi(p,t)\ e^{\frac{i}{\hbar}px}}_{\psi(x,t)}$$

$$= \int dx\ \psi^*(x,t)\ f(\tfrac{\hbar}{i}\tfrac{\partial}{\partial x})\ \psi(x,t)$$

<u>example</u>

$$\psi(x) = 2\alpha\sqrt{\alpha}\, x\, e^{-\alpha x} \qquad x>0$$
$$= 0 \qquad x<0$$



(i) normalized:

$$\int_{-\infty}^{\infty} dx\, |\psi(x)|^2$$
$$= \int_0^{\infty} dx\, 4\alpha^2 \cdot \alpha\, x^2 e^{-2\alpha x}$$
$$= 4\alpha^3 \int_0^{\infty} x^2 e^{-2\alpha x} dx$$
$$= 4\alpha^3 \frac{d^2}{d\beta^2} \underbrace{\int_0^{\infty} e^{-\beta x} dx}_{= \frac{1}{\beta}} \Big|_{\beta=2\alpha}$$
$$= 4\alpha^3 \frac{2}{\beta^3} \Big|_{\beta=2\alpha} = 1$$

(ii) $\langle x \rangle$

$$= \int_{-\infty}^{\infty} dx\, x\, |\psi(x)|^2$$
$$= 4\alpha^3 \int_0^{\infty} dx\, x^3 e^{-2\alpha x}$$
$$= 4\alpha^3 \frac{d^3}{d\beta^3} \int_0^{\infty} dx\, e^{-\beta x} \Big|_{\beta=2\alpha}$$
$$= 4\alpha^3 \frac{d^3}{d\beta^3}\left(\frac{1}{\beta}\right) \Big|_{\beta=2\alpha} = 4\alpha^3 \frac{1\cdot 2\cdot 3}{(2\alpha)^4}$$
$$= \frac{3}{2\alpha}$$

$$\langle x^2\rangle = \int_0^\infty dx\; x^4 e^{-2\alpha x}\cdot 4\alpha^3$$

$$= 4\alpha^3 \frac{d^4}{d\beta^4}\frac{1}{\beta}\Big|_{\beta=2\alpha} = 4\alpha^3 \frac{4!}{(2\alpha)^5} = \frac{3}{\alpha^2}$$

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

標準差

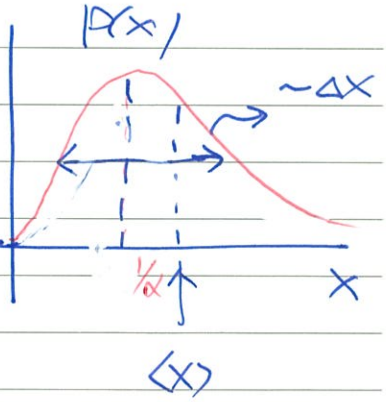
(Standard deviation)

$$= \langle x^2\rangle - \langle x\rangle^2$$

$$= 3/\alpha^2 - \frac{9}{4\alpha^2} = \frac{3}{4\alpha^2}$$

⇓

Δx = uncertainty of x $= \frac{\sqrt{3}}{2}\frac{1}{\alpha}$



注意：並不是所有波函數之Δx都可以如此算出的
如fig 2.1之波函數即不行！

(iii) $\frac{dP(x)}{dx} = 0$

$$\frac{d}{dx}\left(x^2 e^{-2\alpha x}\right) = 2x(1-\alpha x)e^{-2x\alpha} = 0$$

$\therefore x_{max} = \frac{1}{\alpha}$ (注意 $x_{max} \neq \langle x\rangle$)

(iv)

$$\Phi(p) = \frac{1}{\sqrt{2\pi\hbar}}\int_0^\infty dx\; e^{-\frac{ipx}{\hbar}}(2\alpha\sqrt{\alpha})\,x\,e^{-\alpha x}$$

$$= \sqrt{\frac{4\alpha^3}{2\pi\hbar}}\underbrace{\int_0^\infty dx\; e^{-(\alpha+\frac{ip}{\hbar})x}\cdot x}_{} = \sqrt{\frac{4\alpha^3}{2\pi\hbar}}\frac{1}{(\alpha+ip/\hbar)^2}$$

$$\left(-\frac{d}{d\alpha}\right)\underbrace{\int_0^\infty e^{-(\alpha+\frac{ip}{\hbar})x}dx}_{\frac{1}{\alpha+ip/\hbar}}$$

22 hours

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(U)

$$\langle p\rangle = \int_{-\infty}^{\infty} dp\ p\ |\Phi(p)|^2$$

$$= \frac{4\alpha^3}{2\pi\hbar}\int_{-\infty}^{\infty} dp\ \frac{p}{(\alpha^2+p^2/\hbar^2)^2} = 0$$

← odd in p

由 operator :

if ψ = real

$\langle p\rangle = 0$ 類似係之理

$$\langle p\rangle = \int dx\ \psi^*(x)\ \frac{\hbar}{i}\frac{d}{dx}\psi(x)$$

$$= \int_0^{\infty} dx\ (2\alpha\sqrt{\alpha})^2\ x e^{-\alpha x}\ \underbrace{\frac{\hbar}{i}\frac{d}{dx} x e^{-\alpha x}}_{\frac{\hbar}{i}[e^{-\alpha x}](1-\alpha x)}$$

$$= \frac{\hbar}{i} 4\alpha^3 \underbrace{\int_0^{\infty} dx\ x(1-\alpha x)\ e^{-2\alpha x}}$$

$$\int_0^{\infty} dx\ x e^{-2\alpha x} - \alpha\int_0^{\infty} dx\ x^2 e^{-2\alpha x}$$

$$\frac{1}{(2\alpha)^2} - \alpha\cdot\frac{2}{(2\alpha)^3} = 0$$

$$\langle p^2\rangle = \int_{-\infty}^{\infty} dp\ p^2\cdot\frac{4\alpha^3}{2\pi\hbar}\frac{1}{(\alpha^2+p^2/\hbar^2)^2}$$

$$= \frac{8\alpha^3}{2\pi\hbar}\int_0^{\infty} dp\ \frac{p^2}{(p^2/\hbar^2+\alpha^2)^2}$$

$p = \hbar\alpha\tan\theta$

$dp = \hbar\alpha\sec^2\theta\, d\theta$

$$= \frac{8\alpha^3}{2\pi\hbar}\int_0^{\pi/2} \hbar\alpha\sec^2\theta\, d\theta\ \frac{(\hbar\alpha)^2\tan^2\theta}{\alpha^4\sec^4\theta}$$

$\Delta p = \hbar\alpha$

$$= \frac{8\alpha^3}{2\pi\hbar}\cdot\frac{\hbar^3}{\alpha}\int_0^{\pi/2}\sin^2\theta\, d\theta = \frac{8\hbar^2\alpha^2}{2\pi}\cdot\frac{\pi}{4} = \hbar^2\alpha^2$$

Question: 何以 $\psi(x,t) = A e^{-\alpha(x-v_g t)^2}$ 為 real 但會動?
$(\alpha = \text{real})$

$\langle p \rangle = 0$
$\nparallel$

$\because \psi = \text{real}$

一個 wave function 會不會動? 與 $\langle p \rangle$ 之關係是由

$\langle p \rangle = m \frac{d\langle x \rangle}{dt}$ 來的.

但 $\langle p \rangle = m \frac{d\langle x \rangle}{dt}$ 則是假設 $\psi(x,t)$ 滿足 Schrödinger equation: $i\hbar \frac{d\psi(x,t)}{dt} = \frac{-\hbar^2}{2m} \frac{d^2}{dx^2}\psi(x,t) + V(x,t)\psi(x,t)$

with real $V(x,t)$

$\psi(x,t)$ 並不滿足 Schrödinger eq.!

$$i\hbar \frac{d\psi}{dt} = i\hbar (+\alpha) 2(x-v_g t)(v_g)\psi$$

$$\frac{-\hbar^2}{2m}\nabla^2\psi = \frac{-\hbar^2}{2m}\frac{d^2}{dx^2} A e^{-\alpha(x-v_g t)^2}$$

$$= \frac{-\hbar^2}{2m} A \frac{d}{dx}\left[-2\alpha(x-v_g t) e^{-\alpha(x-v_g t)^2}\right]$$

$$= \frac{-\hbar^2}{2m}\left\{-2\alpha + (2\alpha)^2(x-v_g t)^2\right\}\psi$$

$$\therefore V = 2\alpha i\hbar(x-v_g t)v_g - \frac{\alpha\hbar^2}{m} + \frac{2\alpha^2\hbar^2}{m}(x-v_g t)^2$$

不為 real!

真正的解為

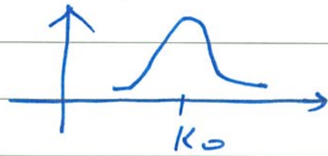
$$\psi(x,t) = A(t)\, e^{i(k_0x-\omega_0 t)}\, e^{-\frac{(x-v_g t)^2}{4(\alpha+i\beta t)}}$$ (可以 check 這是解)

其中 $v_g = \frac{d\omega}{dk}\Big|_{k_0}$ $2\beta = \frac{d^2\omega}{dk^2}\Big|_{k=k_0}$

free particles: $\omega = \frac{p^2}{2m\hbar} = \frac{\hbar k^2}{2m}$

$\therefore \frac{2\hbar}{2m} = \frac{d^2\omega}{dk^2}\Big|_{k=k_0} = 2\beta$ $\therefore \beta = \hbar/m$

α 為 k space 中之寬度，為給定的 $g(k) = e^{-\alpha(k-k_0)^2}$



若 $k_0=0 \Rightarrow \omega_0 = 0$ $v_g = \frac{d\omega}{dk}\Big|_{k_0=0} = 0$

$$\therefore \psi(t) = A(t)\, e^{-\frac{x^2}{4(\alpha+i\beta t)}}$$

此時 $\langle p \rangle$ 確實 $=0$，但 $\langle x \rangle$ 也 $=0$

$\therefore \langle p \rangle = m\frac{d\langle x \rangle}{dt}$ 是滿足的.

所以，若 Gaussian 部分要有 $(x-v_g t)^2$，才能動，

則必須乘以 $e^{i(k_0x-\omega_0 t)}$ 之因子.

此時 $v_g = \frac{d\omega}{dk} = \frac{\hbar k}{m}$

$$\frac{\hbar}{i}\frac{\partial}{\partial x}\psi = \hbar k_0 \psi + e^{i(k_0x-\omega_0 t)} A(t) \frac{\hbar}{i}\frac{\partial}{\partial x} e^{-\frac{(x-v_g t)^2}{4(\alpha+i\beta t)}}$$

在如 $v_g=0$ 之情形，知第二項之 $\langle p \rangle = 0$

但第一項 $= \hbar k_0$ $\therefore \langle p \rangle = \hbar k_0$，又 $\langle x \rangle = v_g t$

$\therefore \langle p \rangle = m\frac{d\langle x \rangle}{dt}$

以 operator (在 x 空間) 中計算 $\langle p^2 \rangle$

$$\langle p^2 \rangle = \int_{-\infty}^{\infty} dx \; \psi^*(x) \, -\hbar^2 \frac{d^2}{dx^2} \, \psi(x)$$

$$= -\hbar^2 (2\alpha\sqrt{\alpha})^2 \left\{ \int_{0^+}^{\infty} dx \; x e^{-\alpha x} \underbrace{\frac{d^2}{dx^2} x e^{-\alpha x}}_{\begin{array}{c} \| \\ \frac{d}{dx}\left[e^{-\alpha x}(1-\alpha x)\right] \\ \| \\ \alpha e^{-\alpha x}(\alpha x - 2) \end{array}} \right\} \quad \text{— (i)}$$

$$+ \int_{0^-}^{0^+} dx \; \psi^*(x) \left[-\hbar^2 \frac{d^2}{dx^2} \psi(x) \right] \quad \text{— (ii)}$$

$$\text{(i)} = -4\hbar^2 \alpha^3 \underbrace{\int_0^\infty dx \; \alpha x \, e^{-2\alpha x} (\alpha x - 2)}_{\begin{array}{c} \| \\ \frac{1}{\alpha} \underbrace{\int_0^\infty dy \; y(y-2) e^{-2y}}_{-1/4} \end{array}} = \hbar^2 \alpha^2$$

$$\text{(ii)} \quad \frac{d}{dx} x e^{-\alpha x} \Big|_{x=0} = e^{-\alpha x}(1-\alpha x) \Big|_{x=0} = 1$$

$$\therefore \frac{d^2 \psi(x)}{dx^2} \Big|_{x=0} = \underset{2\alpha\sqrt{\alpha}}{\wedge} \frac{1-0}{\Delta x \to 0} = \delta(x) \cdot 2\alpha\sqrt{\alpha}$$

$$\therefore \text{(ii)} = -\hbar^2 (2\alpha\sqrt{\alpha})^2 \int_{0^-}^{0^+} x e^{-\alpha x} \delta(x) \, dx = 0.$$

$$\therefore \langle p^2 \rangle = \hbar^2 \alpha^2$$

我們看到 $\langle p \rangle$ 的求法有2種:

在 x-space $\langle p \rangle = \int_{-\infty}^{\infty} dx \; \psi^*(x) \frac{\hbar}{i}\frac{\partial}{\partial x} \psi(x)$

在 p 空間 $\langle p \rangle = \int_{-\infty}^{\infty} dp \; \phi^*(p) \, p \, \phi(p)$

∵ x 和 p 是類似的，一個空間的問題是:

在 x 空間 $\langle x \rangle = \int_{-\infty}^{\infty} dx \; \psi^*(x) \, x \, \psi(x)$

則在 p 〃 〃 $\langle x \rangle = ?$

答案是 $\langle x \rangle = \int_{-\infty}^{\infty} dp \; \phi^*(p) \, i\hbar \frac{\partial}{\partial p} \phi(p)$ (Ex 3.8)

* The operators in the Schrödinger equation.

1. Free particle: $i\hbar \frac{\partial \psi(x,t)}{\partial t} = \underbrace{\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2}}_{\frac{p^2}{2m}} \psi(x,t)$

∴ $\hat{p} = \frac{\hbar}{i}\frac{\partial}{\partial x}$ 似乎是对應 momentum 之 operator

這也表現在求 $\langle p \rangle = \int_{-\infty}^{\infty} dx \; \psi^*(x) \, \hat{p} \, \psi(x)$

同理可以定 $\hat{x} = x$ ∴ $\langle x \rangle = \int_{-\infty}^{\infty} dx \; \psi^*(x) \, \hat{x} \, \psi(x)$

注意：以上的表示方法 (representation) 是在 x 空間中！在 p 空間中，$\hat{p} = p$，$\hat{x} = i\hbar \frac{\partial}{\partial p}$

$X = i\hbar \frac{d}{dp}$ 之例：

$$\psi(x) = \begin{cases} 2\alpha\sqrt{\alpha}\, x e^{-\alpha x} & x>0 \\ 0 & x<0 \end{cases}$$

$$\phi(p) = \sqrt{\frac{4\alpha^3}{2\pi\hbar}} \quad \frac{1}{(\alpha + ip/\hbar)^2}$$

$$\langle x \rangle = \int_{-\infty}^{\infty} dp \quad \phi^*(p) \; i\hbar \frac{d}{dp} \phi(p)$$

$$= \frac{4\alpha^3}{2\pi\hbar} \int_{-\infty}^{\infty} dp \frac{1}{(\alpha - ip/\hbar)^2} \; i\hbar \frac{-2}{(\alpha+ip/\hbar)^3} \quad \left(\frac{+i}{\hbar}\right)$$

$$= \frac{4\alpha^3}{\pi\hbar} \int_{-\infty}^{\infty} dp \frac{1}{(\alpha^2 + p^2/\hbar^2)^2} \quad \frac{1}{\alpha + ip/\hbar}$$

$$= \frac{4\alpha^3}{\pi} \int_{-\infty}^{\infty} \frac{dz}{\alpha + iz} \quad \frac{1}{(\alpha^2 + z^2)^2}$$

$$= \frac{4\alpha^3}{\pi} \frac{2\pi i}{i} \left\{ \frac{-d}{dz} \left[\frac{1}{(z-i\alpha)^3 (z+i\alpha)^2} \right] (z+i\alpha)^2 \Big|_{z=-i\alpha} \right\}$$

$$= \frac{4\alpha^3}{\pi} \times 2\pi \times \frac{3}{(z-i\alpha)^4} \Big|_{z=-i\alpha}$$

$$= \frac{4\alpha^3}{\pi} \times 2\pi \quad \frac{3}{(2\alpha)^4}$$

$$= \frac{3}{2\alpha}$$

由 $\hat{x}$ 和 $\hat{p}$ 可以組合其他的 operator.

如

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

$$\hat{H} = \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V$$

$$= \frac{\hat{p}^2}{2m} + V(\hat{x})$$ Hamiltonian (energy operator)

似乎沒有什麼新的東西!

事實上,上面的例子是比較單純的
真正比較複雜的例子為古典中像 xp 之類有 x 和 p 混合的量。

原因是 $\hat{x}$ 和 $\hat{p}$ 是 non commute: $\hat{A}\hat{B}\psi$ 指的是先作用 $\hat{B}$ 再作用 $\hat{A}$

$$[\hat{A},\hat{B}] \equiv \hat{A}\hat{B}-\hat{B}\hat{A} = \text{Commutator}$$

如 $[\hat{p},\hat{x}]\psi(x,t)$ $\qquad \hat{x}\psi(x,t) = x\psi(x,t)$

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

$$\because \frac{\partial}{\partial x}(x\psi(x,t)) = \frac{\partial x}{\partial x}\psi(x,t) + x\frac{\partial}{\partial x}\psi(x,t)$$

$$\therefore [\hat{p},\hat{x}]\psi(x,t) = \frac{\hbar}{i}\psi(x,t) \quad \text{for any } \psi(x,t)$$

$$\therefore [\hat{p},\hat{x}] = \frac{\hbar}{i}$$ ⇐ Commutation relation ← check in p-space

即和一般數不同 $\hat{p}\hat{x} \neq \hat{x}\hat{p}$! ⇒ 這是 $\Delta x \Delta p \geq \hbar/2$ 之根源

因此，古典中像 x p 之量在量子力學中之表示就

有很大的 "ambiguity"！事實上，這反應了古典的表示，與量子之表示並非一對一的！

Symmetrization rule:

$$\left[\begin{aligned} xp &\to \frac{1}{2}(\hat{x}\hat{p}+\hat{p}\hat{x}) \\ x^2p &\to \frac{1}{4}(\hat{x}^2\hat{p}+2\hat{x}\hat{p}\hat{x}+\hat{p}\hat{x}^2) \end{aligned}\right\} \text{∵ 真正的 form 必須由實驗數據確定}$$

為何不用 $\hat{x}\hat{p}$ 代表呢？（見習題）

2. <u>Hermitian operators</u>

由以上可知在 x 空間，$\hat{p}=\frac{\hbar}{i}\frac{\partial}{\partial x}$，乍看之下，∵ $\hat{p}$ 帶了一個 i，所以會有疑慮：

$$\langle p\rangle = \int dx\, \psi^*(x,t)\frac{\hbar}{i}\frac{\partial}{\partial x}\psi(x,t)$$ 是測量的平均值 ⇒ 要是實數！

有 i 會是實數嗎？

Check
$$\langle p\rangle^* = \int dx\, \psi(x,t)\left[-\frac{\hbar}{i}\frac{\partial}{\partial x}\psi^*(x,t)\right]$$

$$\therefore \langle p\rangle - \langle p\rangle^* = \int_{-\infty}^{\infty} dx\, \frac{\hbar}{i}\underbrace{\left[\psi^*\frac{\partial}{\partial x}\psi + \psi\frac{\partial}{\partial x}\psi^*\right]}_{=\frac{\partial}{\partial x}\psi^*\psi}$$

$$= \frac{\hbar}{i}\,\psi^*(x,t)\,\psi(x,t)\Big|_{x=-\infty}^{x=\infty} = 0$$

∵ $|\psi|^2 \to 0$ as $x\to\pm\infty$ (square integrable 一定要求 $|\psi|^2\to 0$ as $x\to\pm\infty$)

$\langle xp \rangle$ 之仔細探討 ⇒ 習題

不過這裏有一個重要的問題：

It's tempting to find the probability density of find particles at x & p ⇒ $|\Psi(x,p)|^2$

so that

$$\langle xp \rangle = \int dx \int dp \; xp \, |\Psi(x,p)|^2$$

這在量子力學中是不能作到的！

主要是測不準原理的關係，$\Delta x \Delta p \geq \hbar/2$

⇒ 我們無法定出找到質點在 x 與 p 之機率！

正確的作法是將 p 換為 $\frac{\hbar}{i}\frac{d}{dx}$，計算 $\langle \frac{\hat{x}\hat{p}+\hat{p}\hat{x}}{2} \rangle$

或是 $x \to i\hbar\frac{d}{dp}$

問題是怎樣的實驗值對應 $\langle \frac{\hat{x}\hat{p}+\hat{p}\hat{x}}{2} \rangle$？

這對應到 observable 嗎？

Algebra of commutator

Ex 3.8.

$$e^{\frac{i\hat{p}a}{\hbar}}\hat{x}\,e^{-\frac{i}{\hbar}\hat{p}a} = ?$$

$$\hat{x} = i\hbar\frac{\partial}{\partial p}$$

考慮：$e^{\frac{i\hat{p}a}{\hbar}}\hat{x}\,e^{-\frac{i}{\hbar}\hat{p}a}\,\psi(p)$ 作用在任意 $\psi(\,)$ 上

$$= e^{\frac{ipa}{\hbar}}\underbrace{i\hbar\frac{\partial}{\partial p}\left[e^{-\frac{i}{\hbar}pa}\,\psi(p)\right]}_{\displaystyle \parallel} \qquad \hat{p}\,\psi(p) = p\,\psi(p)$$

$$e^{-\frac{i}{\hbar}pa}\underbrace{i\hbar\frac{\partial}{\partial p}}_{\hat{x}}\psi(p) + a\,e^{-\frac{i}{\hbar}pa}\,\psi(p)$$

$$= (\hat{x}+a)\,\psi(p)$$

$$\therefore\ e^{\frac{i}{\hbar}\hat{p}a}\,\hat{x}\,e^{-\frac{i}{\hbar}\hat{p}a} = \hat{x}+a$$

Ex

$$[\hat{A},\hat{B}\hat{C}] = \hat{A}\hat{B}\hat{C} - \hat{B}\hat{C}\hat{A} = \hat{A}\hat{B}\hat{C} - \hat{B}\hat{A}\hat{C} + \hat{B}\hat{A}\hat{C} - \hat{B}\hat{C}\hat{A}$$

$$= [\hat{A},\hat{B}]\hat{C} + \hat{B}[\hat{A},\hat{C}]$$

Ex

$$[A,B] = -[B,A]$$

$$[\alpha A,B] = \alpha[A,B]$$

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

~~此類 operator ($\langle p\rangle - \langle p\rangle^* = 0$ for any ψ)~~

$\Rightarrow$ Hermitian operators !

(More advanced topics for linear operators can be found in Appendix B)

Hermitian operators 之定義 與 boundary conditions 有很大的關係。如上 $|\psi|^2 \to 0$ 是一個例子.

Another example : $0 \le x \le L$, periodic boundary condition

$$\psi(x) = \psi(x+L)$$

$$\therefore \langle p\rangle - \langle p\rangle^* = \frac{\hbar}{i}\int_0^L dx \frac{d}{dx}|\psi(x)|^2$$

$$= \frac{\hbar}{i}\left[|\psi(L)|^2 - |\psi(0)|^2\right] = 0 \quad \text{too !}$$

Other examples :

$\hat{x} = x \Rightarrow \langle x\rangle - \langle x\rangle^* = 0 \quad \therefore x = \text{Hermitian}$

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

$$\langle H\rangle - \langle H\rangle^* = \int dx\, \psi^*(x,t)\left[\frac{-\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right]\psi(x,t)$$

$$- \int dx\, \psi(x,t)\left[\frac{-\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right]\psi^*(x,t)$$

$$= \int dx \, \frac{\hbar^2}{2m}\left[\psi\frac{d^2}{dx^2}\psi^* - \psi^*\frac{d^2}{dx^2}\psi\right]$$

$$= \int dx \, \frac{\hbar^2}{2m} \frac{d}{dx} \left[\psi \frac{d}{dx} \psi^* - \psi^* \frac{d}{dx} \psi \right]$$

$= 0.$

$\therefore \hat{H} =$ Hermitian

可以証明 $\hat{p}$ = Hermitian

$\hat{p}^n$ = 〃

我們在 Chapter 6 會再回來談 Hermitian operators.

目前，最重要的結論：量子力學中可以測量的量一定以 Hermitian Operators，$\hat{O}$ 來表示.

如此 $\langle O \rangle = \langle O \rangle^*$ = 實數.