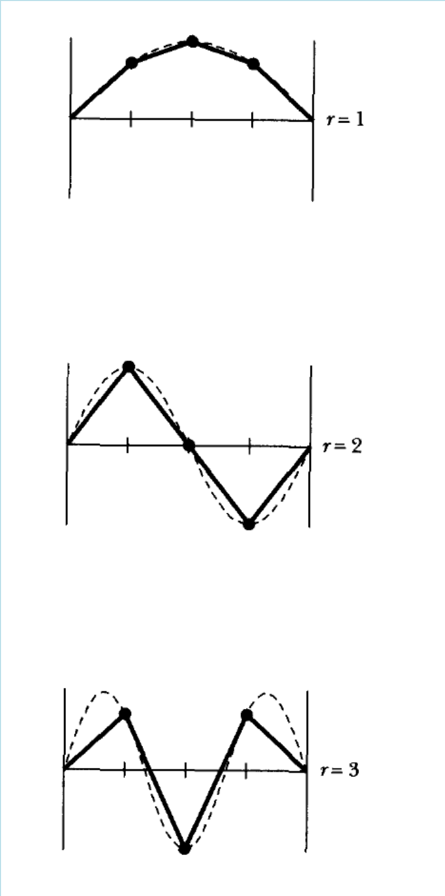
Schrodinger Wave Equation in large infinite space

Free state and scattering 散射

Fourier Transformation

若介質大小有限，連續介質就如大數目的彈簧組，有一系列模式振動。

彈簧組運動：一個本徵向量就對應一個可獨立振盪的模式。



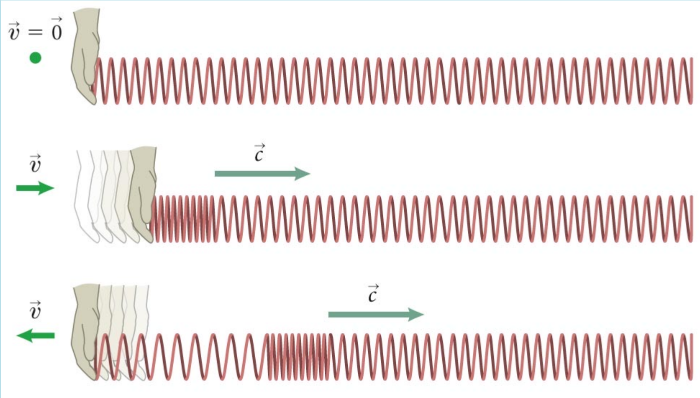
$$\boldsymbol{a}^{(1)} \sim \begin{pmatrix} \frac{1}{\sqrt{2}} \\ 1 \\ \frac{1}{\sqrt{2}} \end{pmatrix}$$

$$\boldsymbol{a}^{(2)} \sim \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}$$

$$\boldsymbol{a}^{(3)} \sim \begin{pmatrix} \frac{1}{\sqrt{2}} \\ -1 \\ \frac{1}{\sqrt{2}} \end{pmatrix}$$

連續介質的波方程式Wave Equation

$$\frac{\partial^2\phi}{\partial t^2} = v^2\frac{\partial^2\phi}{\partial x^2}$$



Initial Condition: 起始的弦位移$\phi(x,0)$，起始的弦垂直方向速度$\frac{\partial\phi}{\partial t}(x,0)$。

是不是要考慮邊界差別很大！

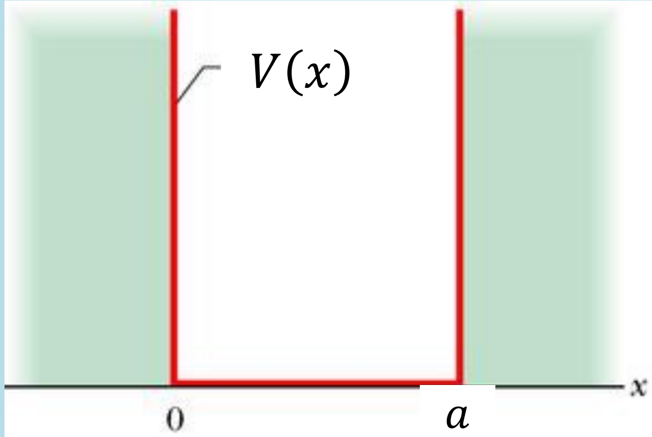
若不需考慮邊界、離開邊界很遠，介質中會有行進波的傳播 d'Alembert solution：

$$\phi(x,t) = f(x - vt) + g(x + vt)$$

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

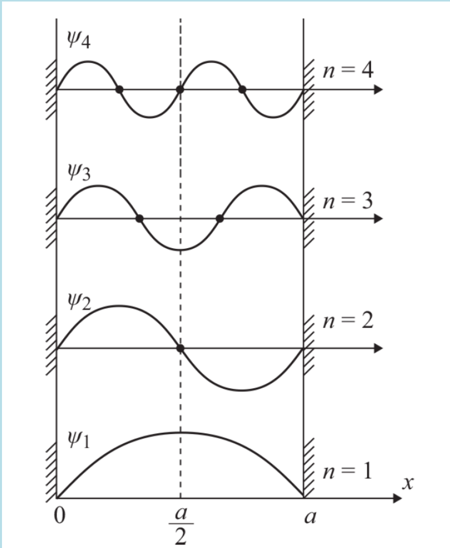
若不需考慮邊界、離開邊界很遠，電子的狀態如何描述：

可以討論有邊界之自由電子，再取邊界為無限遠的極限！ $a \to \infty$



邊界條件：

$\psi_E(0) = 0$ $\psi_E(a) = 0$



$$\psi_n = C \sin\left(\frac{n\pi}{a}x\right)$$

但這不是很方便的極限。

We can displace the infinite space without physical result, called displacement symmetry.

無限大無邊界的空間，可以平移而不產生可測量的物理結果，稱平移對稱。

This symmetry makes the solutions very simple and general.

It would be great to use a boundary condition that keep this symmetry during the limiting process. The simplest one is Periodic Boundary Condition.

Consider a function $f(x)$ that is periodic, with period $2L$, so that

$$f(x) = f(x + 2L) \qquad L \to \infty \qquad \text{(2A-1)}$$

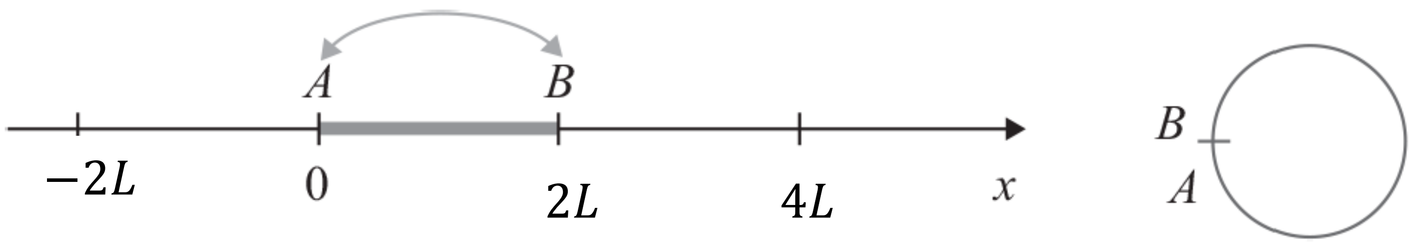


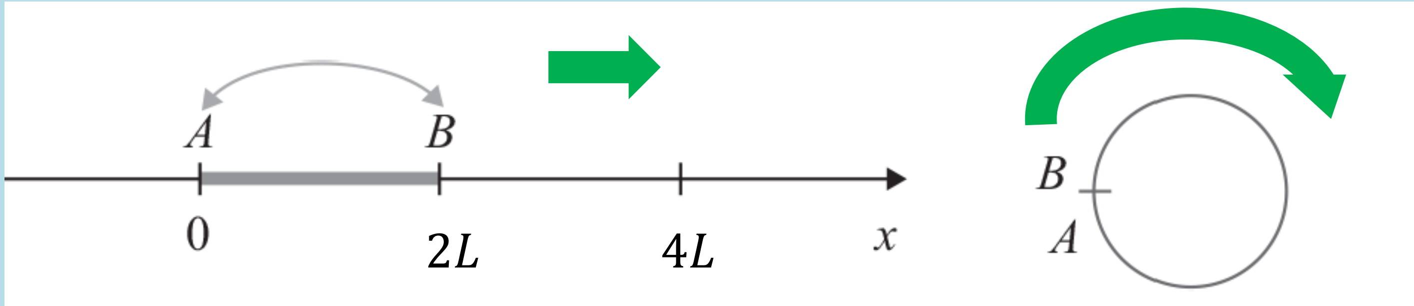
Figure 5.1
A circle of circumference L presented as the real line x with the identification $x \sim x + L$. After the identification, all points on the line are represented by those on $[0, L]$, with point A at $x = 0$ declared identical to point B at $x = L$. The result is the circle shown to the right.

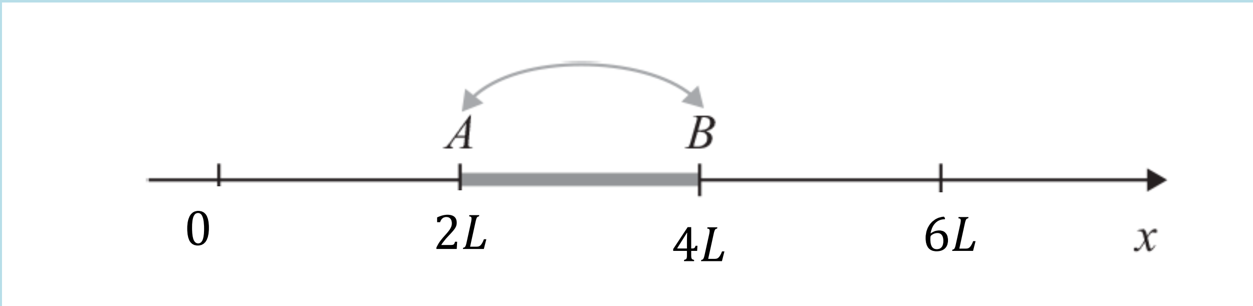
$$\psi_E(x) = \psi_E(x + 2L)$$

Free particle in a circle 圓周上的自由粒子

Periodic Boundary Condition

$$\psi_E(x) = \psi_E(x + 2L)$$





空間部分微分方程式，或稱本徵函數方程式：

$$\frac{d^2\psi_E}{dx^2} = -\frac{2mE}{\hbar^2}\psi_E \qquad \equiv -k^2\psi_E \qquad k \equiv \sqrt{\frac{2mE}{\hbar^2}}$$

$$\frac{d^2\psi_E}{dx^2} = -k^2\psi_E$$

$$\psi_E(x) = Ae^{ikx} + Be^{-ikx}$$

週期性條件很容易被滿足：

$$\psi_E(x) = Ae^{ikx} + Be^{-ikx} = \psi_E(x+2L) = Ae^{ik(x+2L)} + Be^{-ik(x+2L)}$$

只要：

$kL = n\pi$ 即可！

這就是滿足週期性條件的自由空間電子波函數的解：

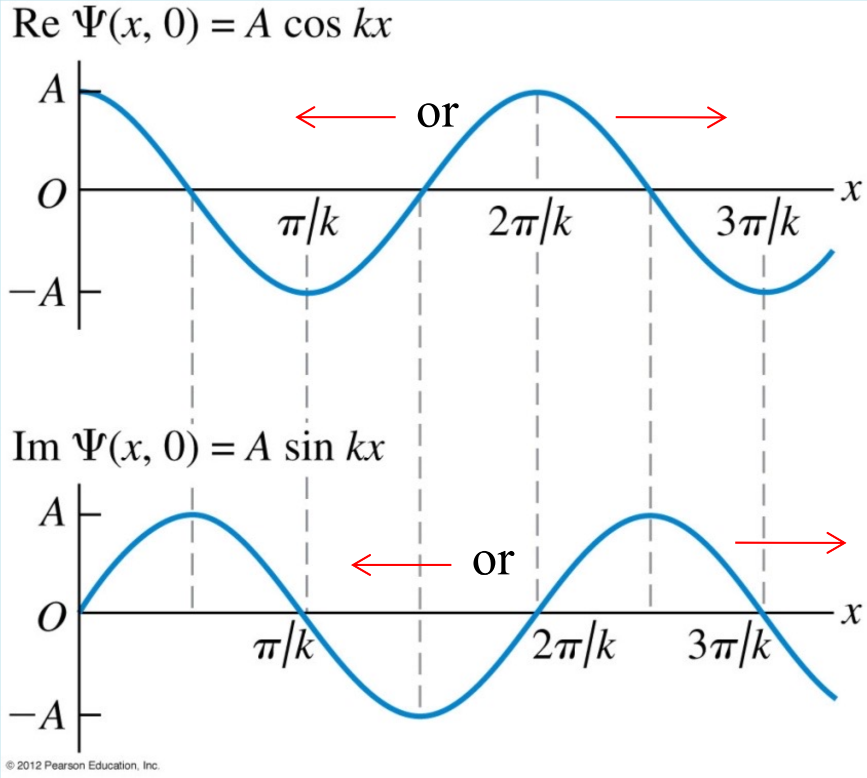
$$u_n(x) = Ae^{i\frac{n\pi}{L}x} + Be^{-ik\frac{n\pi}{L}x} \qquad n = 1,2,\cdots\infty$$

能量、也就是本徵值，等於：

$$E_n = -\frac{\hbar^2}{2m}\frac{n^2\pi^2}{L^2}$$

自由空間的電子定態 $\Psi(x,t)=\left(Ae^{i\frac{n\pi}{L}x}+Be^{-ik\frac{n\pi}{L}x}\right)e^{-i\frac{E_n}{\hbar}t}$

$$\Psi(x,t)=Ae^{i(kx-\omega t)}+Be^{i(kx+\omega t)}\sim Ae^{ik(x-vt)}+Be^{ik(x+vt)}$$



這其實就是古典d'Alembert solution

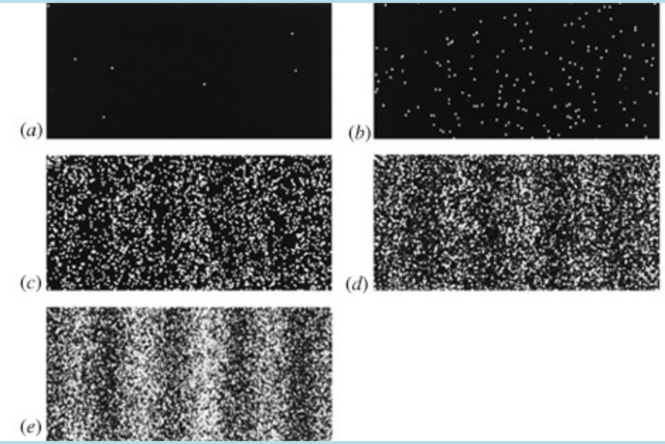
$$\phi(x,t)=f(x-vt)+g(x+vt)$$

只是現在色散關係不同，

波速不再是常數。

實數部與虛數部有一個相同的波長λ：

$$\lambda=\frac{2\pi}{k}=\frac{2\pi\hbar}{\sqrt{2mE}}=\frac{h}{\sqrt{2mE}}=\frac{h}{p}$$



這是可以觀察到的量。

$$\lambda = \frac{h}{p} = \frac{h}{\sqrt{2mE}}$$

以$0.1c$光速移動的電子 $\lambda \sim 7.28 \times 10^{-11}\mathrm{m}$

電子波的波長大致是原子尺度，極小，因此在日常生活無法察覺！

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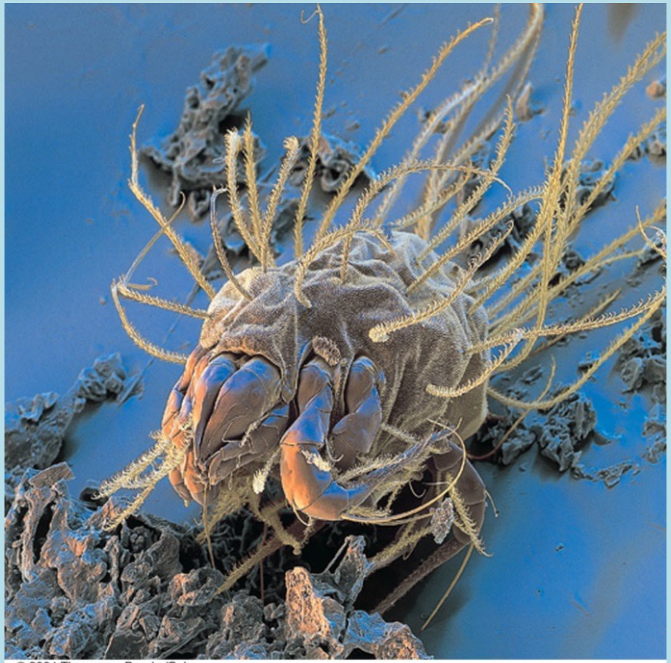

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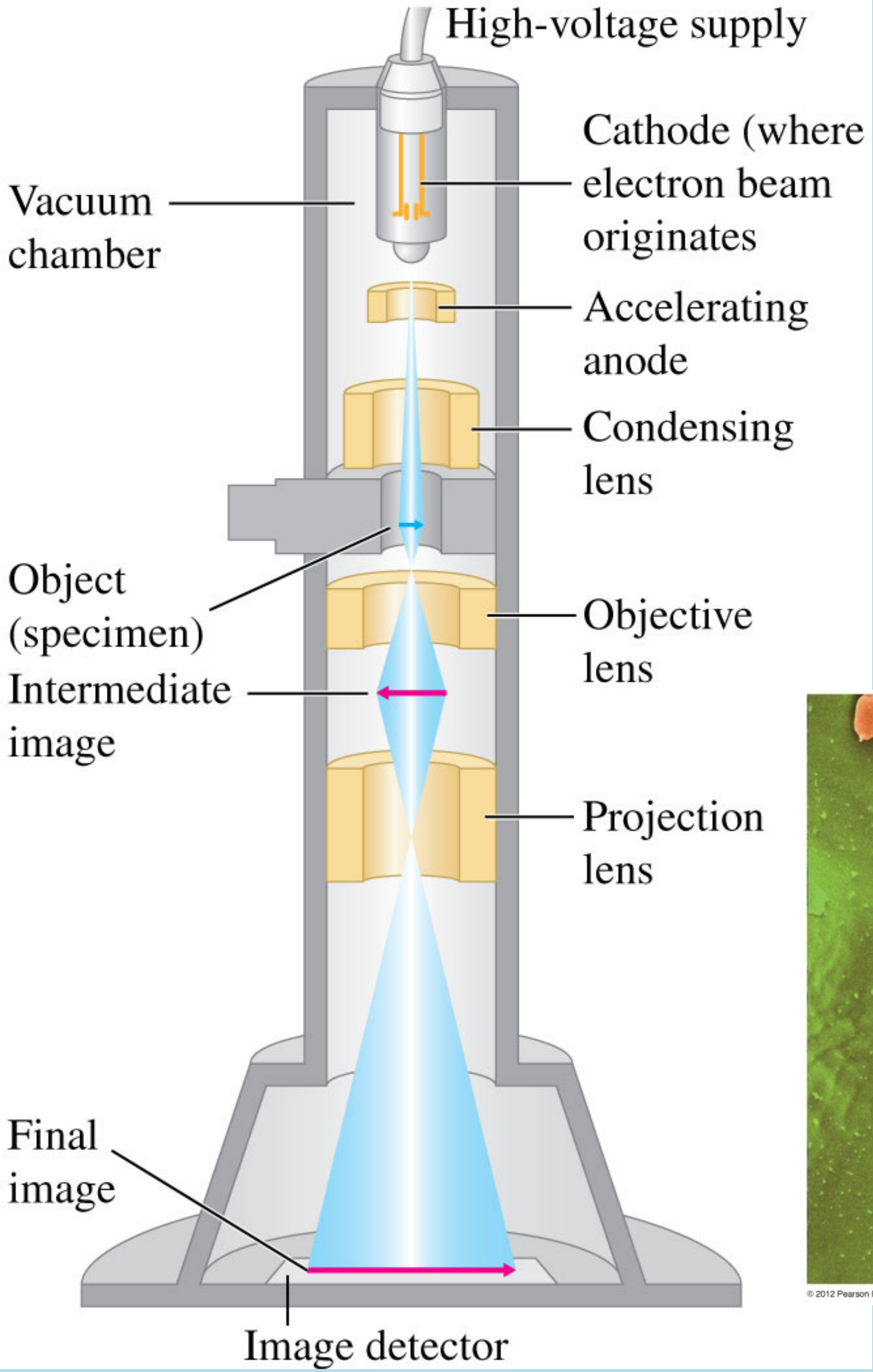
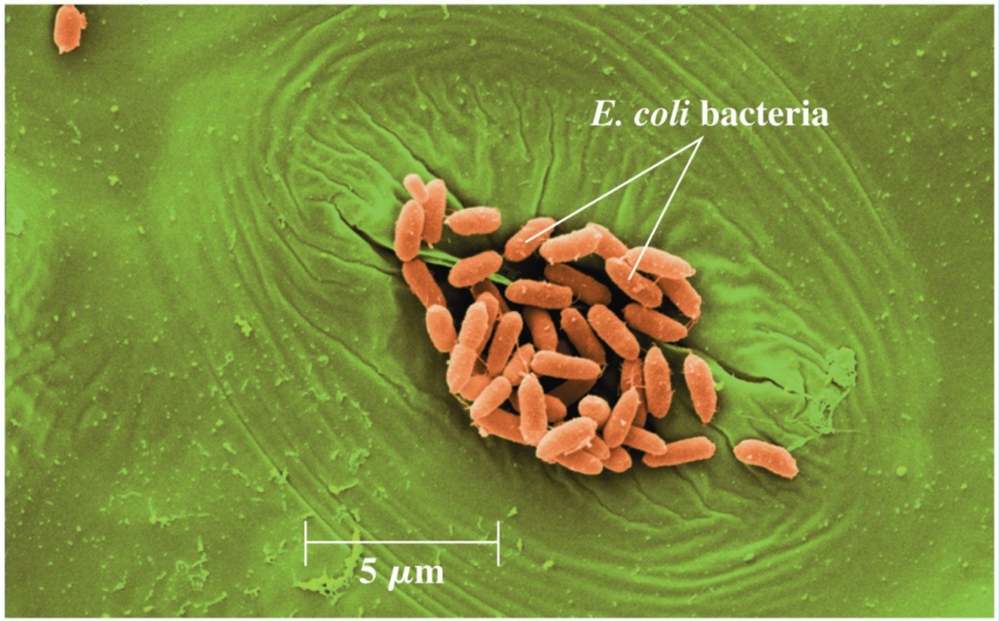
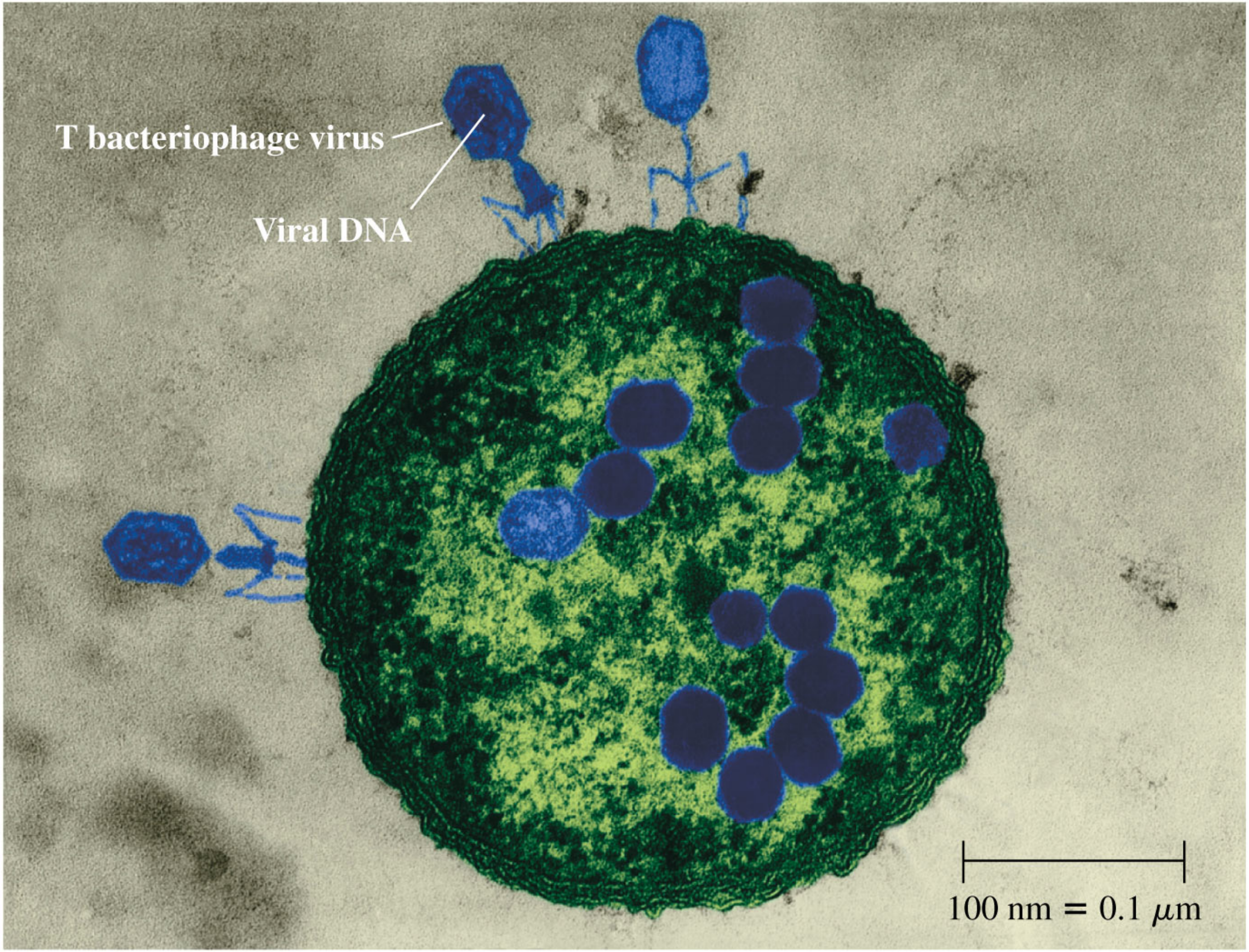
極小的波長，使電子波顯微鏡鑑別度極高！


High-voltage supply
Cathode (where electron beam originates
Vacuum chamber
Accelerating anode
Condensing lens
Object (specimen)
Objective lens
Intermediate image
Projection lens
Final image
Image detector


E. coli bacteria
5 μm


T bacteriophage virus
Viral DNA
100 nm = 0.1 μm

將$t=0$時的波函數，即起始條件，對定態解展開如下：

$$\Psi(x,0)\equiv\phi(x)=\sum_{n=1}^{\infty}c_n\left(Ae^{i\frac{n\pi}{L}x}+Be^{-ik\frac{n\pi}{L}x}\right)=\sum_{n=-\infty}^{\infty}a_ne^{i\frac{n\pi}{L}x}=\sum_{n=-\infty}^{\infty}a_nu_n(x)$$

$e^{-ik\frac{n\pi}{L}x}$設為$u_{-n}(x)$，級數和就延伸到負無限大。

若u_n是完備的，這永遠可以做到！ $u_n(x)\sim e^{i\frac{n\pi}{L}x},\qquad n=-\infty\cdots-1,0,1,\cdots\infty$

$t=0$時此狀態可以視為定態u_n的如上疊加，

接著定態隨時間個自演化，位能下薛丁格方程式要求u_n乘上$e^{-i\frac{E_n}{\hbar}t}$。

乘完之後依同樣方式疊加，整個波函數也就滿足薛丁格波方程式。

$$\Psi(x,t)=\sum_{n=-\infty}^{\infty}a_nu_n(x)e^{-i\frac{E_n}{\hbar}t}$$

我們已經在自由薛丁格方程式用了這樣的策略！當時的正弦波就是定態。

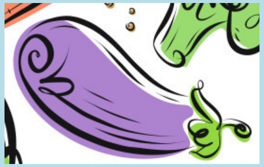
很明顯，這個程序不只適用於無限大位能井，原則上適用於任何位能。

起始各個配料$u_n(x)$依配方c_n收集

各個配料按分離烹煮$e^{-i\frac{E_n}{\hbar}t}$

各自演化後，最後合體！

=



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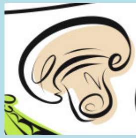

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⋮

$$\Psi(x,t) = \sum_{n=-\infty}^{\infty} a_n u_n(x) e^{-i\frac{E_n}{\hbar}t}$$

這樣的波函數顯然滿足波方程式，又滿足起始條件，就是唯一解。

不同本徵值的本徵函數彼此正交！

The coefficients can be determined with the help of the orthonormality relation

$$\frac{1}{2L}\int_{-L}^{L} dx\, e^{in\pi x/L}e^{-im\pi x/L} = \delta_{mn} = \begin{cases} 1 & m = n \\ 0 & m \neq n \end{cases} \tag{2A-4}$$

$$\int_{-L}^{L} dx\ u_{-m}(x)u_n(x) = \delta_{mn}$$

推廣的函數內積

$$\int_{-L}^{L} dx\, e^{-i\frac{m\pi}{L}x}e^{i\frac{n\pi}{L}x} = 2L\cdot\delta_{mn}$$

$$\Psi(x,0) = \sum_{n=-\infty}^{\infty} a_n e^{ik_n x}$$

$$u_n(x) \equiv \frac{1}{\sqrt{2L}}e^{i\frac{n\pi}{L}x}$$

forms a set of orthonormal functions.

係數可以以投影算出

$$a_n = \frac{1}{\sqrt{2L}}\int_{-L}^{L} dx\, e^{-i\frac{n\pi}{L}x}\Psi(x,0)$$

根據傅立葉級數定理，$u_n(x)$也是完備的，它們等價於傅立葉級數的三角函數。

傅立葉級數Fourier Series

任一週期函數可以分解成一系列正弦函數與餘弦函數的級數和：

$$f(x') = \sum_{n=1}^{\infty} [a_n \cdot \cos nx' + b_n \cdot \sin nx']$$

$$f(x') = f(x' + 2\pi)$$

做一個變數變換： $x' = \frac{n\pi}{L} x$

$$\phi(x) = a_0 + \sum_{n=1}^{\infty} \left[a_n \cdot \cos\frac{n\pi}{L} x + b_n \cdot \sin\frac{n\pi}{L} x\right]$$

$$a_n \cdot \cos\frac{n\pi}{L} x + b_n \cdot \sin\frac{n\pi}{L} x = Ae^{i\frac{n\pi}{L}x} + Be^{-ik\frac{n\pi}{L}x}$$

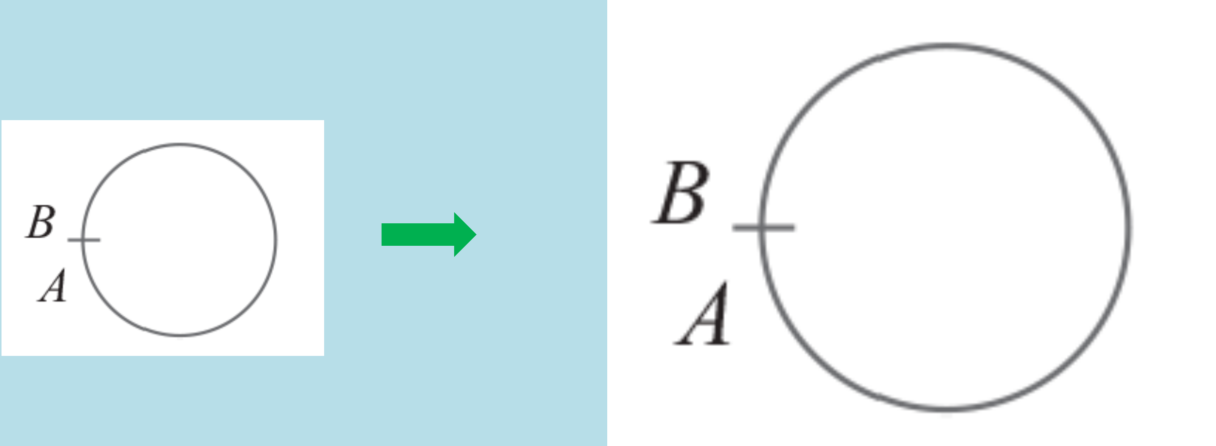
$$\phi(x) = \sum_{n=1}^{\infty} \left[Ae^{i\frac{n\pi}{L}x} + Be^{-ik\frac{n\pi}{L}x}\right]$$

$$\phi(x) = \phi(x + 2L)$$

Jean-Baptiste Joseph Fourier

1768-1830

$u_n(x)$是完備的，任一週期函數可以分解成$u_n(x)$的級數和！



$$\Psi(x,0) \equiv \phi(x) = \sum_{n=1}^{\infty} c_n \left(A e^{i\frac{n\pi}{L}x} + B e^{-ik\frac{n\pi}{L}x} \right) = \sum_{n=-\infty}^{\infty} a_n e^{i\frac{n\pi}{L}x} = \sum_{n=-\infty}^{\infty} a_n e^{ik_n x}$$

現在讓空間大小趨近無限大$L \to \infty$，畢竟無邊界宇宙不應有大小限制！

$$k_n = \frac{n\pi}{L}$$

$$k_n = \frac{n\pi}{L} \to k$$

離散可數的角波數k_n近似趨近連續變數k。

與n相關的係數a_n，也就與連續變數k相關，因此近似趨近一個k的函數。

而級數近似趨近函數積分：

$$\phi(x) \sim \int_{-\infty}^{\infty} dk\, A(k) e^{ikx}$$

$A(k)$就稱為$\phi(x)$的傅立葉變換Fourier Transform。

更細緻的推導：

$$\Delta n = 1$$

$$\phi(x) = \sum_{n=-\infty}^{\infty} a_n e^{i\frac{n\pi}{L}x} = \frac{L}{\pi}\sum_{n=-\infty}^{\infty} a_n e^{i\frac{n\pi}{L}x}\frac{\pi}{L}\Delta n = \frac{L}{\pi}\sum_{n=-\infty}^{\infty} a_n e^{i\frac{n\pi}{L}x}\Delta k$$

$$k_n = \frac{n\pi}{L} \to k$$

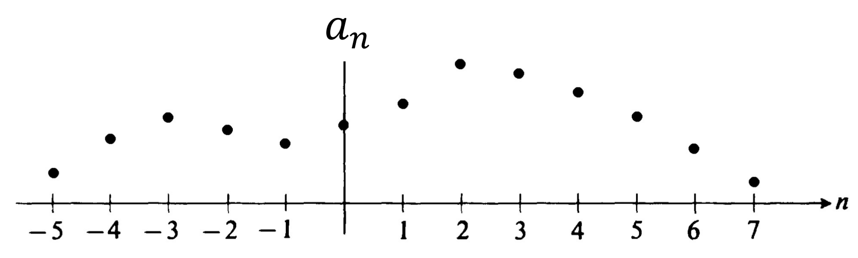


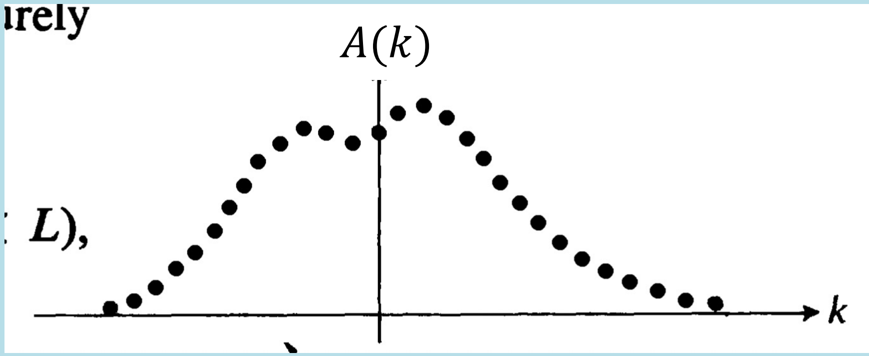
Figure 7.1

重新定義係數：

$$\frac{L}{\pi}a_n \equiv \frac{1}{\sqrt{2\pi}}A_n$$

$$\phi(x) = \frac{1}{\sqrt{2\pi}}\sum_{n=-\infty}^{\infty} A_n e^{i\frac{n\pi}{L}x}\Delta k$$

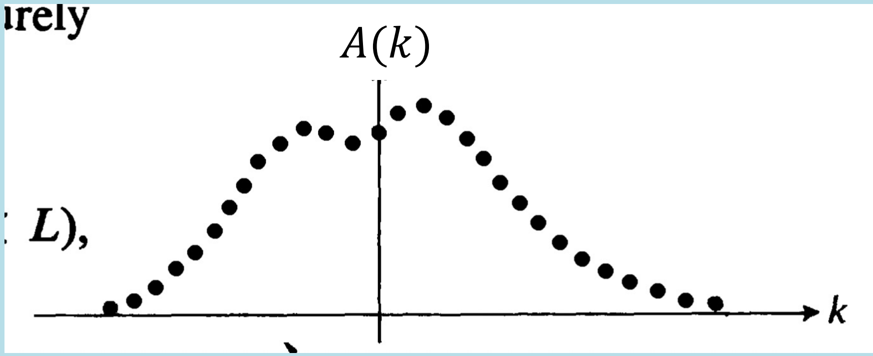
$$\phi(x) = \int_{-\infty}^{\infty} dk\, A(k) e^{ikx}$$



A_n可以以推廣式函數內積的投影計算：

$$A_n = \sqrt{2\pi}\frac{L}{\pi}a_n = \frac{1}{\sqrt{2\pi}}\int_{-L}^{L} dx\, e^{-i\frac{n\pi}{L}x}\Psi(x,0)$$

$$A(k) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \phi(x)\cdot e^{-ikx}\cdot dx$$



$$\phi(x) = \int_{-\infty}^{\infty} dk\, A(k) e^{ikx}$$

$A(k)$就稱為$\phi(x)$的傅立葉變換Fourier Transform。

$$A(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(x) \cdot e^{-ikx} \cdot dx$$

$\phi(x)$就稱為$A(k)$的反傅立葉變換Inverse Fourier Transform。

$$\Psi(x,0) = \int_{-\infty}^{\infty} A(k) \cdot e^{ikx} \cdot dk$$

$A(k)$是以e^{ikx}疊加出$\Psi(x,0)$時的配重係數。

與$\Psi(x,0)$互為Fourier Transform，兩者對應同樣的資訊內容。

若有了$A(k)$，薛丁格方程式的解$\Psi(x,t)$就可以直接寫下！

$A(k)$還有另一個物理意義：

我們可以把對k的積分換成對p的積分！因為兩者成正比。 $p = \hbar k$

$$\Psi(x,0) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \phi(p) \cdot e^{ipx/\hbar} \cdot dp$$

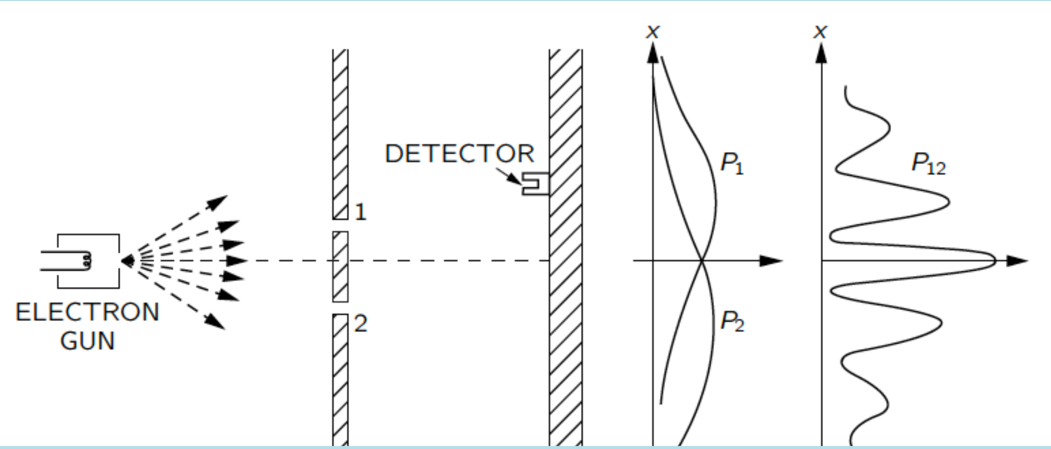
$e^{ipx/\hbar}$是$t = 0$時，有固定動量p的瞬間電子波函數，測量動量永遠得到p值。

因此$\phi(p)$是疊加波函數時，動量為p的配重。稱為動量空間的波函數。

利用Fourier Transformation：$\phi(p)$可以由$\Psi(x,0)$得到。

電子在本質上就有不同的面貌！

自由空間中運動的電子，有特定的動量，但無特定位置，電子像波！

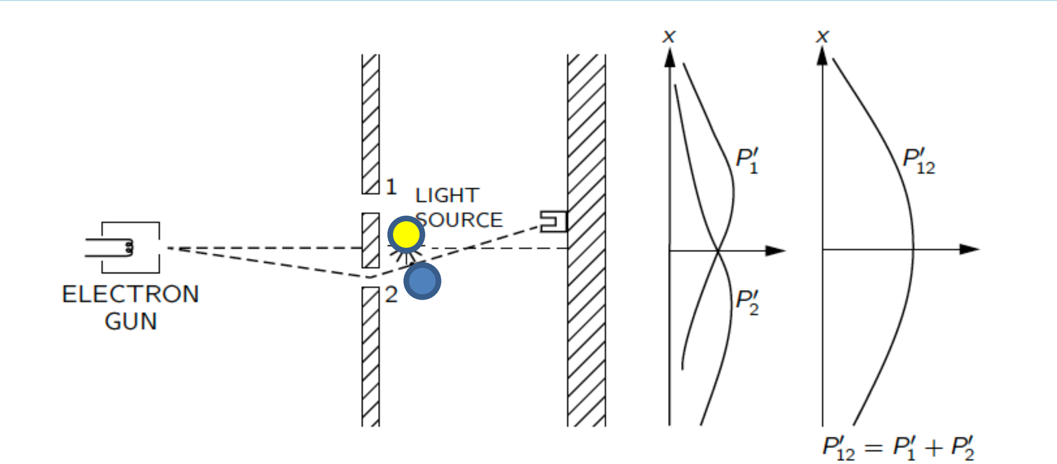


波狀的態

$\Delta x \to \infty, \Delta p = 0$

在狹縫屏幕被觀測位置後，電子像粒子，有特定的位置，

但被光子隨機撞擊改變動量，原本動量的確定性已消失。



粒子狀的態

$\Delta x = 0, \Delta p \to \infty$

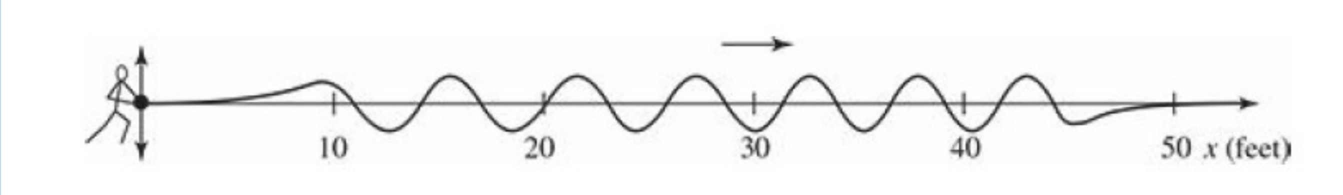
有點像蝙蝠俠，

You can look at the world with q-eyes and you can look at the world with p-eyes. But if you want to open both eyes at the same time, you will go crazy!

Pauli

用波動力學來說明非常直接！電子的兩種面貌都能以波函數來描述：

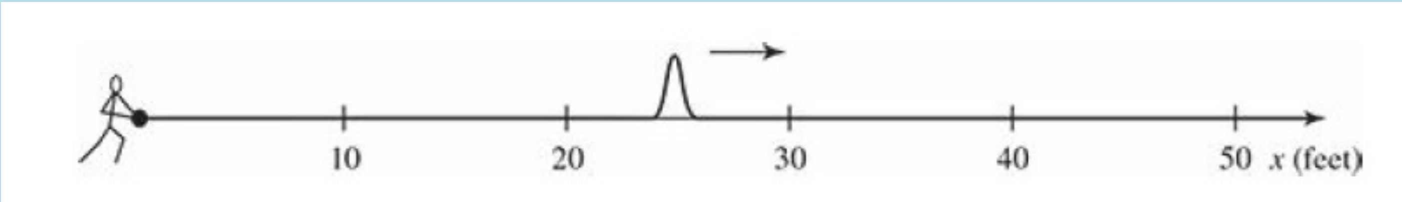
波狀的態的波函數就是自由電子波：$Ae^{i(k_0x-\omega t)}$ 。



正弦波波長特定，動量特定： $\Delta p = 0$

波的強度是一個常數，因此在各處發現此粒子的機率都一樣： $\Delta x \to \infty$

粒子狀的態的波函數則是一個尖針般的波，極窄的波包就是很好的近似。

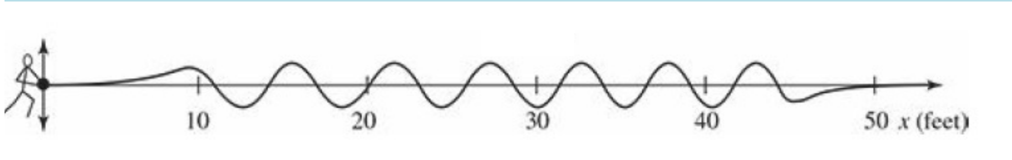


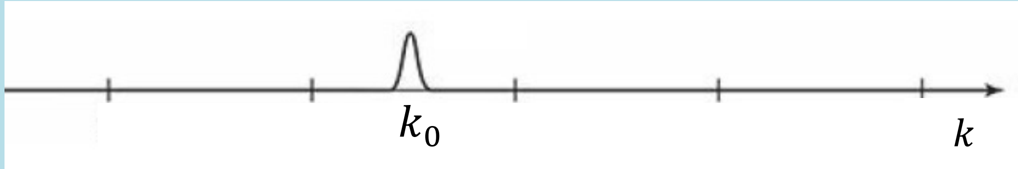
波函數幾乎只在一個位置有值： $\Delta x = 0$

這是由眾多不同波長的正弦波疊加而成，動量完全未定： $\Delta p \to \infty$

電子的動量與位置似乎不能同時維持確定性。

波狀的態的波函數就是自由電子波：Ae^{ik_0x}。





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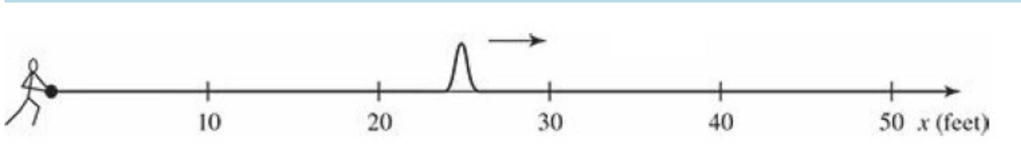
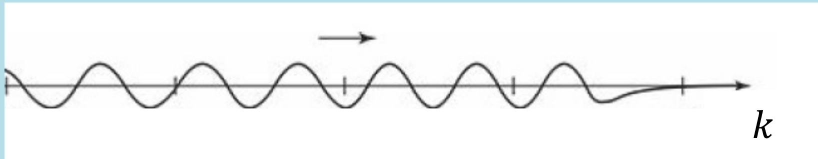
動量空間的波函數$A(k)$or $\phi(p)$ 則是一個如尖針般的函數。





粒子狀的態的波函數則是一個尖針般的波，極窄的波包就是很好的近似。

波函數幾乎只在一個位置有值：$\Delta x = 0$

這是由眾多不同波長的正弦波疊加而成，動量完全未定：$\Delta p \to \infty$

動量空間的波函數$A(k)$or $\phi(p)$ 則是一個正弦函數。

這種如尖針般的函數在無限大空間中的狀態函數研究上非常有用。稱為Delta Function。

6.1 STRONGLY PEAKED FUNCTIONS AND THE DIRAC DELTA FUNCTION

In physics, we often encounter the concept of a pulse of "infinitely short" duration. For instance, a body set in motion (from rest) by a sudden blow attains a momentum equal to the impulse of the blow, namely,

$$mv = I = \int_{t_0}^{t_0+\tau} F(t)\, dt,$$

where $F(t)$ is the force and τ is the duration of the action of the force. The term "blow" implies that τ is so small that the change in momentum occurs instantaneously. However, since such a change in momentum is a finite number, it follows that $F(t)$ should have been infinite during the blow and zero otherwi

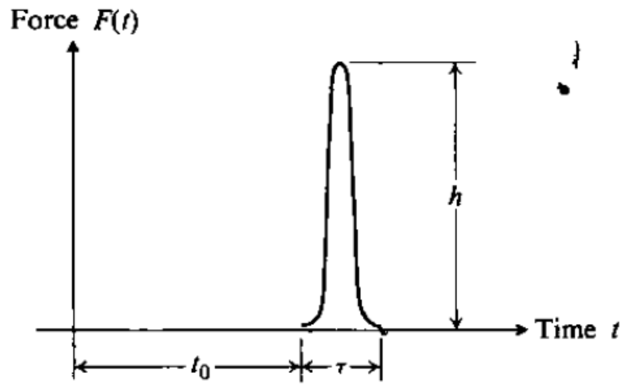


Figure 6.1

This kind of description is not proper in terms of common mathematical concepts. For that matter, it may not even be physically rigorous. Indeed, the actual graph of force is more likely to be a strongly peaked function, as in Fig. 6.1, where h is very large while τ is very small such that the area under the curve is equal to a given value of I. In many cases, a great majority, as a matter of fact, the exact shape of the strongly peaked function [$F(t)$ in this case] is not known. However, insofar as the observable physical effects of such functions are concerned, this lack of information does not usually matter. What is significant, though, is the intensity of the impulse, namely, the value of the integral

$$\int_{t_0}^{t_0+\tau} F(t)\, dt,$$

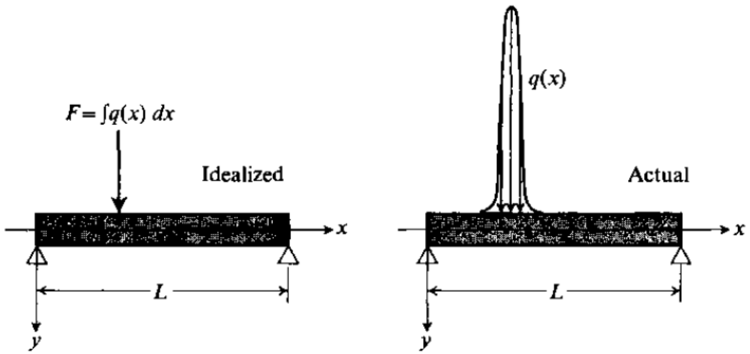


Figure 6.2

and the time when the impulse occurred, namely t_0 (or, perhaps, $t_0 + \tau/2$, but that hardly matters if τ is sufficiently small).

Strongly peaked functions are common to all branches of physics. For instance, a concentrated force acting on a beam is actually a strongly peaked distribution of load (Fig. 6.2). In electrical circuits, strongly peaked currents of extremely short duration often occur in switching processes, like the redistribution of charges between the two capacitors shown in Fig. 6.3 when the switch S is closed. Initially, the voltages $V_1 = Q_1/C_1$ and $V_2 = Q_2/C_2$ are assumed to be different. When the switch is closed, there is a rush of current through it until the charges Q_1 and Q_2 are redistributed into

$$Q_1' = \frac{C_1(Q_1 + Q_2)}{C_1 + C_2}, \qquad Q_2' = \frac{C_2(Q_1 + Q_2)}{C_1 + C_2}.$$

If the resistance of the leads is negligible, then this current pulse is of infinitely short duration and the current is infinitely large. Needless to say, this cannot be rigorously true; apart from the inevitable resistance (small, but never zero), there will also be a self-inductance L of the loop which will tend to moderate the steep rise of the current to its peak value after the switch is closed. In short, the current pulse will be a strongly peaked function of time.

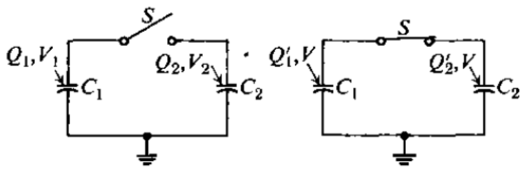


Figure 6.3

In order to facilitate a variety of operations in mathematical physics, and particularly in quantum mechanics, Dirac proposed the introduction of the so-called *delta function* $\delta(x)$ which will be a representative of an infinitely sharply

Equations (2A-11) and (2A-12) define the Fourier integral transformations. If we insert the second equation into the first we get

$$f(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk\, e^{ikx} \int_{-\infty}^{\infty} dy\, f(y) e^{-iky} \tag{2A-13}$$

Suppose now that we interchange, without question, the order of integrations. We then get

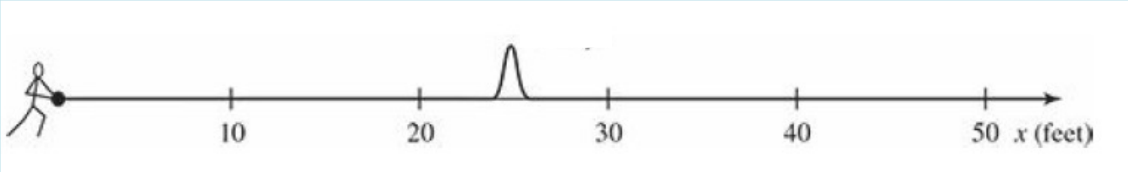
$$f(x) = \int_{-\infty}^{\infty} dy\, f(y) \left[\frac{1}{2\pi} \int_{-\infty}^{\infty} dk\, e^{ik(x-y)} \right] \tag{2A-14}$$

For this to be true, the quantity $\delta(x - y)$ defined by

$$\delta(x - y) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk\, e^{ik(x-y)} \tag{2A-15}$$

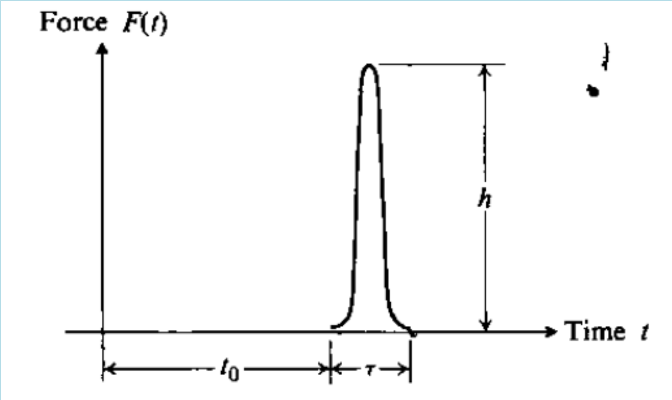
and called the *Dirac delta function* must be a very peculiar kind of function; it must vanish when $x \neq y$, and it must tend to infinity in an appropriate way when $x - y = 0$, since the range of integration is infinitesimally small. It is therefore not a function of the usual

Delta Function - Distribution



粒子狀的態的波函數則是一個尖針般的波，極窄的波包就是很好的近似。

波函數幾乎只在一個位置有值：$\Delta x = 0$ $\Psi(x,0) = \psi(x) \equiv \delta(x - x_0)$



$F(t) \equiv \delta(t - t_0)$

$\delta(x) = 0, x \neq 0$

$\delta(x - x_0) = 0, x \neq x_0$

我們期待脈衝的總衝量是固定的，我們設定$\delta(x)$的積分等於1。

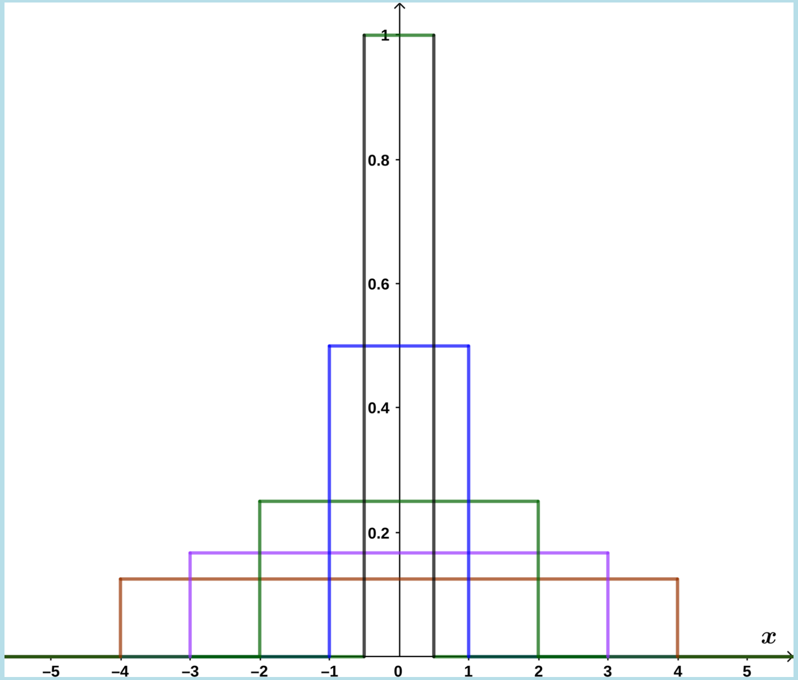
$$\int_{-\infty}^{\infty} dx \cdot \delta(x - x_0) = 1$$

如此，則 $\delta(x) = \infty, x = 0$

$\delta(x - x_0) = \infty, x = x_0$

定義為以下函數取極限$\varepsilon \to 0$：

$$\delta^{(\varepsilon)}(x) = \frac{1}{\varepsilon} \quad \text{for} \quad -\frac{\varepsilon}{2} < x < \frac{\varepsilon}{2}$$
$$= 0 \quad \text{for} \quad |x| > \frac{\varepsilon}{2}$$



$$\int_{-\infty}^{\infty} dx \cdot \delta(x) = 1$$

當$\varepsilon \to 0$，$\delta(x) = 0, x \neq 0$ $\delta(x) = \infty, x = 0$

$$\int_{-\infty}^{\infty} dx \cdot \delta(x) = 1$$

與ε無關，當$\varepsilon \to 0$，依舊成立！

由以上可得，將$\delta(x-a)$與任一函數$f(x)$相乘積分，會得到該函數的值$f(a)$：

$$\int_{-\infty}^{\infty} dx \cdot \delta(x-a) f(x) = \int_{a-\frac{\epsilon}{2}}^{a+\frac{\epsilon}{2}} dx \cdot \frac{1}{\epsilon} f(x) \sim \frac{1}{\epsilon} \cdot \epsilon f(a) \to f(a)$$

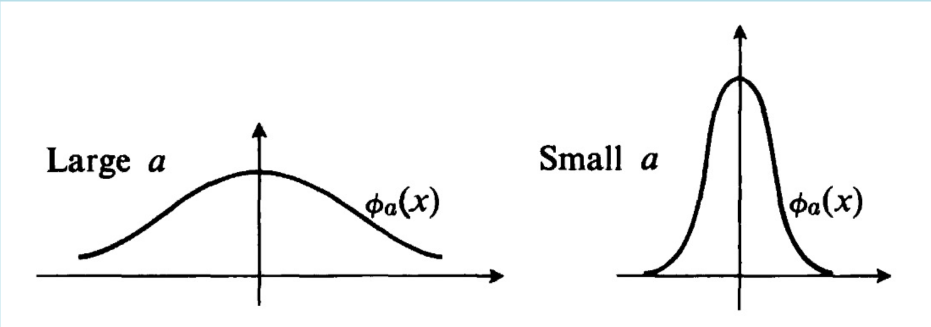
Delta Function $\delta(x)$顯然不是一個正常函數，而是極限的結果。

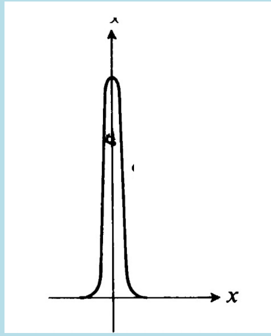
除了上一頁的定義，它有許多極限表示法。

我們可以用極窄的波包來近似：

$$\Psi(x,0) = \sqrt{\frac{2\pi}{\alpha}}\, e^{-\frac{x^2}{2\alpha}} \xrightarrow[\alpha\to 0]{} 2\pi\delta(x)$$

注意：
$$\int_{-\infty}^{\infty} dx \cdot \Psi(x,0) = 2\pi$$





另一方面，波包可以展開為高斯函數與平面波的積分：

$$\Psi(x,0) = \int_{-\infty}^{\infty} e^{-\alpha k^2/2} \cdot e^{ikx} \cdot dk \xrightarrow[\alpha\to 0]{} \int_{-\infty}^{\infty} e^{ikx} \cdot dk$$

這裏得到一非常有用的公式，稱為$\delta(x)$的積分表現。

$$\int_{-\infty}^{\infty} e^{ikx} \cdot dk = 2\pi\delta(x)$$

自由電子波函數e^{ikx}對k無限積分可以得到$\delta(x)$。

無論你取哪一種極限來定義： $\delta(x-a)=0, x\neq a$

$$\int_{-\infty}^{\infty} dx\cdot\delta(x-a)f(x)=\int_{-\infty}^{\infty} dx\cdot\delta(x-a)f(a)=f(a)\int_{-\infty}^{\infty} dx\cdot\delta(x-a)=f(a)$$

$\delta(x)=0, x\neq 0$ $\delta(x)=\infty, x=0$

$$\int_{-\infty}^{\infty} dx\cdot\delta(x)=1$$

Summary

$$\int_{-\infty}^{\infty} dx\cdot\delta(x-a)f(x)=f(a)$$

$$\int_{-\infty}^{\infty} dx\cdot[\delta(x)]^2=\delta(0)=\infty$$

$\delta(x)$不是一個正常的、平方可積的函數，這一類函數被稱為 distribution.

Example 3. Verify the rule

$$\delta(ax) = (1/|a|)\,\delta(x),\ a \neq 0.$$

Assume that $a > 0$ and write, using $ax = \xi$, $dx = (1/a)\,d\xi$:

$$\int_{-\infty}^{+\infty} \delta(ax)f(x)\,dx = \int_{-\infty}^{+\infty} \delta(\xi)f(\xi/a)(1/a)\,d\xi = (1/a)f(0).$$

If $a < 0$, use $ax = \xi$, $dx = (1/a)\,d\xi$ again; now, however, the limits of integration are interchanged and

$$\int_{-\infty}^{+\infty} \delta(ax)f(x)\,dx = \int_{+\infty}^{-\infty} \delta(\xi)f(\xi/a)(1/a)\,d\xi = -(1/a)f(0).$$

In either case, the result is $(1/|a|)f(0)$, thus establishing the rule.

Remark: From this it follows that $\delta(x)$ is an even function (set $a = -1$).

Example 4. Verify the rule

$$\delta(x^2 - a^2) = (1/2a)[\delta(x + a) + \delta(x - a)] \qquad (a > 0).$$

Observe that $\delta(x^2 - a^2) = \delta[(x + a)(x - a)]$. Since $\delta(\xi) = 0$ unless $\xi = 0$, it follows that $\delta(x^2 - a^2) = 0$ except at the points $x = \pm a$. Therefore, we can write

$$\int_{-\infty}^{+\infty} \delta(x^2 - a^2)f(x)\,dx = \int_{-a-\epsilon}^{-a+\epsilon} \delta[(x + a)(x - a)]f(x)\,dx + \int_{a-\epsilon}^{a+\epsilon} \delta[(x + a)(x - a)]f(x)\,dx \qquad (a > 0),$$

where $0 < \epsilon < 2a$ and ϵ can be arbitrarily small. Now, in the neighborhood of $x = -a$, the factor $(x - a)$ may be replaced by $-2a$. Then

$$\begin{aligned}\int_{-a-\epsilon}^{-a+\epsilon} \delta[(x + a)(x - a)]f(x)\,dx &= \int_{-a-\epsilon}^{-a+\epsilon} \delta[(-2a)(x + a)]f(x)\,dx \\ &= \int_{-a-\epsilon}^{-a+\epsilon} \frac{1}{|-2a|}\,\delta(x + a)f(x)\,dx \\ &= \int_{-\infty}^{+\infty} \frac{1}{2a}\,\delta(x + a)f(x)\,dx.\end{aligned}$$

The infinite limits can be used again because $\delta(x + a) = 0$ except at $x = -a$.

In a similar manner,

$$\int_{a-\epsilon}^{a+\epsilon} \delta[(x + a)(x - a)]f(x)\,dx = \int_{-\infty}^{+\infty} \frac{1}{2a}\,\delta(x - a)f(x)\,dx,$$

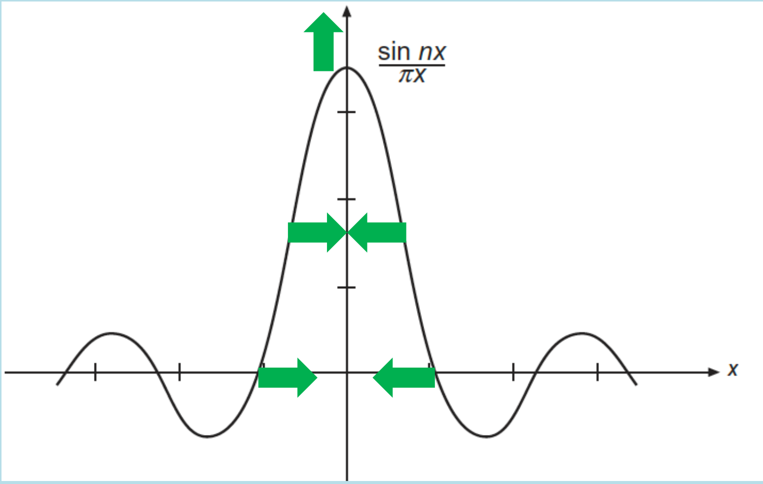
and the rule is established.

Remark. This rule breaks down for $a = 0$. There is apparently no way of interpreting the expression $\delta(x^2)$.

$$\delta(x) \equiv \lim_{n\to\infty} \frac{1}{2\pi} \int_{-n}^{n} dk \cdot e^{ikx} = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk \cdot e^{ikx}$$

有限積分可以直接具體算出來：

$$\frac{1}{2\pi} \int_{-n}^{n} dk \cdot e^{ikx} = \frac{1}{2\pi} \frac{1}{ik} e^{ikx} \Big|_{-n}^{n} = \frac{\sin nx}{\pi x}$$



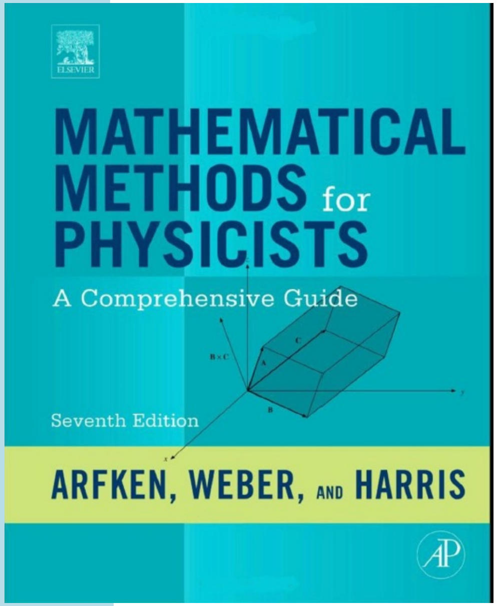
$$\int_{-\infty}^{\infty} e^{ikx} \cdot dk = 2\pi\delta(x)$$

$n \to \infty$時中央的Peak會變窄又變高，類似$\delta(x)$只有$x = 0$最重要。

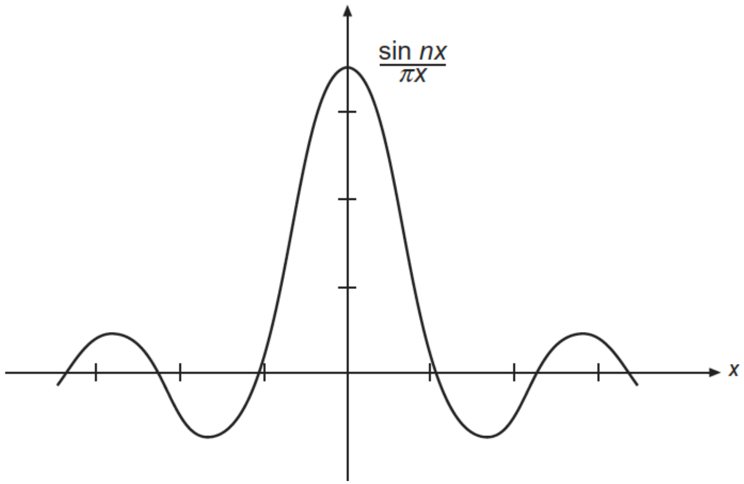
而且可以證明函數底下總面積、如同$\delta(x)$、為1：

$$\int_{-\infty}^{\infty} dx \cdot \frac{\sin nx}{\pi x} = 1$$

From Eq. (1.150), $\delta(x)$ must be an infinitely high, thin spike at $x = 0$, as in the description of an impulsive force or the charge density for a point charge. The problem is that **no such function exists**, in the usual sense of function. However, the crucial property in Eq. (1.150) can be developed rigorously as the limit of a **sequence** of functions, a distribution. For example, the delta function may be approximated by any of the sequences of functions, Eqs. (1.152) to (1.155) and Figs. 1.21 and 1.22:



$$\delta_n(x) = \frac{\sin nx}{\pi x} = \frac{1}{2\pi}\int_{-n}^{n} e^{ixt}\,dt. \tag{1.155}$$



The forms for $\delta_n(x)$ given in Eqs. (1.152) to (1.155) all obviously peak strongly for large n at $x = 0$. They must also be scaled in agreement with Eq. (1.151). For the forms in Eqs. (1.152) and (1.154), verification of the scale is the topic of Exercises 1.11.1 and 1.11.2. To check the scales of Eqs. (1.153) and (1.155), we need values of the integrals

$$\int_{-\infty}^{\infty} e^{-n^2x^2}\,dx = \sqrt{\frac{\pi}{n}} \quad \text{and} \quad \int_{-\infty}^{\infty} \frac{\sin nx}{x}\,dx = \pi.$$

Delta Function $\delta(x)$的積分表示式：

$$\int_{-\infty}^{\infty} dk \cdot e^{ikx} = 2\pi\delta(x)$$

這可以改寫成動量積分的版本：

$$\int_{-\infty}^{\infty} dp \cdot e^{ipx/\hbar} = 2\pi\hbar\delta(x)$$

$$p = \hbar k$$

把動量變數與位置變數互換，也是對的，畢竟兩者都是一樣的連續變數。

$$\int_{-\infty}^{\infty} dx \cdot e^{ipx/\hbar} = 2\pi\hbar\delta(p)$$

自由電子波函數對x無限積分可以得到$\delta(k)$。

有一個比較不嚴格但直覺地推導：

If $p \neq 0$, $$\int_{-\infty}^{\infty} dx \cdot e^{ipx} = 0$$

因為e^{ipx}，是週期函數，加總一個週期，值就抵消為零，

積分邊界趨近無限大，積分會跨越無限多個e^{ipx}的週期，積分值趨近零。

If $p = 0$, $$\int_{-\infty}^{\infty} dx \cdot e^{ipx} \to \infty$$

這是$\delta(p)$的典型表現，因此可以寫成： $$\int_{-\infty}^{\infty} dx \cdot e^{ipx/\hbar} = 2\pi\hbar\delta(p)$$

$$\Psi(x,0) = \int_{-\infty}^{\infty} A(k) \cdot e^{ikx} \cdot dk$$

$A(k)$是以e^{ikx}疊加出$\Psi(x,0)$時的配重係數。

我們可以把對k的積分換成對p的積分！因為兩者成正比。 $p = \hbar k$

$$\Psi(x,0) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \phi(p) \cdot e^{ipx/\hbar} \cdot dp$$

$e^{ipx/\hbar}$是$t = 0$時，有固定動量p的瞬間電子波函數，測量動量永遠得到p值。

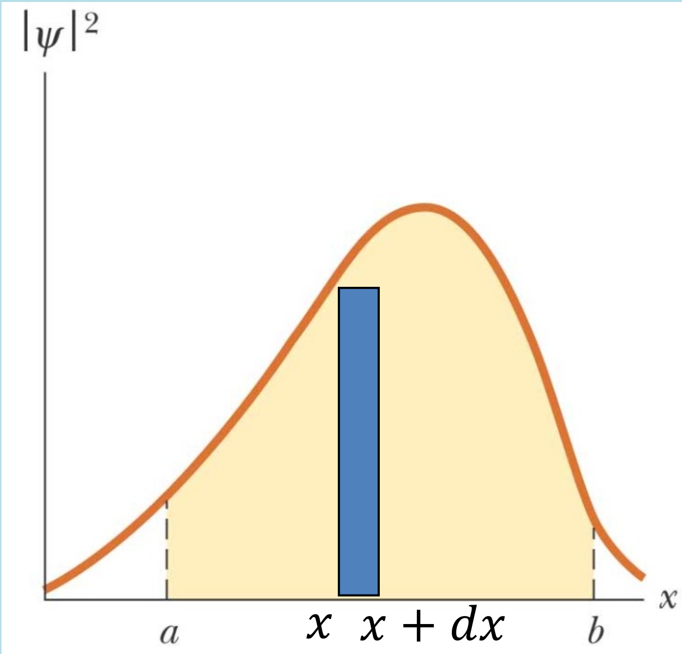
因此$\phi(p)$是疊加波函數時，動量為p的配重。稱為動量空間的波函數。

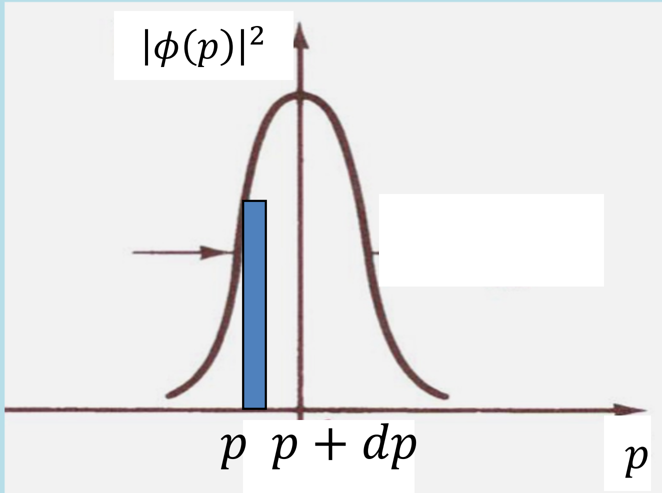
利用Fourier Transformation：$\phi(p)$可以由$\Psi(x,0)$得到。

量子力學的機率基本假設

在x與$x+dx$之間發現該粒子的機率，可以寫成：

$$|\psi(x)|^2 \cdot dx = \psi^*(x) \cdot \psi(x) \cdot dx$$





動量測量結果在p與$p+dp$之間的機率，可以寫成：

$$|\phi(p)|^2 \cdot dp = \phi^*(p) \cdot \phi(p) \cdot dp$$

以上的假設也可以等價用期望值來表示，就更能推廣到其他物理量！

Delta Function 典型用法是將$\delta(p-p')$與任一函數$f(p')$積分，它會強迫$p'=p$。

$$\int_{-\infty}^{\infty} dp' \cdot \delta(p'-p) f(p') = f(p)$$

將此式運用於動量空間的波函數：

$$\phi(p) = \int_{-\infty}^{\infty} dp' \cdot \phi(p')\delta(p'-p) =$$

$$\int_{-\infty}^{\infty} dx \cdot e^{\frac{i(p'-p)x}{\hbar}} = 2\pi\hbar\delta(p'-p)$$

$$= \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dp' \cdot \phi(p') \cdot \int_{-\infty}^{\infty} dx\, e^{\frac{i(p'-p)x}{\hbar}}$$

$$\Psi(x,0) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} \phi(p') \cdot e^{\frac{ip'x}{\hbar}} \cdot dp'$$

$$= \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} dx\, e^{\frac{-ipx}{\hbar}} \left[\frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} dp' \cdot \phi(p') e^{\frac{ip'x}{\hbar}}\right]$$

交換積分順序！

$\phi(p)$可以由$\Psi(x,0)$得到的具體計算式：

$$\phi(p) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} \Psi(x,0) \cdot e^{\frac{-ipx}{\hbar}} \cdot dx$$

這是數物中標準的傅立葉變換！

動量空間波函數$\phi(p)$與波函數$\psi(x)$互為傅立葉變換：

$$\phi(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \psi(x) \cdot e^{-ipx/\hbar} \cdot dx$$

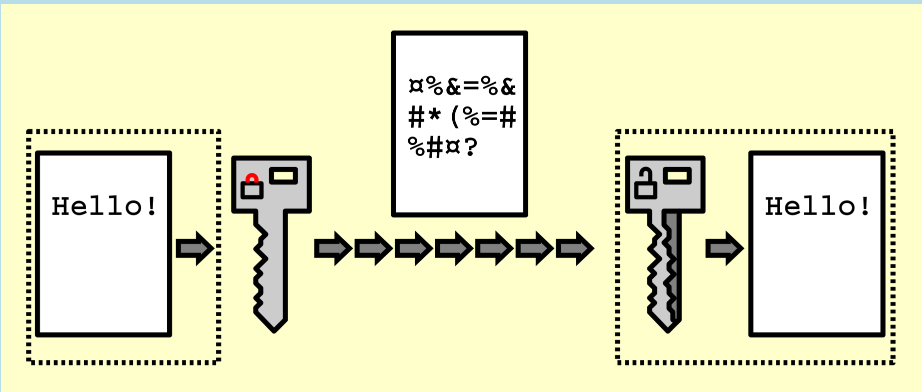
$\Psi(x,0)$就是$\phi(p)$的反傅立葉變換Inverse Fourier Transform：

$$\psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \phi(p) \cdot e^{ipx/\hbar} \cdot dp$$

將平面波以動量波函數$\phi(p)$為權重疊加就得到空間波函數$\psi(x)$。

我們常說$\psi(x)$的所有資訊都存在$\phi(p)$之中。

有了$\phi(p)$就能算出$\psi(x)$，反之亦然！有點像Encryption加密。



1. Given that $A(k) = N/(k^2 + \alpha^2)$, calculate $\psi(x)$. Plot $A(k)$ and $\psi(x)$ and show that $\Delta k\, \Delta x > 1$, independent of the choice of α.

EXAMPLE 2-1

Consider a wave packet for which

$$A(k) = N \qquad -K \le k \le K$$
$$= 0 \qquad \text{elsewhere}$$

Calculate $\psi(x, 0)$, and use some reasonable definition of the width to show that (2-8) is satisfied.

SOLUTION We have

$$\psi(x, 0) = \int_{-K}^{K} dk\, N e^{ikx} = \frac{N}{ix}(e^{iKx} - e^{-Kx}) = 2N\frac{\sin Kx}{x}$$

The definition of $A(k)$ easily shows that $\Delta k = 2K$. A reasonable definition of Δx might be the distance between the two points at which $\psi(x)$ first vanishes as it gets away from $x = 0$. This happens when $Kx = \pm\pi$, so that $\Delta x = 2\pi/K$. It follows that

$$\Delta k\, \Delta x = 4\pi$$

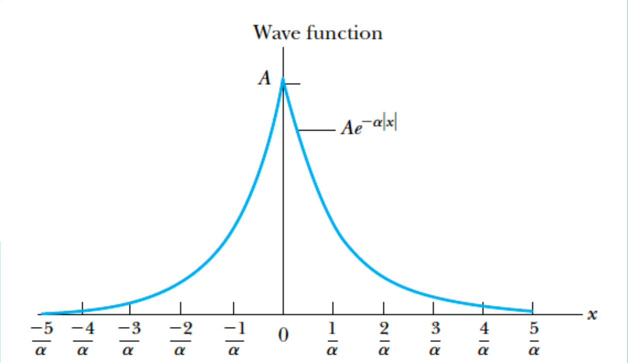
which certainly satisfies (2-8).

$$\int_0^\infty \frac{\cos(mx)}{x^2 + a^2}\, dx = \frac{\pi}{2|a|} e^{-|ma|}$$

Consider a wave function of the form

$$\Psi(x, 0) = Ae^{-\mu|x|}$$

Calculate the wave function in momentum space $\phi(p)$.



$\phi(p)$是動量波函數，而動量測量總機率也必須為1，$\phi(p)$必定滿足歸一化條件。

$$\int_{-\infty}^{\infty} dx\, \Psi^*(x)\Psi(x) = \int_{-\infty}^{\infty} dx \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Phi^*(k)e^{-ikx}dk \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Phi(k')e^{ik'x}dk'. \tag{4.4.7}$$

We rearrange the integrals to do the x integration first:

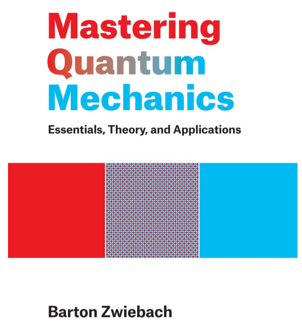
$$\int_{-\infty}^{\infty} dx\, \Psi^*(x)\Psi(x) = \int_{-\infty}^{\infty} dk\, \Phi^*(k) \int_{-\infty}^{\infty} dk'\, \Phi(k') \frac{1}{2\pi} \int_{-\infty}^{\infty} dx\, e^{i(k'-k)x}. \tag{4.4.8}$$

The x integral, with the $1/(2\pi)$ prefactor, is precisely a delta function, and it makes the k' integration immediate:

$$\begin{aligned} \int_{-\infty}^{\infty} dx\, \Psi^*(x)\Psi(x) &= \int_{-\infty}^{\infty} dk\, \Phi^*(k) \int_{-\infty}^{\infty} dk'\, \Phi(k')\, \delta(k'-k) \\ &= \int_{-\infty}^{\infty} dk\, \Phi^*(k)\Phi(k). \end{aligned} \tag{4.4.9}$$

Our final result is therefore

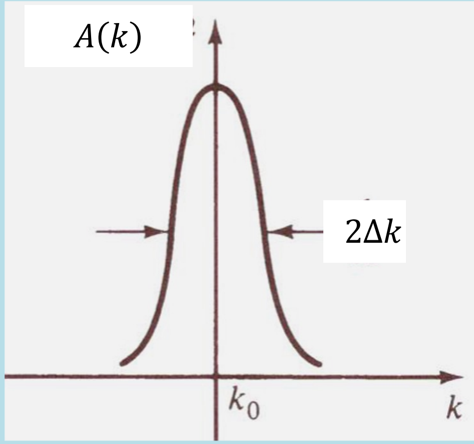
$$\boxed{\int_{-\infty}^{\infty} dx\, |\Psi(x)|^2 = \int_{-\infty}^{\infty} dk\, |\Phi(k)|^2.} \tag{4.4.10}$$



波包是最有用的疊加態了，它是疊加稍微不同角波數k的正弦波。

具體可以考慮一高斯分佈Gaussian form $A(k)$：

$$A(k) = Ce^{-\frac{\alpha(k-k_0)^2}{2}}$$



這表示是以為k_0中心，形成一離開此值就快速降低的分佈，

若取極值的1/3左右位置，寬度大約是$\Delta k \sim \sqrt{2}/\sqrt{\alpha}$。

k與動量成正比，所疊加出的狀態，在測量動量時，$p_0 = \hbar k_0$的機率應該最大，

合理的猜想：測量結果會有不準度$\Delta p = \hbar \Delta k \sim \hbar\sqrt{2}/\sqrt{\alpha}$ 。

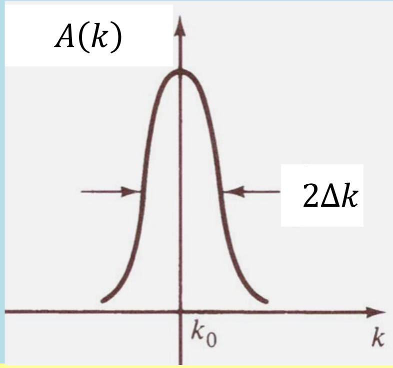
暫時忽略常數C，最後再用歸一化條件來訂。

$$\psi(x) = \int_{-\infty}^{\infty} e^{-\frac{\alpha(k-k_0)^2}{2}} \cdot e^{ikx} \cdot dk$$

已知高斯函數的無限積分：

因此要將指數湊成平方：

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



首先變換變數： $q \equiv k - k_0$ 　將$k = q + k_0$代入

$$\psi(x) = \int_{-\infty}^{\infty} e^{-\frac{\alpha(k-k_0)^2}{2}} \cdot e^{ikx} \cdot dk = \int_{-\infty}^{\infty} e^{-\frac{\alpha q^2}{2}} \cdot e^{i(q+k_0)x} \cdot dq$$

與q無關！

$$= e^{ik_0x} \int_{-\infty}^{\infty} e^{-\frac{\alpha q^2}{2}+iqx} \cdot dq$$

接下來湊成平方。

$$= e^{ik_0x} \int_{-\infty}^{\infty} e^{-\frac{x^2}{2\alpha}} \cdot e^{-\frac{\alpha}{2}\left(q^2-2\frac{ix}{\alpha}q-\frac{x^2}{\alpha^2}\right)} \cdot dq$$

$$q' \equiv q - i\frac{x}{\alpha}$$

$$= e^{ik_0x} e^{-\frac{x^2}{2\alpha}} \int_{-\infty}^{\infty} e^{-\frac{\alpha q'^2}{2}} \cdot dq' = \sqrt{\frac{2\pi}{\alpha}}\, e^{ik_0x} e^{-\frac{x^2}{2\alpha}}$$

積分已經與x無關了!就是一個常數。

計算前一頁的常數 $\int_{-\infty}^{\infty} dx \cdot e^{-ax^2}$

先平方：

$$\int_{-\infty}^{\infty} dx \cdot e^{-ax^2} \cdot \int_{-\infty}^{\infty} dy \cdot e^{-ay^2} = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} dxdy \cdot e^{-ax^2-ay^2}$$

換極座標：

$$= \int_{0}^{2\pi}\int_{0}^{\infty} rdr \cdot d\theta \cdot e^{-ar^2} = 2\pi \int_{0}^{\infty} rdr \cdot e^{-ar^2} = \pi \int_{0}^{\infty} dr^2 \cdot e^{-ar^2} = \frac{\pi}{a}$$

開根號：

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

$$\psi(x) = C\sqrt{\frac{2\pi}{\alpha}}\, e^{ik_0 x} e^{-\frac{x^2}{2\alpha}}$$

$$= C\sqrt{\frac{2\pi}{\alpha}}\left(e^{-\frac{x^2}{2\alpha}}\cos k_0 x + i e^{-\frac{x^2}{2\alpha}}\sin k_0 x\right)$$

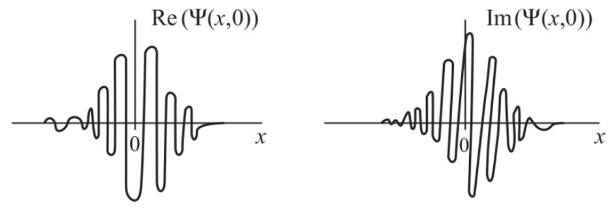
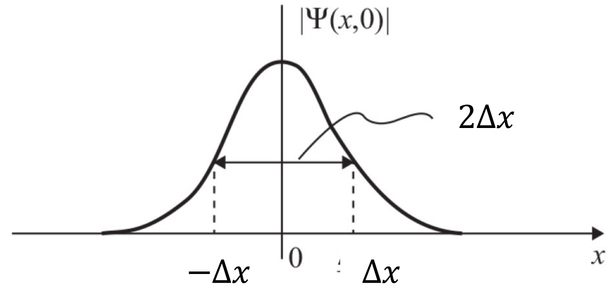


Figure 4.2
The real and imaginary parts of Ψ(x, 0).



在時間為零，波函數是一類似自由電子波$e^{ik_0 x}$的振盪函數，乘上一高斯函數。

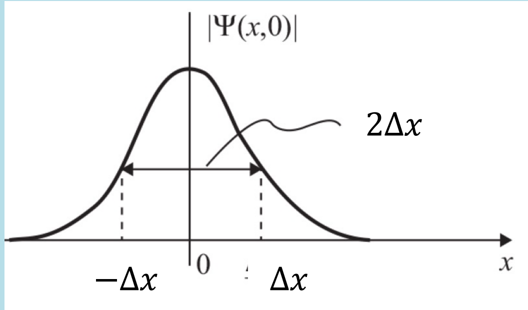
高斯函數 $e^{-\frac{x^2}{2\alpha}}$ 決定了振盪的振幅，也就是波強度：$|\Psi(x,0)|$ 。

因此振幅集中於以原點為中心，寬度由α決定的packet內。稱為波包Wave Packet。

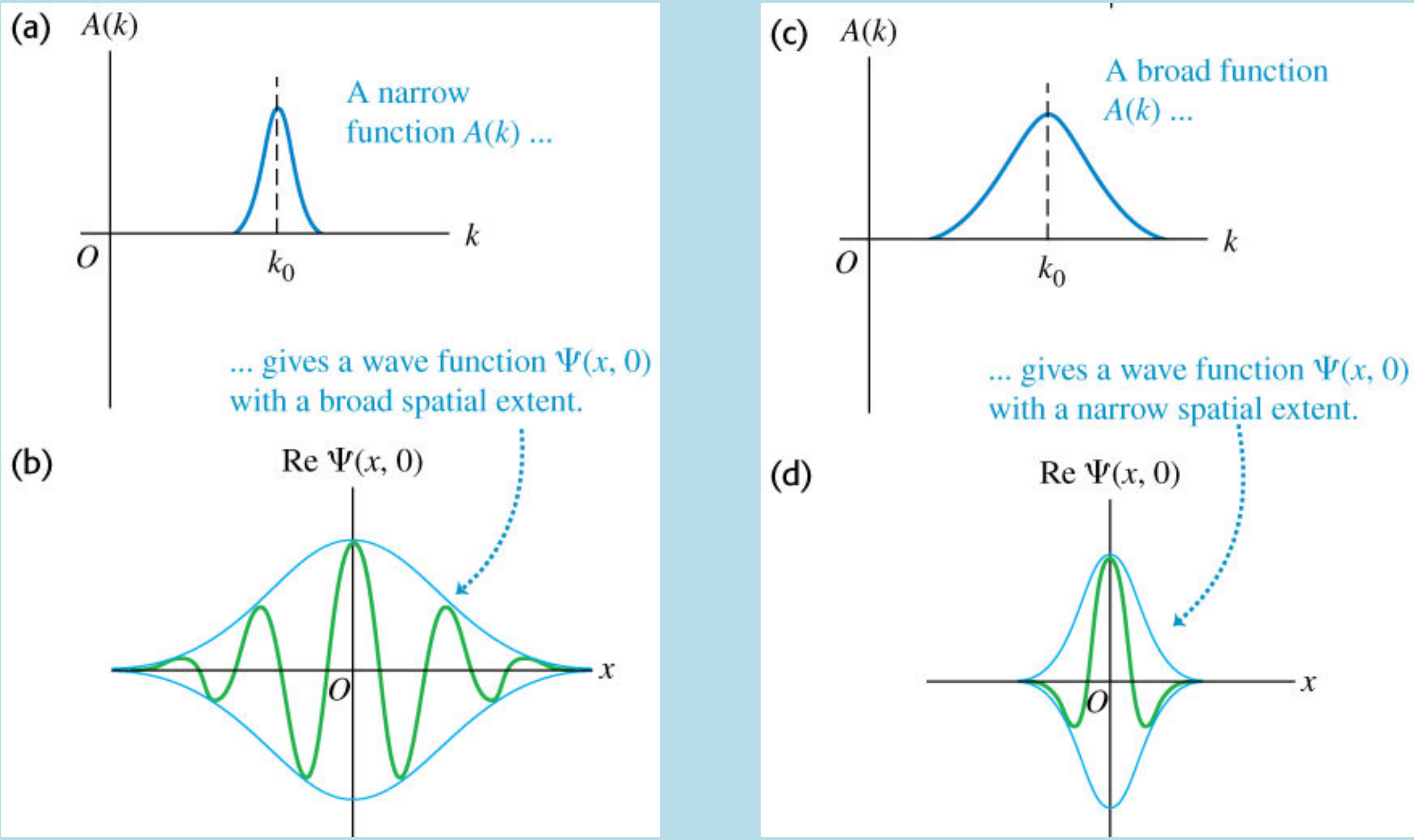
$A(k)$與$|\psi(x)|$都是高斯分佈。若取極值的e^{-1}左右位置為寬度：

$A(k) \sim e^{-\frac{\alpha(k-k_0)^2}{2}}$ 寬度大約是$k - k_0 = \Delta k \sim \sqrt{2}/\sqrt{\alpha}$。

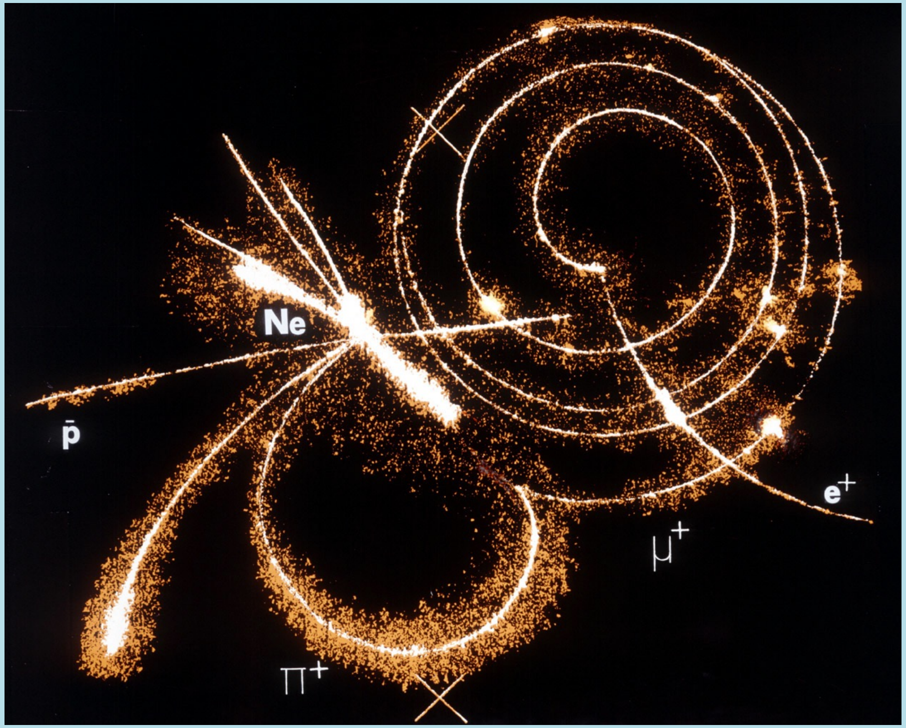
$|\psi(x)| \sim e^{-\frac{x^2}{2\alpha}}$ 波函數振幅寬度大約是$\Delta x = \sqrt{2}\sqrt{\alpha}$。



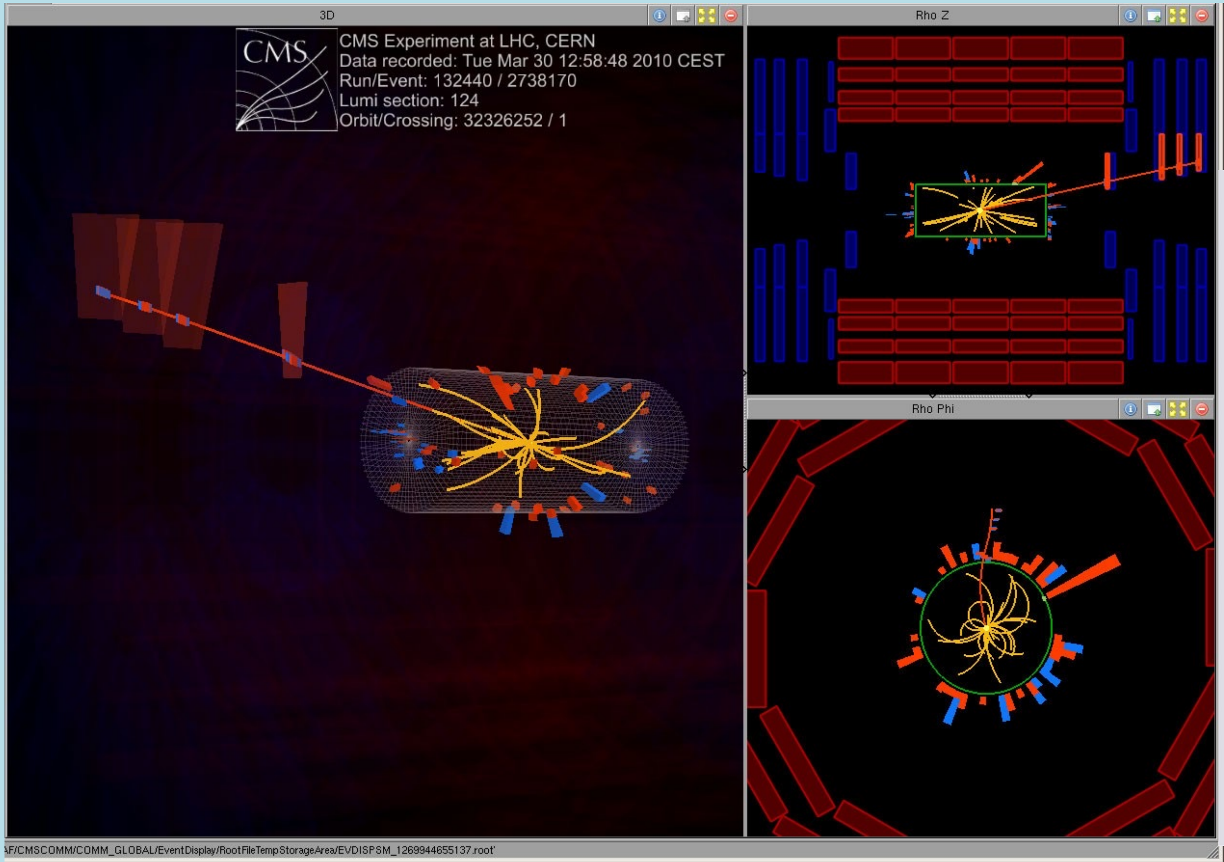
$$\Delta x \cdot \Delta k = 2$$

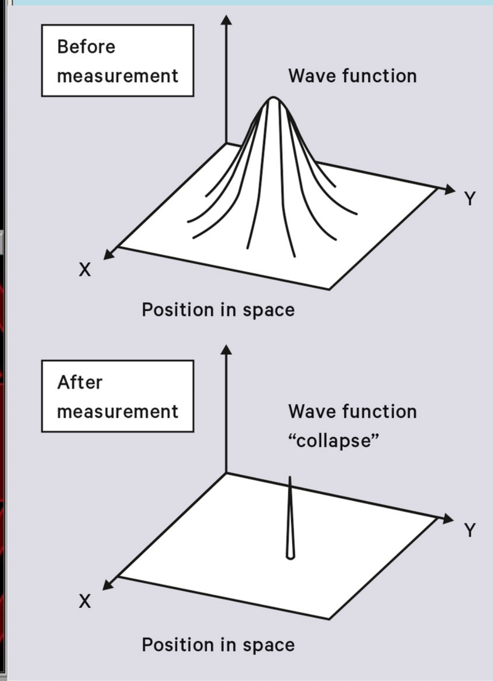


角波數k範圍越寬，製造出的波包的空間x範圍就可以越窄！



波包的意義就是在全球化的波動現象中，實現區域性的波函數！





波包的應用最具體的應用就是粒子的散射！

粒子在散射後一出現路徑就等於對位置作了測量，

作了測量，波函數就崩潰為極窄的波包，接著波包的演化就是等速移動。

函數$F(p)$為函數$f(x)$的傅立葉變換：

$$f(x) \to F(k) \equiv \mathcal{F}\{f(x)\}$$

$$F(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) \cdot e^{-ikx} \cdot dx$$

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f'(x) e^{-ikx} dx = \frac{1}{\sqrt{2\pi}} f(x) e^{-ikx} \Big|_{-\infty}^{\infty} - \frac{ik}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) e^{-ikx} dx$$

函數的微分在變換後只是乘上$-ik$。

$$\mathcal{F}\{f'(x)\} = -ik \cdot \mathcal{F}\{f(x)\}$$

此結果可以推廣為：

$$\mathcal{F}\left\{f^{(n)}(x)\right\} = (-ik)^n \cdot \mathcal{F}\{f(x)\}$$

Chapter 20

Integral Transforms

20.1 Introduction

Frequently in mathematical physics we encounter pairs of functions related by an expression of the form

$$g(x) = \int_a^b f(t)K(x,t)dt, \qquad (20.1)$$

$$\mathcal{F}\{f'(x)\} = -ik \cdot \mathcal{F}\{f(x)\}$$

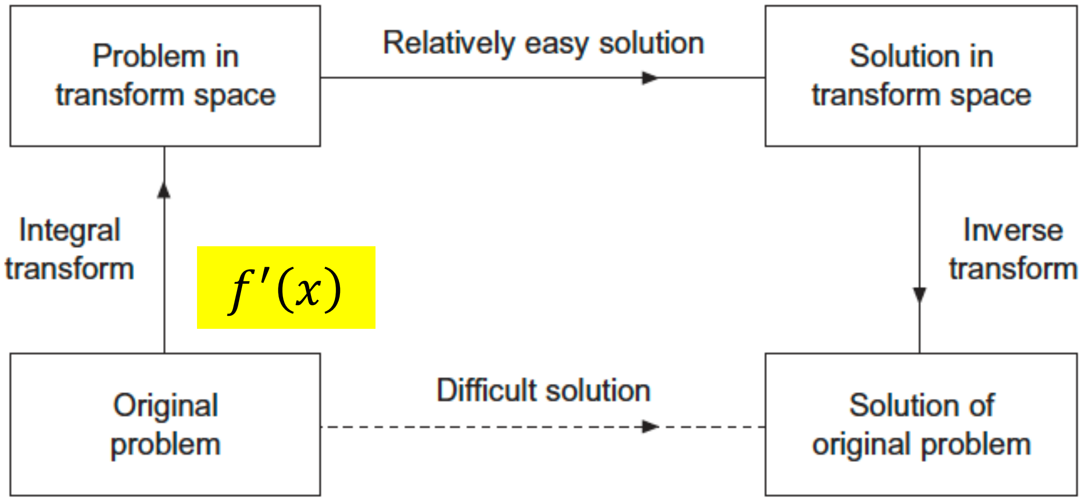


Figure 20.1 Schematic: use of integral transforms.

7.7 APPLICATIONS OF FOURIER TRANSFORMS. THE PRINCIPLE OF CAUSALITY

Example 1. Consider a damped harmonic oscillator acted on by an external force $g(t)$. The motion of the oscillator is then governed by the differential equation

$$\ddot{x}(t) + 2\alpha\dot{x}(t) + \omega_0^2 x(t) = f(t),$$

where $f(t) = (1/m)g(t)$. This problem has been treated in Section 2.5 for the case where $f(t)$ is a sinusoidally varying function of frequency ω. By means of Fourier transforms, we can extend this result to an arbitrary function $f(t)$. In all cases of practical interest, $f(t)$ will possess a Fourier transform;† then

$$f(t) = (1/\sqrt{2\pi})\int_{-\infty}^{+\infty} F(\omega)e^{-i\omega t}\,d\omega,$$

where

$$F(\omega) = (1/\sqrt{2\pi})\int_{-\infty}^{+\infty} f(t)e^{i\omega t}\,dt.$$

The solution $x(t)$ is also expected, on physical grounds, to possess a Fourier transform [which we shall denote by $A(\omega)$] so that

$$x(t) = (1/\sqrt{2\pi})\int_{-\infty}^{+\infty} A(\omega)e^{-i\omega t}\,d\omega.$$

We can easily find $A(\omega)$ by subjecting the differential equation to a Fourier transformation and using $\mathfrak{F}\{\dot{x}\} = -i\omega\mathfrak{F}\{x\}$, and $\mathfrak{F}\{\ddot{x}\} = -\omega^2\mathfrak{F}\{x\}$. *Note:* These formulas assume that $x(\pm\infty) = \dot{x}(\pm\infty) = 0$. In many cases this will be true. However, if $x(t)$ is treated as a *distribution*, no such restriction is needed. We have, *by definition,**

$$\int_{-\infty}^{+\infty} \frac{d}{dt} x(t) e^{i\omega t}\, dt = -\int_{-\infty}^{+\infty} x(t) \frac{d}{dt} e^{i\omega t}\, dt.$$

The transformed differential equation reads

$$-\omega^2 A(\omega) - 2\alpha\omega i A(\omega) + \omega_0^2 A(\omega) = F(\omega)$$

and yields

$$A(\omega) = \frac{F(\omega)}{(\omega_0^2 - \omega^2) - 2\alpha\omega i}\cdot$$

The solution of the problem is then

$$x(t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \frac{F(\omega) e^{-i\omega t}}{(\omega_0^2 - \omega^2) - 2\alpha\omega i}\, d\omega.$$

Theorem. If $\mathfrak{F}\{h(x)\} = F(k)G(k)$, then

$$h(x) = (f * g) = (g * f) = (1/\sqrt{2\pi}) \int_{-\infty}^{+\infty} f(\xi)g(x - \xi)\, d\xi,$$

where $F(k) = \mathfrak{F}\{f(x)\}$ and $G(k) = \mathfrak{F}\{g(x)\}$.

Indeed (denote the inverse Fourier transform by $\mathfrak{F}^{-1}$),

$$\mathfrak{F}^{-1}\{F(k)G(k)\} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} F(k)G(k)e^{-ikx}\, dk$$

$$= \frac{1}{2\pi} \int_{-\infty}^{+\infty} F(k)e^{-ikx}\, dk \int_{-\infty}^{+\infty} g(\xi)e^{ik\xi}\, d\xi.$$

If the interchanging of the order of integrations is permissible, then

$$\mathfrak{F}^{-1}\{F(k)G(k)\} = \frac{1}{2\pi} \int_{-\infty}^{+\infty} g(\xi)\, d\xi \int_{-\infty}^{+\infty} F(k)e^{-ik(x-\xi)}\, dk$$

$$= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} g(\xi)f(x - \xi)\, d\xi,$$

as stated.

5.2 THE LAPLACE INTEGRAL

If a function $f(t)$ is defined in the region $0 \leq t < \infty$, where t and $f(t)$ are real, then the function $F(s)$, defined by the *Laplace integral*

$$F(s) = \int_0^\infty e^{-st} f(t)\, dt \qquad (s = \text{complex}),$$

is known as the *Laplace transform* of $f(t)$. Symbolically,

$$F(s) = \mathcal{L}\{f(t)\},$$

emphasizing the point of view that $F(s)$ is a result of a certain operation (as defined above) performed on a function $f(t)$.

Examples

1. $f(t) = t, \qquad F(s) = \int_0^\infty te^{-st}\,dt = 1/s^2 \quad (\text{Re } s > 0).$

   Observe that if s is complex and $s = \sigma + i\omega$, then

$$F(s) = \int_0^\infty te^{-\sigma t}e^{-i\omega t}\,dt$$
$$= \int_0^\infty te^{-\sigma t}\cos\omega t\,dt - i\int_0^\infty te^{-\sigma t}\sin\omega t\,dt.$$

Both integrals converge if $\sigma > 0$ and diverge if $\sigma \leq 0$. For $\sigma > 0$, the actual evaluation is conveniently done in the complex form (using integration by parts).

2. $f(t) = 1, \qquad F(s) = \int_0^\infty e^{-st}\,dt = 1/s \quad (\text{Re } s > 0),$

Using integration by parts and induction,

3. $f(t) = t^n \quad (n = \text{integer}), \qquad F(s) = \int_0^\infty t^n e^{-st}\,dt = n!/s^{n+1} \quad (\text{Re } s > 0).$

Using the definition of gamma function,

4. $f(t) = t^\alpha \quad (\alpha > -1), \qquad F(s) = \dfrac{\Gamma(\alpha+1)}{s^{\alpha+1}} \quad (\text{Re } s > 0).$

5. $f(t) = e^{at}, \qquad F(s) = \dfrac{1}{s-a} \quad (\text{Re } s > a),$

6. $f(t) = \sin kt, \qquad F(s) = \dfrac{k}{s^2+k^2} \quad (\text{Re } s > 0),$

7. $f(t) = \cos kt, \qquad F(s) = \dfrac{s}{s^2+k^2} \quad (\text{Re } s > 0).$

From these examples, it is evident that the Laplace integral converges, as a rule, for a restricted region of s (in the complex s-plane). It is a general feature of the Laplace integral that this region can be characterized by Re $s > \alpha$, where α is some real constant. In other words, the Laplace integral converges to the right of some vertical line in the s-plane (Fig. 5.1).

and integrate the Laplace integral by parts:

$$\int_0^\infty e^{-st} f(t)\,dt = -(1/s)e^{-st} f(t)\Big|_0^\infty + 1/s \int_0^\infty e^{-st} f'(t)\,dt$$

or

$$s\int_0^\infty e^{-st} f(t)\,dt = f(0) + \int_0^\infty e^{-st} f'(t)\,dt.$$

Assuming that $\mathfrak{L}\{f'(t)\}$ exists, this may be written as

$$\mathfrak{L}\{f'(t)\} = s\mathfrak{L}\{f(t)\} - f(0)$$

and is known as the *derivative property*.

It is not difficult now to derive a formula for the Laplace transform of the second derivative and, for that matter, of the derivative of any order. Replace $f(t)$ by $f'(t)$ and $f'(t)$ by $f''(t)$ in the derivative property and obtain

$$\mathfrak{L}\{f''(t)\} = s\mathfrak{L}\{f'(t)\} - f'(0)$$

or

$$\mathfrak{L}\{f''(t)\} = s^2\mathfrak{L}\{f(t)\} - sf(0) - f'(0).$$

This formula is valid, of course, provided $f'(t)$ is continuous (and f, f', and f'' have a Laplace transform).

The general formula for the nth derivative, established by induction, reads

$$\mathfrak{L}\{f^{(n)}(t)\} = s^n\mathfrak{L}\{f(t)\} - \sum_{k=1}^{n} s^{k-1} f^{(n-k)}(0),$$

where $f^{(m)}(t)$ is the mth derivative of $f(t)$ and $f^{(m)}(0)$ is its value at $t = 0$.

5.4 THE INVERSION PROBLEM

The example of the preceding section involving a DE provides a blueprint for the use of the Laplace transform in solving similar problems: The relation satisfied by the unknown function $f(t)$ is subjected to the Laplace transform. The result is a relation satisfied by $F(s) = \mathcal{L}\{f(t)\}$. From this relation $F(s)$ can (in principle) be determined. The third step is to find the unknown function $f(t)$ from its Laplace transform $F(s)$. This last problem involves performing the so-called *inverse Laplace transformation*.

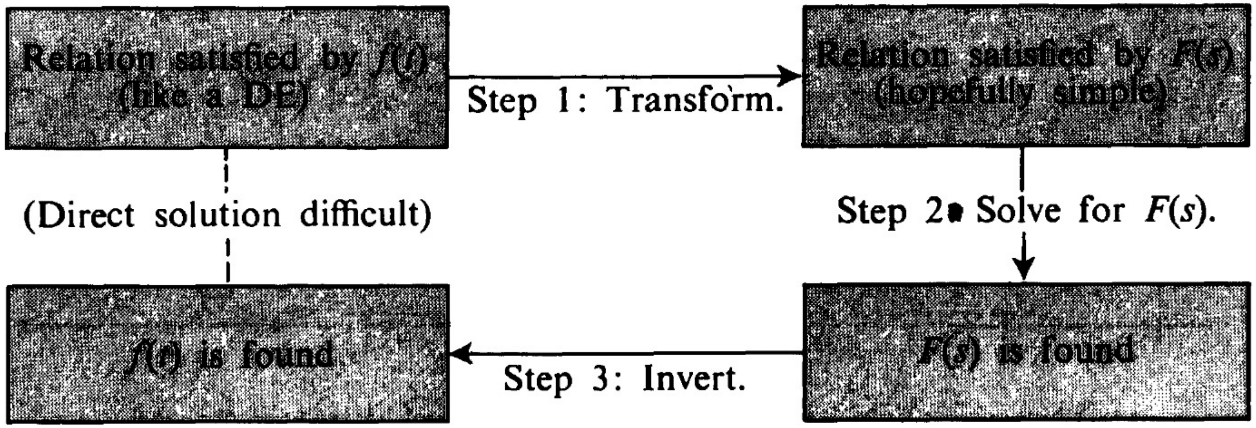
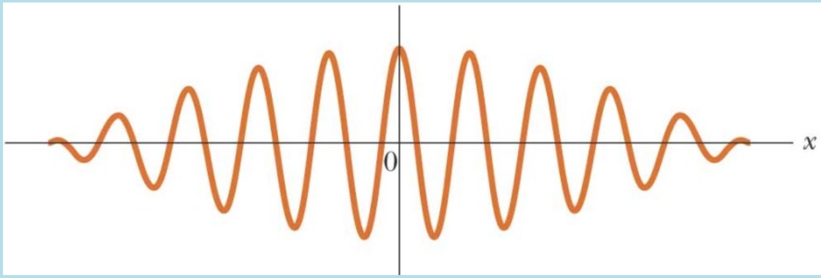


Figure 5.4

期望值 Expectation Value

波函數$\Psi(x,0)$代表一個粒子的狀態。

$|\Psi(x,0)|^2$代表在測量位置時得到x的機率。

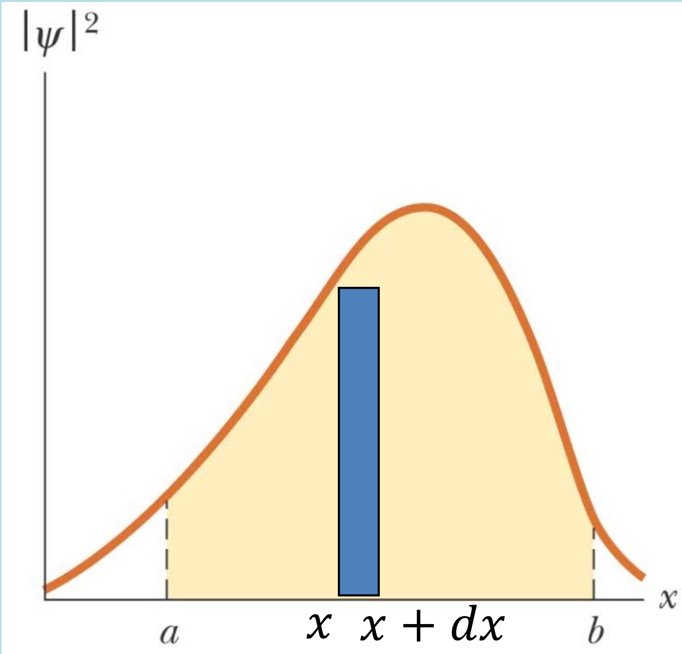


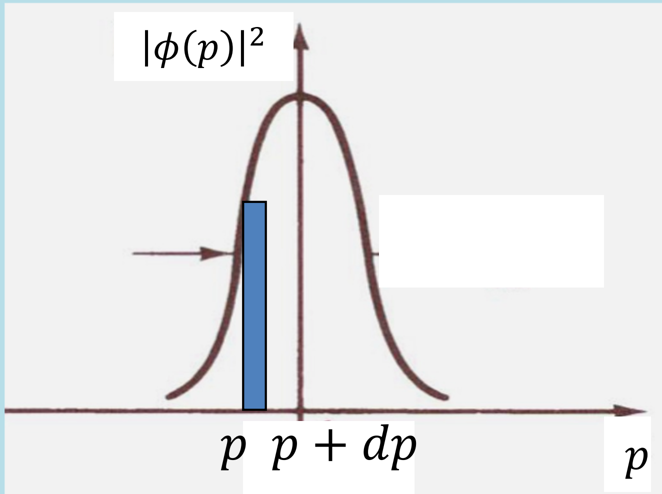
那如何預測對這個狀態、其他物理量例如動量、能量的測量？

量子力學的機率基本假設

在x與$x + dx$之間發現該粒子的機率，可以寫成：

$$|\psi(x)|^2 \cdot dx = \psi^*(x) \cdot \psi(x) \cdot dx$$





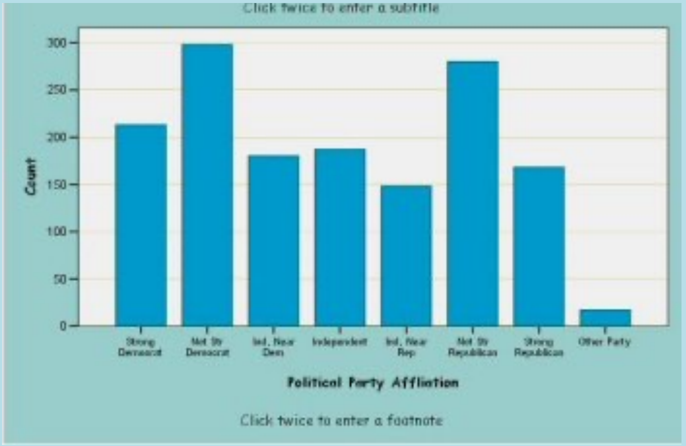
動量測量結果在p與$p + dp$之間的機率，可以寫成：

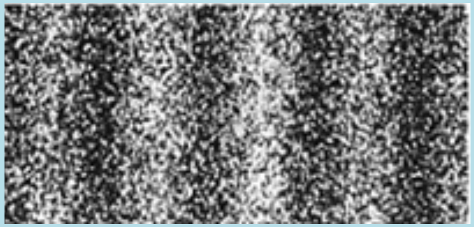
$$|\phi(p)|^2 \cdot dp = \phi^*(p) \cdot \phi(p) \cdot dp$$

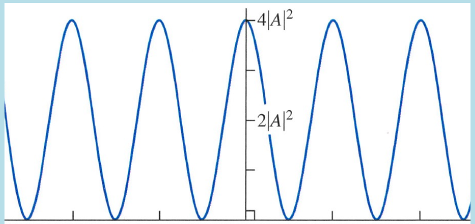
以上的假設也可以等價用期望值來表示，就更能推廣到其他物理量！

對單一電子的物理量，測量結果不一定確定！

但多次測量後，不確定的結果形成一個可預測的分布！







此分布可以計算出平均值，特別稱為期望值 Expectation Value。

Consider a random variable Q. This variable takes values in the set $\{Q_1, \ldots, Q_n\}$ and does so randomly with respective, nonzero probabilities $\{p_1, \ldots, p_n\}$ adding to one. The *expectation value* $\langle Q \rangle$, or the expected value of Q, is defined to be

$$\langle Q \rangle = \sum_{i=1}^{n} Q_i P_i \tag{5.1.1}$$

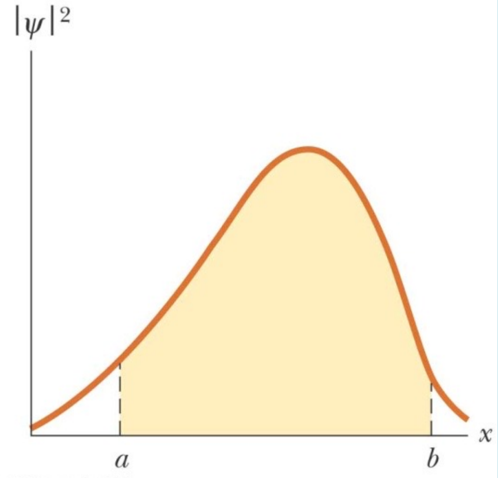
The expected value can be thought of heuristically as a *long-run mean*: as more and more values of the random variable are collected, the mean of that set approaches the expected value.

$$\langle Q \rangle = \sum_{i=1}^{n} Q_i P_i$$

位置的期望值即是以機率為權重對位置求和：

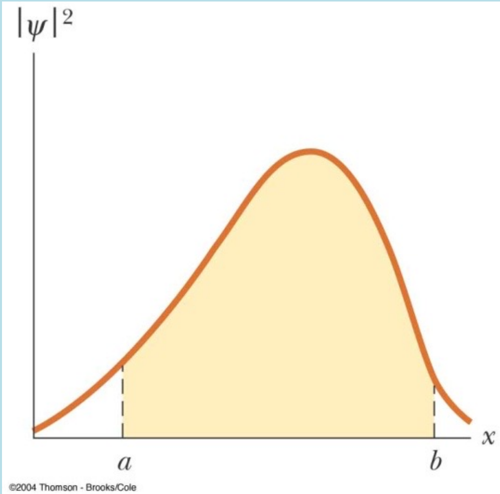
位置為連續變數，因此需做積分。

$$\langle x \rangle = \int_{-\infty}^{\infty} x \cdot |\psi(x)|^2 dx = \int_{-\infty}^{\infty} dx \cdot \psi^*(x) \cdot x \cdot \psi(x)$$



有了位置期望值的計算式：

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



任何位置函數、比如位能的期望值就可以用類似方式寫下。

$$\langle f(x)\rangle = \int_{-\infty}^{\infty} f(x) \cdot |\psi(x)|^2 dx = \int_{-\infty}^{\infty} dx \cdot \psi^*(x) \cdot f(x) \cdot \psi(x)$$

我們可以用此式來計算位置的不確定性Δx！

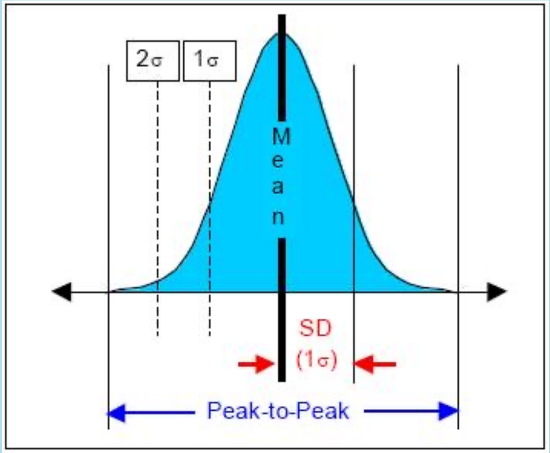
測量一個物理量$\hat{A}$時的不確定性，由測量結果分布的標準差ΔA來描述 ：

可定義為「測量值與期望值的差」的平方的期望值的開根號。

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

此式可化簡：

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



這兩個期望值都可以用波函數計算：

$$= \int_{-\infty}^{\infty} dx \cdot \psi^*(x) \cdot x^2 \psi(x) - \left(\int_{-\infty}^{\infty} dx \cdot \psi^*(x) \cdot x \psi(x) \right)^2$$

位置的不確定性Δx，現在可以精確定義與計算了。

$$(\Delta x)^2 \equiv \langle \hat{x}^2 \rangle - \langle \hat{x} \rangle^2$$

那我可以用位置空間波函數$\psi(x)$來算動量期望值嗎？$\psi(x)$與$\phi(p)$互為傅立葉變換。

$$\langle p\rangle = \int_{-\infty}^{\infty} dp\cdot\phi^*(p)\cdot p\cdot\phi(p)$$

$$\phi(p) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty}\psi(x)\cdot e^{-ipx/\hbar}\cdot dx$$

$$= \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dp\cdot\left[\int_{-\infty}^{\infty} dx\cdot\psi^*(x)\cdot e^{\frac{ipx}{\hbar}}\right]\cdot p\cdot\left[\int_{-\infty}^{\infty} dx'\cdot\psi(x')\cdot e^{-\frac{ipx'}{\hbar}}\right]$$

dp積分先作

$$= \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dx\cdot\psi^*(x)\int_{-\infty}^{\infty} dx'\cdot\psi(x')\int_{-\infty}^{\infty} dp\cdot pe^{-\frac{ip(x'-x)}{\hbar}}$$

$$= \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dx\cdot\psi^*(x)\frac{\hbar}{i}\frac{\partial}{\partial x}\left[\int_{-\infty}^{\infty} dx'\cdot\psi(x')\int_{-\infty}^{\infty} dp\cdot e^{-\frac{ip(x'-x)}{\hbar}}\right]$$

$$= \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dx\cdot\psi^*(x)\frac{\hbar}{i}\frac{\partial}{\partial x}\int_{-\infty}^{\infty} dx'\cdot\psi(x')\cdot\delta(x'-x)$$

$$\int_{-\infty}^{\infty} dp\cdot e^{ipx/\hbar} = 2\pi\hbar\delta(x)$$

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

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

$$\langle p\rangle = \int_{-\infty}^{\infty} dx \cdot \psi^*(x) \cdot \left(-i\hbar\frac{\partial}{\partial x}\right)\psi(x) = \int_{-\infty}^{\infty} dx \cdot \psi^*(x) \cdot \left(-i\hbar\frac{\partial \psi}{\partial x}\right)(x)$$

這個表示式中的微分有點熟悉！

終極翻譯表，直接由粒子圖像翻譯為波函數的運算！

$$\frac{\partial}{\partial x} \leftrightarrow ik$$

$$\frac{\partial}{\partial t} \leftrightarrow -i\omega$$

$$p = \hbar k$$

$$E = \hbar\omega$$

$$-i\hbar\frac{\partial}{\partial x} \leftrightarrow p$$

$$i\hbar\frac{\partial}{\partial t} \leftrightarrow E$$

動量翻譯為空間微分運算

能量翻譯為時間微分運算

這可能不是巧合！

很自然的：動量的函數（比如動能）的期望值，也可以這樣算：

$$\langle f(p)\rangle = \int_{-\infty}^{\infty} dx \cdot \psi^*(x) \cdot f\left(-i\hbar\frac{\partial}{\partial x}\right)\psi(x)$$

例如漢米爾頓量的期望值$\langle E\rangle$：

$$\langle E\rangle = \left\langle\frac{p^2}{2m}\right\rangle = \int_{-\infty}^{\infty} dx \cdot \psi^*(x) \cdot \frac{1}{2m}\left(-i\hbar\frac{\partial}{\partial x}\right)^2 \psi(x) = \int_{-\infty}^{\infty} dx \cdot \psi^*(x) \cdot \frac{-\hbar^2}{2m}\left(\frac{\partial^2\psi(x)}{\partial x^2}\right)$$

以上的對應提供一個處方來計算其他物理量測量的期望值。

所有古典物理量都可以寫成位置與動量的多項式函數： $f(x,p)$

因此，何不假設所有古典物理量的期望值都可以寫成.....

$$\langle f(x,p)\rangle = \int_{-\infty}^{\infty} dx \cdot \psi^*(x) \cdot f\left(x, -i\hbar\frac{\partial}{\partial x}\right)\psi(x)$$

例如z方向角動量：

$$\langle(\vec{r}\times\vec{p})_z\rangle = \langle xp_y - yp_x\rangle = \int_{-\infty}^{\infty} d^3\vec{r} \cdot \psi^*(\vec{r}) \cdot \left[x \cdot \left(-i\hbar\frac{\partial}{\partial y}\right) - y \cdot \left(-i\hbar\frac{\partial}{\partial x}\right)\right]\psi(\vec{r})$$

當初只是幫助猜想的翻譯表，現在可以稍加修改，正式地搬上量子力學檯面，

我們將波函數的空間微分運算，直接定義為量子力學的動量算子Operator $\hat{p}$ ！

$$-i\hbar\frac{\partial}{\partial x}\equiv\hat{p}$$

將波函數乘上位置的運算定義為量子力學的位置算子Operator $\hat{x}$ ！

$$\hat{x}\equiv x$$

有古典對應的物理量就用與古典一樣的形式，來組合位置與動量算子：

$$f(x,p)\rightarrow\hat{f}\left(x,-i\hbar\frac{\partial}{\partial x}\right)\equiv f(\hat{x},\hat{p})$$

大膽地假設，所有物理量本質上，都對應作用於波函數的運算算子！

該物理量測量的期望值，就是此運算作用於狀態的波函數，

乘上波函數的複數共軛，最後對空間積分！

$$\langle p\rangle=\int_{-\infty}^{\infty}dx\cdot\psi^*(x)\cdot\left(-i\hbar\frac{\partial}{\partial x}\right)\psi(x)=\int_{-\infty}^{\infty}dx\cdot\psi^*(x)\cdot\hat{p}\psi(x)$$

$$\langle f(x,p)\rangle=\int_{-\infty}^{\infty}dx\cdot\psi^*(x)\cdot f\left(x,-i\hbar\frac{\partial}{\partial x}\right)\psi(x)$$

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

古典

$$\hat{H} \equiv \frac{\hat{p}^2}{2m} + V(\hat{x}) = \frac{-\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}\right) + V(x)$$

量子

漢米爾或稱能量算子就定義為動量算子的平方加上位能算子。

注意這是一個運算子Operator與運算子Operator之間的關係！

與古典力學中，這些物理量的代數關係一致。

薛丁格方程式就可以寫為：

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

$$i\hbar\frac{\partial}{\partial t} \leftrightarrow E$$

能量翻譯為時間微分運算

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

這就是量子力學完整的薛丁格方程式。

漢米爾頓、能量算子$\hat{H}$決定了狀態隨時間的演化，如同翻譯表所暗示的。