# Fourier Transformation

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

$A(k)$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。

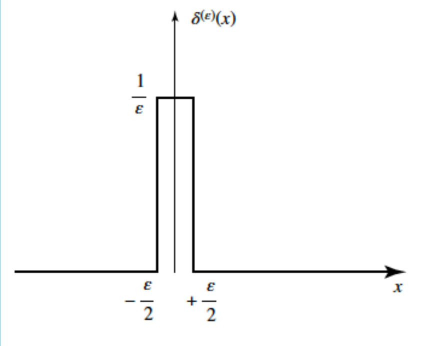
利用Fourier Transformation：$\phi(p)$可以由$\Psi(x,0)$得到。

Fourier Transformation：如何由$\Psi(x,0)$計算得到$\phi(p)$？

一個簡便的方法是利用 Dirac Delta Function $\delta(x)$：

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$\varepsilon$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$f(a)$：

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

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

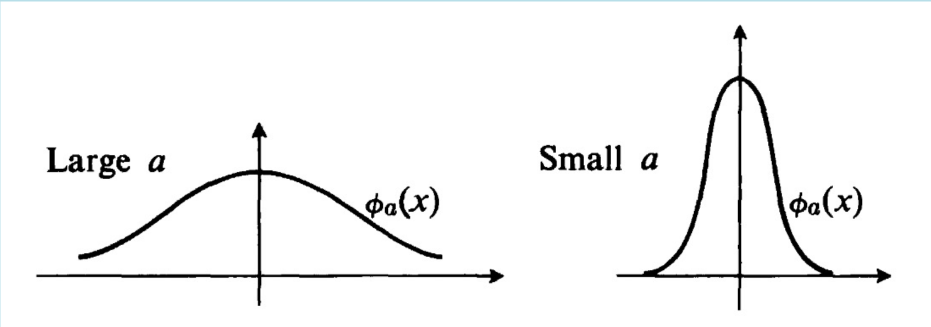
除了上一頁的定義，它有許多極限表示法。

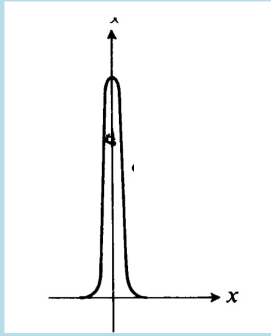
我們可以用極窄的波包來近似：

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

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$\delta(x)$。

Summery

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

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

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

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

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

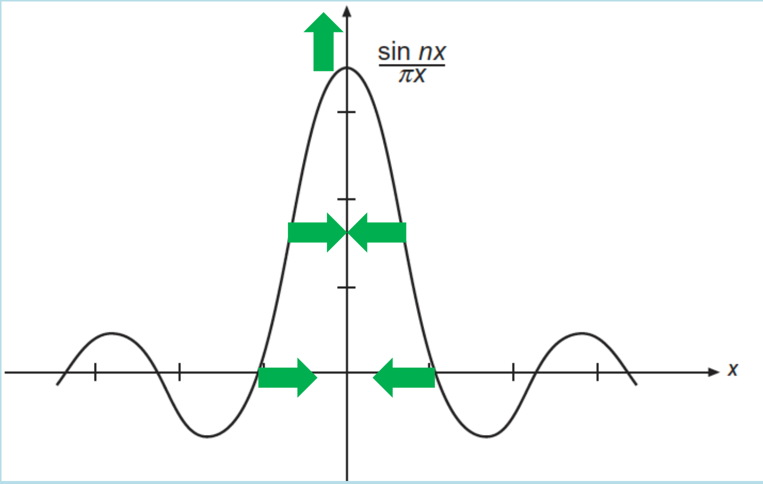
以上論證還可以更嚴格一點，以下參考：

自由電子波函數對$k$的無限積分可以視為有限積分的極限。

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

有限積分可以直接具體算出來：

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

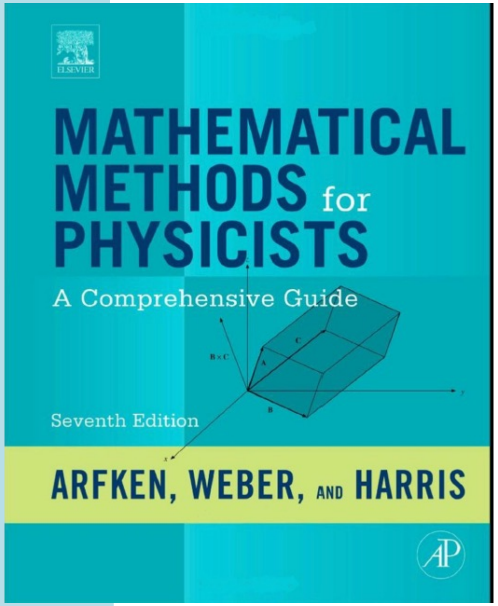



$n \to \infty$時中央的Peak會變窄又變高，類似$\delta(x)$只有$x = 0$最重要。

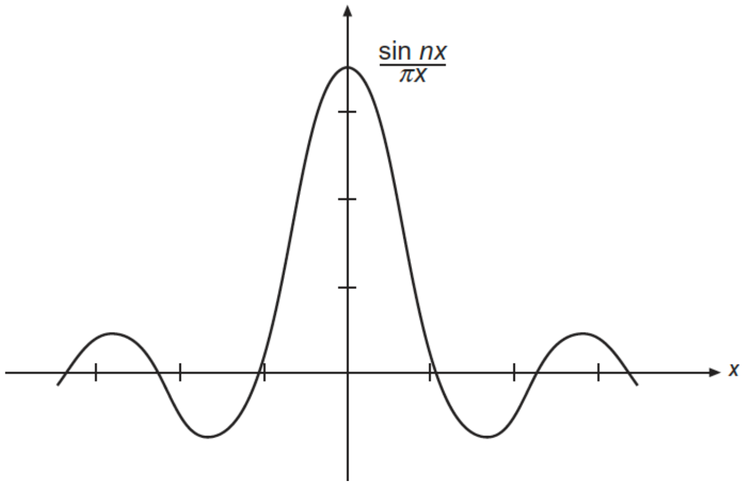
而且可以證明函數底下總面積、如同$\delta(x)$、為1：

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

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

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$\Psi(x,0)$互為傅立葉變換：

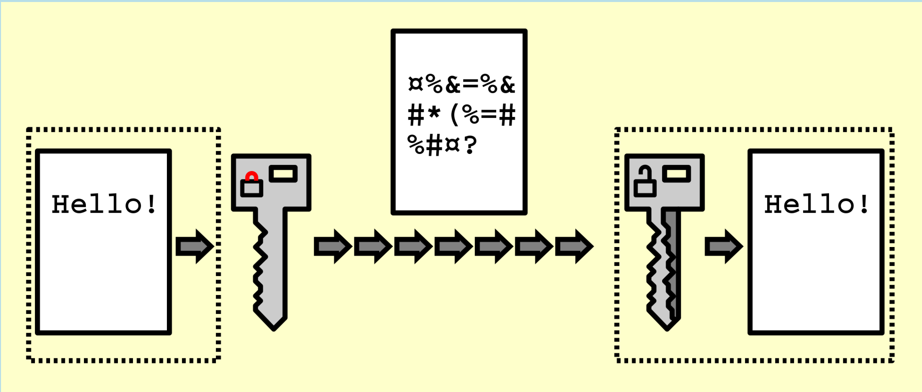
$$\phi(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \Psi(x,0) \cdot e^{-ipx/\hbar} \cdot dx$$

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

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

我們常說$\Psi(x,0)$的所有資訊都存在$\phi(p)$之中。

有了$\phi(p)$就能算出$\Psi(x,0)$，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 $\alpha$.

**EXAMPLE 2-1**

Consider a wave packet for which

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

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 $\Delta x$ 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

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

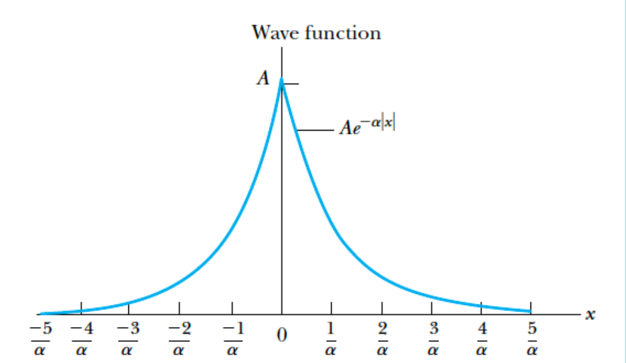
which certainly satisfies (2-8).

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

Consider a wave function of the form

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

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



## Fourier Integral

When we first encountered the delta function, its representation which is the large-$n$ limit of

$$\delta_n(t) = \frac{1}{2\pi}\int_{-n}^{n} e^{i\omega t}\,d\omega, \tag{20.20}$$

was identified as particularly useful in Fourier analysis. We now use that representation to obtain an important result known as the **Fourier integral**. We write the fairly obvious equation,

$$\begin{aligned} f(x) &= \lim_{n\to\infty}\int_{-\infty}^{\infty} f(t)\,\delta_n(t-x)\,dt \\ &= \lim_{n\to\infty}\frac{1}{2\pi}\int_{-\infty}^{\infty} f(t)\left[\int_{-n}^{n} e^{i\omega(t-x)}\,d\omega\right]dt. \end{aligned} \tag{20.21}$$

We now interchange the order of integration and take the limit $n \to \infty$, reaching

$$f(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega \int_{-\infty}^{\infty} dt\, f(t)e^{i\omega(t-x)}.$$

Finally, we rearrange this equation to the form

$$f(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-i\omega x}\,d\omega \int_{-\infty}^{\infty} f(t)e^{i\omega t}\,dt. \tag{20.22}$$

Equation (20.22), the **Fourier integral**, is an integral representation of $f(x)$, and will be more obviously recognized as such if the inner integration (over $t$) is performed, leaving unevaluated that over $\omega$. In fact, if we identify the inner integration as (apart from a factor $\sqrt{1/2\pi}$) the Fourier transform of $f(t)$, and label it $g(\omega)$ as in Eq. (20.10), then Eq. (20.22) can be rewritten

$$f(t) = \sqrt{\frac{1}{2\pi}}\int_{-\infty}^{\infty} g(\omega)e^{-i\omega t}\,d\omega, \tag{20.23}$$

showing that whenever we have the Fourier transform of a function $f(t)$ we can use it to make a **Fourier integral representation** of that function.

# Supplement 2-A
# The Fourier Integral and Delta Functions

以上的結果有一個更嚴格的推導。
先將空間限縮於有限範圍，
再讓空間大小趨近無限大。

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

$$f(x) = f(x + 2L) \tag{2A-1}$$

Such a function can be expanded in a Fourier series in the interval $(-L, L)$, and the series has the form

$$f(x) = \sum_{n=0}^{\infty} A_n \cos\frac{n\pi x}{L} + \sum_{n=1}^{\infty} B_n \sin\frac{n\pi x}{L} \tag{2A-2}$$

We can rewrite the series in the form

$$f(x) = \sum_{n=-\infty}^{\infty} a_n e^{in\pi x/L} \tag{2A-3}$$

$$\cos\frac{n\pi x}{L} = \frac{1}{2}\left(e^{in\pi x/L} + e^{-in\pi x/L}\right)$$

$$\sin\frac{n\pi x}{L} = \frac{1}{2i}\left(e^{in\pi x/L} - e^{-in\pi x/L}\right)$$

If we now let $L \to \infty$, then $k$ approaches a continuous variable, since $\Delta k$ becomes infinitesimally small. If we recall the Riemann definition of an integral, we see that in the limit (2A-10) can be written in the form

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk\, A(k) e^{ikx} \tag{2A-11}$$

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

$$f(x) = f(x + 2L) \tag{2A-1}$$

Such a function can be expanded in a Fourier series in the interval $(-L, L)$, and the series has the form

$$f(x) = \sum_{n=0}^{\infty} A_n \cos\frac{n\pi x}{L} + \sum_{n=1}^{\infty} B_n \sin\frac{n\pi x}{L}$$

We can rewrite the series in the form

$$f(x) = \sum_{n=-\infty}^{\infty} a_n e^{in\pi x/L}$$

which is certainly possible, since

$$\cos\frac{n\pi x}{L} = \frac{1}{2}\left(e^{in\pi x/L} + e^{-in\pi x/L}\right)$$

$$\sin\frac{n\pi x}{L} = \frac{1}{2i}\left(e^{in\pi x/L} - e^{-in\pi x/L}\right)$$

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

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

Thus

$$a_n = \frac{1}{2L}\int_{-L}^{L} dx\, f(x) e^{-in\pi x/L} \tag{2A-5}$$

Let us now rewrite (2A-3) by introducing $\Delta n$, the difference between two successive integers. Since this is unity, we have

$$\begin{aligned} f(x) &= \sum_n a_n e^{in\pi x/L}\,\Delta n \\ &= \frac{L}{\pi}\sum_n a_n e^{in\pi x/L}\,\frac{\pi\,\Delta n}{L} \end{aligned} \tag{2A-6}$$

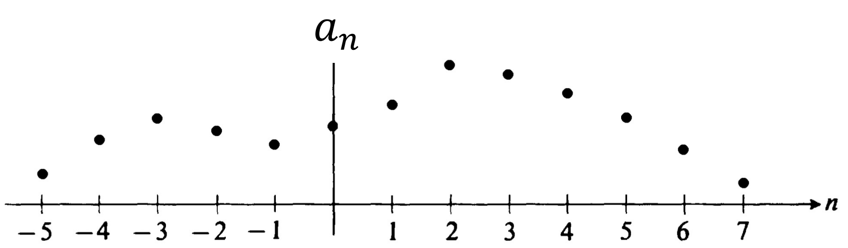



**Figure 7.1**

Let us change the notation by writing

$$\frac{\pi n}{L} = k \tag{2A-7}$$

and

$$\frac{\pi\,\Delta n}{L} = \Delta k \tag{2A-8}$$

We also write

$$\frac{La_n}{\pi} = \frac{A(k)}{\sqrt{2\pi}} \tag{2A-9}$$

Hence (2A-6) becomes

$$f(x) = \sum \frac{A(k)}{\sqrt{2\pi}} e^{ikx}\,\Delta k \tag{2A-10}$$

If we now let $L \to \infty$, then $k$ approaches a continuous variable, since $\Delta k$ becomes infinitesimally small. If we recall the Riemann definition of an integral, we see that in the limit (2A-10) can be written in the form

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk\, A(k) e^{ikx} \tag{2A-11}$$

The coefficient $A(k)$ is given by

$$\begin{aligned} A(k) &= \sqrt{2\pi}\,\frac{L}{\pi} \cdot \frac{1}{2L} \int_{-L}^{L} dx\, f(x) e^{-in\pi x/L} \\ &\to \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx\, f(x) e^{-ikx} \end{aligned} \tag{2A-12}$$

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

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

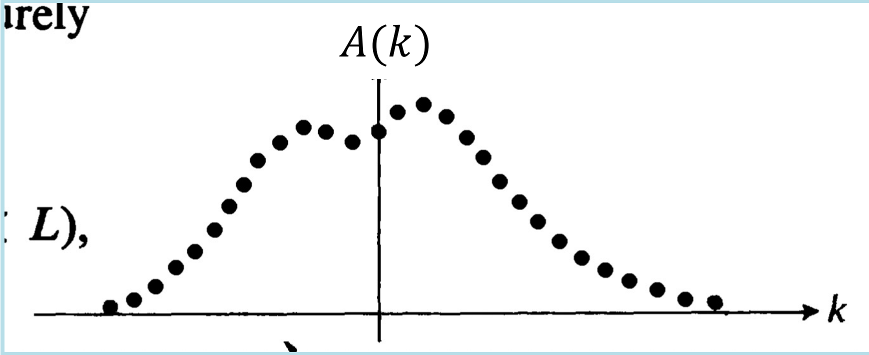
Suppose now that we interchange, without question, the order of integrations. We then get

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

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



$\phi(p)$真的是動量空間的波函數，也滿足歸一化條件。

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

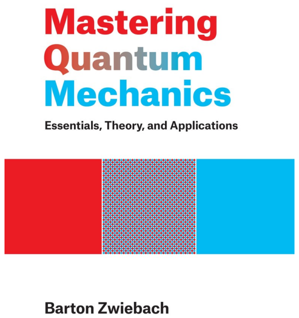
We rearrange the integrals to do the $x$ integration first:

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

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

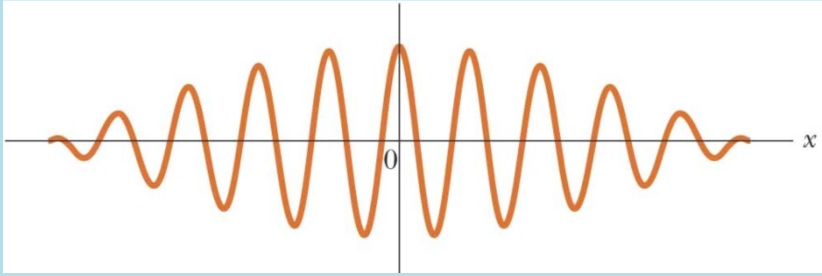



$$\boxed{\int_{-\infty}^{\infty} dx\, |\Psi(x)|^2 = \int_{-\infty}^{\infty} dk\, |\Phi(k)|^2.} \tag{4.4.10}$$

# 期望值 Expectation Value

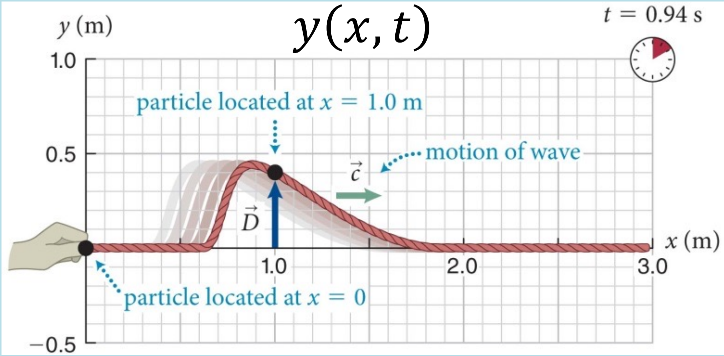
波函數$\Psi(x,0)$代表一個粒子的狀態。

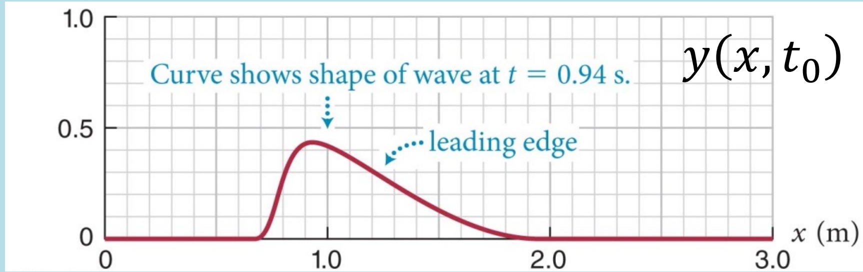
$|\Psi(x,0)|^2$代表在測量位置時得到$x$的機率。




那如何預測對這個狀態、其他物理量例如動量、能量的測量？

固定$t = t_0$，$\Psi(x,t) \to \Psi(x,t_0)$，波函數成為一個$x$的單變數函數。



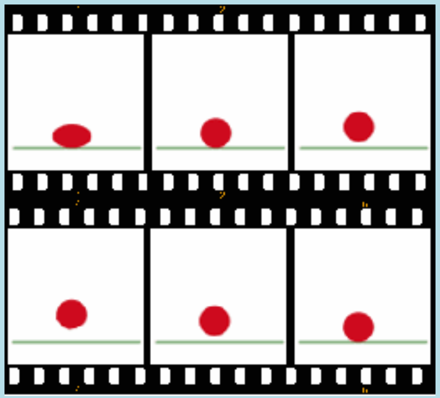



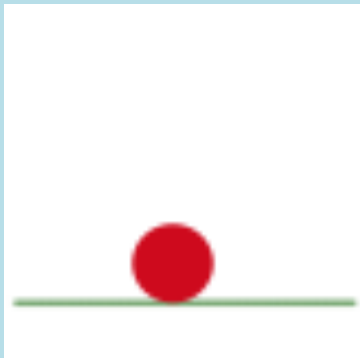

在古典波$y(x,t_0)$就是$t = t_0$時的瞬間波形。

在電子波，$\Psi(x,t_0)$就描述電子在$t = t_0$時瞬間的狀態，可稱為瞬間波函數。

瞬間波函數，有時會以$\psi(x)$表示，又稱為狀態函數！

電子在$t = t_0$時瞬間的狀態，以此狀態函數$\psi(x)$來描述。

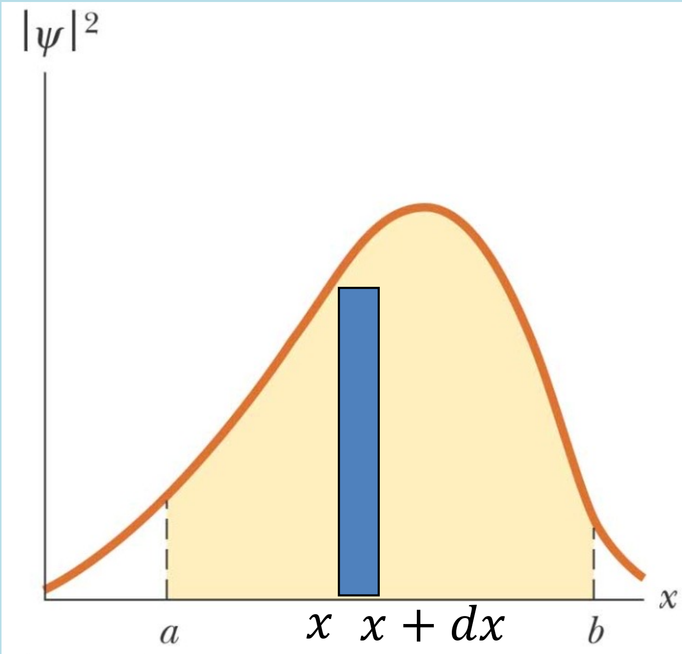


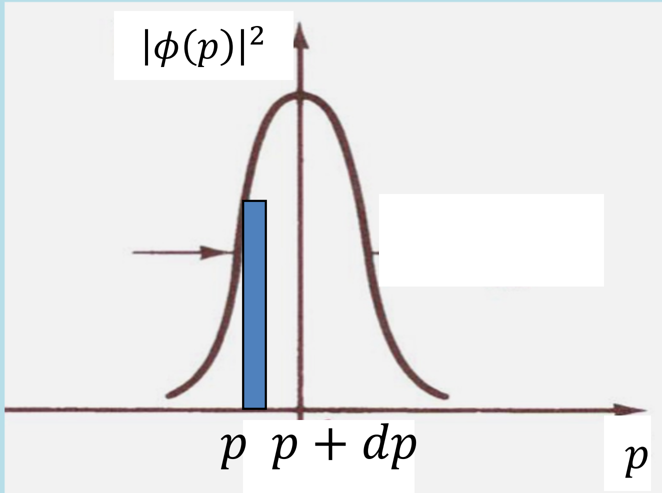


## 量子力學的機率基本假設

在$x$與$x + dx$之間發現該粒子的機率，可以寫成：

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



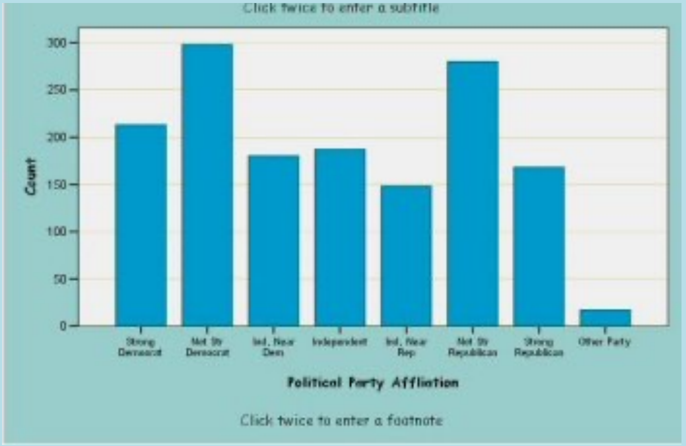

動量測量結果在$p$與$p + dp$之間的機率，可以寫成：

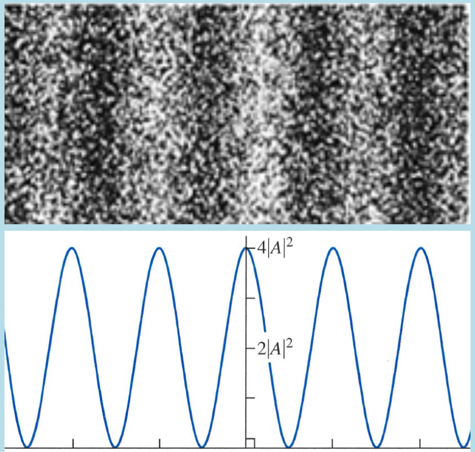
$$|\phi(p)|^2 \cdot dp = \phi^*(p) \cdot \phi(p) \cdot dp$$

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

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

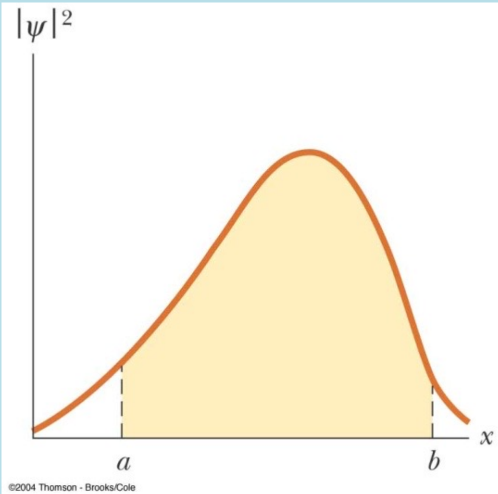
The expected value can be thought of heuristically as a *long-run mean*: as more and more values of the random variable are collected, the mean of that set approaches the expected value.

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

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。

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



例題：利用此式可以計算波包函數的位置期望值：

$$\Psi(x,0) = Ce^{ik_0x}e^{-\frac{x^2}{2\alpha}}$$

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

$$= C^2 \int_{-\infty}^{\infty} dx \cdot xe^{-\frac{x^2}{\alpha}}$$

$$= C^2 \int_{0}^{\infty} dx \cdot xe^{-\frac{x^2}{\alpha}} + C^2 \int_{-\infty}^{0} dx \cdot xe^{-\frac{x^2}{\alpha}}$$

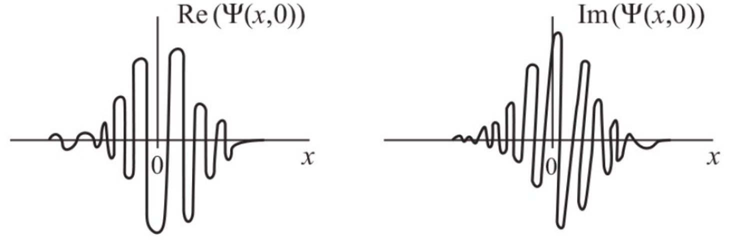
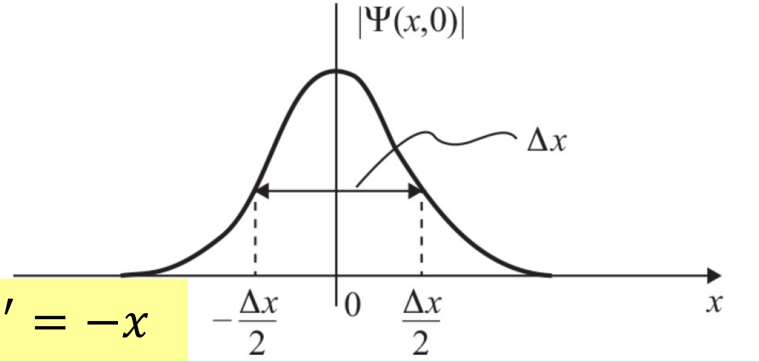



**Figure 4.2**
The real and imaginary parts of $\Psi(x, 0)$.




$$x' = -x$$

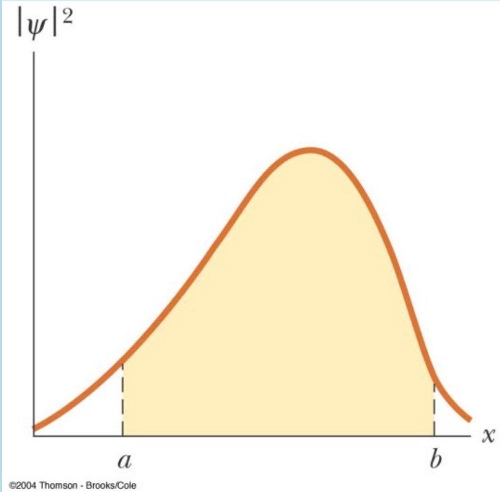
$$= C^2 \int_{0}^{\infty} dx \cdot xe^{-\frac{x^2}{\alpha}} - C^2 \int_{0}^{\infty} dx' \cdot x'e^{-\frac{x'^2}{\alpha}} = 0$$

$$\langle x \rangle = 0$$

波包位置期望值在原點！

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$\Delta x$！

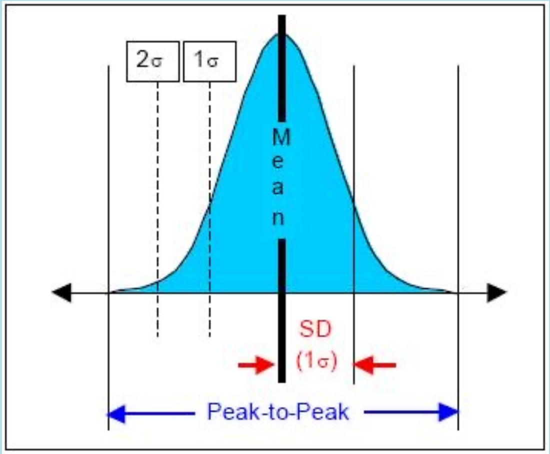
測量一個物理量$\hat{A}$時的不確定性，由測量結果分布的標準差$\Delta A$來描述 ：

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$\Delta x$，現在可以精確定義與計算了。

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

讓我們試一下計算波包的不確定性$\Delta x, \Delta p$。

$$\Delta x \equiv \sqrt{\langle x^2\rangle - \langle x\rangle^2}$$

$$a \equiv \frac{1}{\alpha}$$

$$\Psi(x,0) = \psi(x) = Ce^{ik_0x}e^{-\frac{x^2}{2\alpha}} = Ce^{ik_0x}e^{-\frac{a}{2}x^2}$$

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

首先要將波包函數歸一化： $C = \sqrt[4]{\frac{a}{\pi}}$

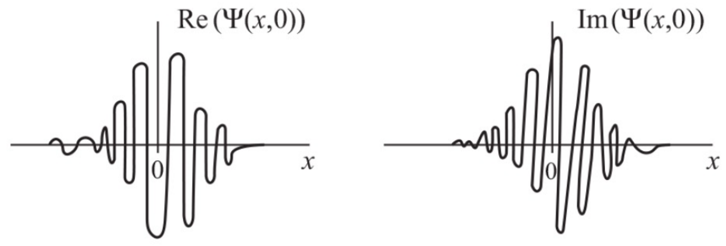
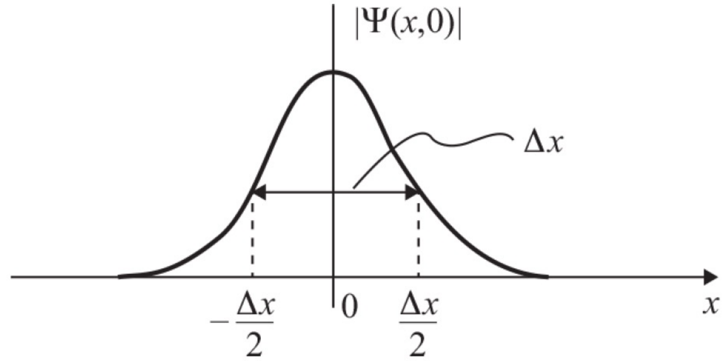



Figure 4.2
The real and imaginary parts of $\Psi(x, 0)$.




$$\langle x^2\rangle = \int_{-\infty}^{\infty} dx \cdot \psi^*(x) \cdot x^2\psi(x) = C^2\int_{-\infty}^{\infty} dx \cdot x^2 e^{-ax^2} = -\sqrt{\frac{a}{\pi}}\frac{\partial}{\partial a}\int_{-\infty}^{\infty} dx \cdot e^{-ax^2}$$

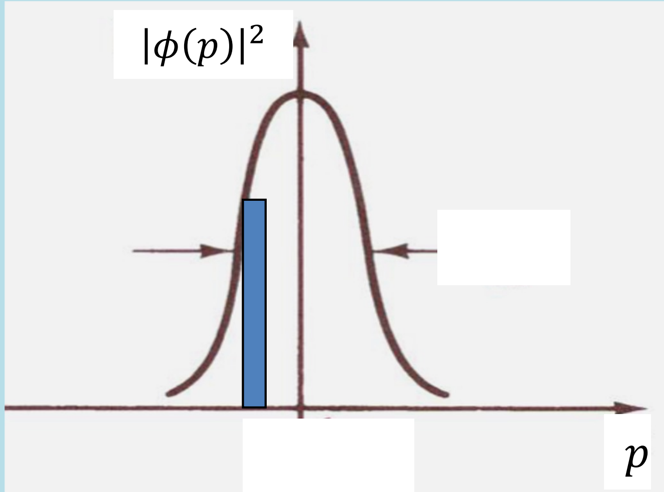
$$= -\sqrt{\frac{a}{\pi}}\frac{\partial}{\partial a}\left(\sqrt{\frac{\pi}{a}}\right) = \frac{1}{2}\sqrt{a}\frac{1}{a\sqrt{a}} = \frac{1}{2a} = \frac{\alpha}{2}$$

$$\Delta x \equiv \sqrt{\langle x^2\rangle - \langle x\rangle^2} = \sqrt{\frac{\alpha}{2}}$$

動量的期望值怎麼算？

動量測量結果在$p$與$p + dp$之間發現的機率：

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




動量的期望值想當然爾：

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

期待：動量的函數，例如動能的期望值也可同樣方式記算：

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

為簡單起見，取$p_0 = k_0 = 0$：

$$\psi(x) = \sqrt[4]{\frac{1}{\alpha\pi}}\, e^{-\frac{x^2}{2\alpha}}$$

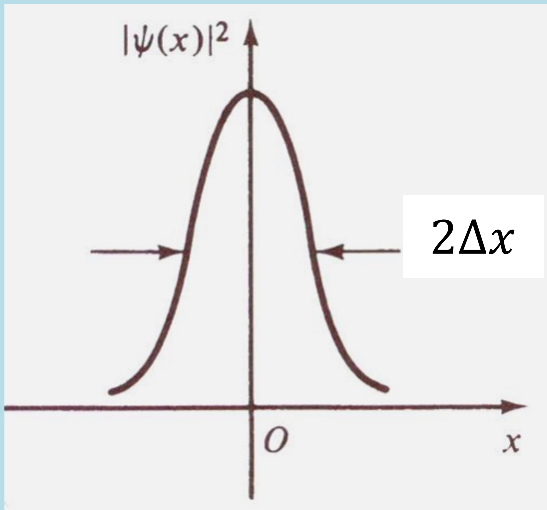
$$\Delta x \equiv \sqrt{\langle x^2\rangle - \langle x\rangle^2} = \sqrt{\frac{\alpha}{2}}$$

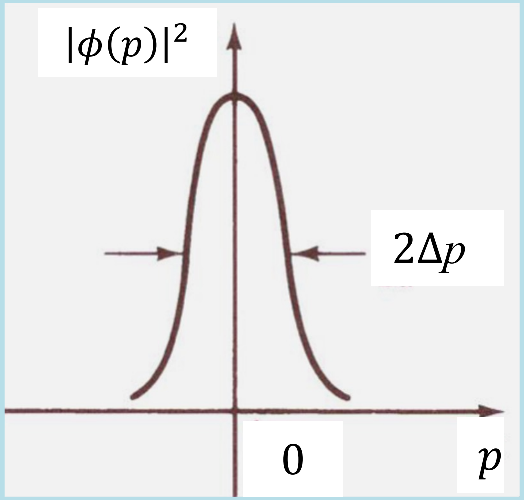
波包的$\phi(p)$也是高斯分佈，也滿足歸一化條件。因此：

現在我們可以用同樣的積分式計算波包的動量不確定性$\Delta p$：

$$\phi(p) = \sqrt[4]{\frac{\alpha}{\pi\hbar^2}}\, e^{-\frac{\alpha p^2}{2\hbar^2}}$$

$$\Delta p \equiv \sqrt{\langle p^2\rangle - \langle p\rangle^2} = \sqrt{\frac{\hbar^2}{2\alpha}}$$




$$\Delta x \cdot \Delta p = \frac{\hbar}{2}$$

**16.** Consider the wave function

$$\psi(x) = (\alpha/\pi)^{1/4} \exp(-\alpha x^2/2)$$

Calculate $\langle x^n \rangle$ for $n = 1, 2$. Can you quickly write down the result for $\langle x^{17} \rangle$?

**17.** Calculate $\phi(p)$ for the wave function in problem 16. Calculate $\langle p^n \rangle$ for $n = 1, 2$.

**18.** Use the definitions $(\Delta x)^2 = \langle x^2 \rangle - \langle x \rangle^2$ and $(\Delta p)^2 = \langle p^2 \rangle - \langle p \rangle^2$ with the results of Problems 16 and 17 to show that $\Delta p \Delta x > \hbar/2$.

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。

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

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

$dp$積分先作

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

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

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

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

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

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

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：

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

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：

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

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

這就是量子力學完整的薛丁格方程式。

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

能量翻譯為時間微分運算

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。