Schrodinger Wave Equation in large infinite space

Free state and scattering 散射

Fourier Transformation

We will extend our results in the infinite quantum well in two directions:

First, you can solve more general partial differential equation in identical way:

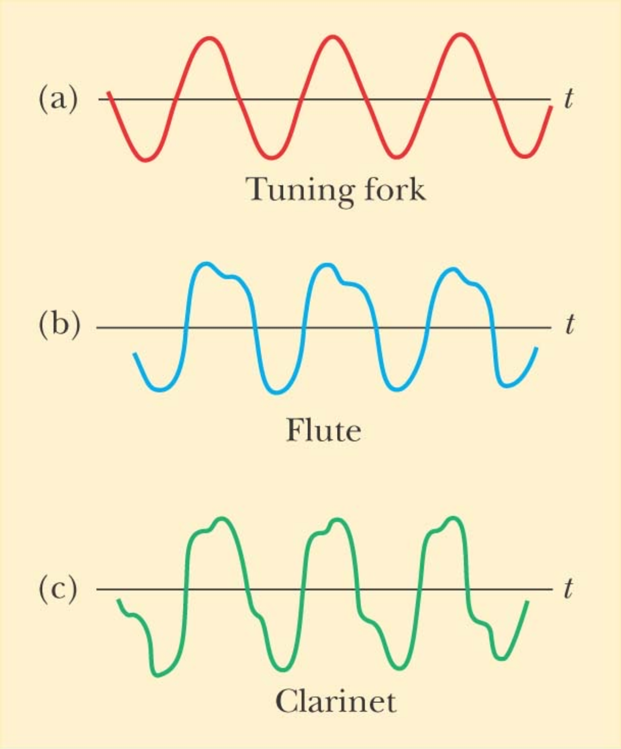
Sturm-Liouville Problem

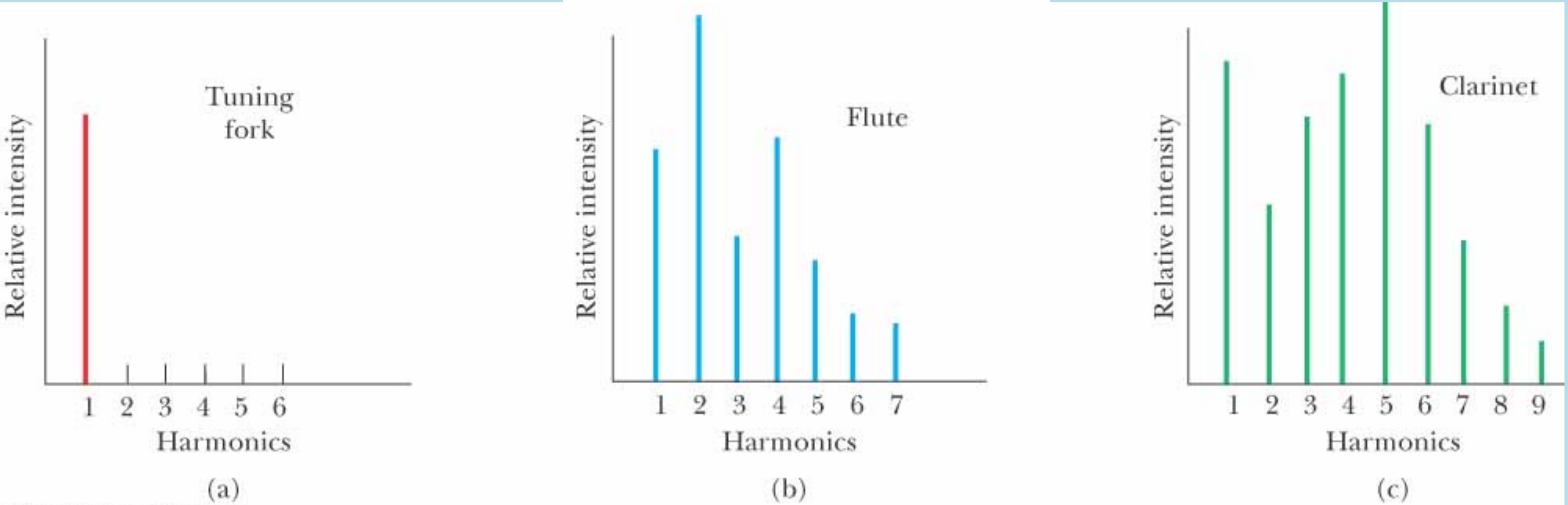
$$\frac{\partial}{\partial x}\left[\tau(x)\frac{\partial y}{\partial x}\right] - v(x)y = \mu(x)\frac{\partial^2 y}{\partial t^2}$$

Any function can be expanded as an linear combination of u_n's.

$$\psi(x) = \sum_{n=1}^{\infty} c_n u_n(x)$$

The information in $\psi(x)$ is equivalent to the information in $c_n, n = 1 \ldots \infty$.


(a)
t
Tuning fork
(b)
t
Flute
(c)
t
Clarinet


Relative intensity
Tuning fork
1 2 3 4 5 6
Harmonics
Relative intensity
Flute
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Harmonics
Relative intensity
Clarinet
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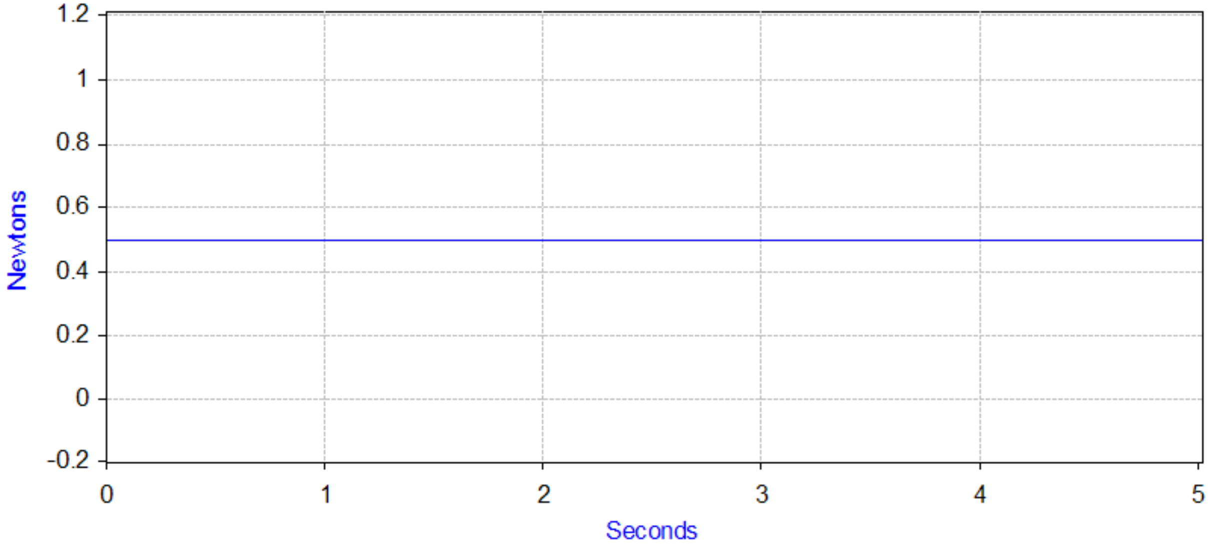
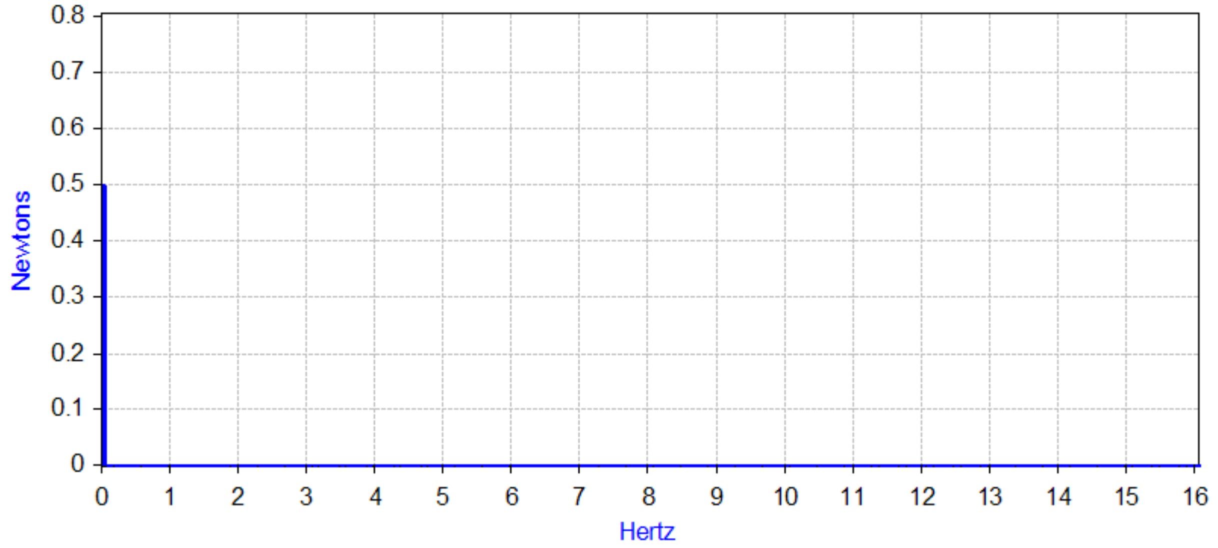
Harmonics

(a) (b) (c)



Square Wave: Generated by Harmonics



Frequency Spectrum: Square Wave

We will extend our results in the infinite quantum well in two directions:

Second, let the boundary go to infinity $a \rightarrow \infty$.

We will find a similar formalism for space without boundary!

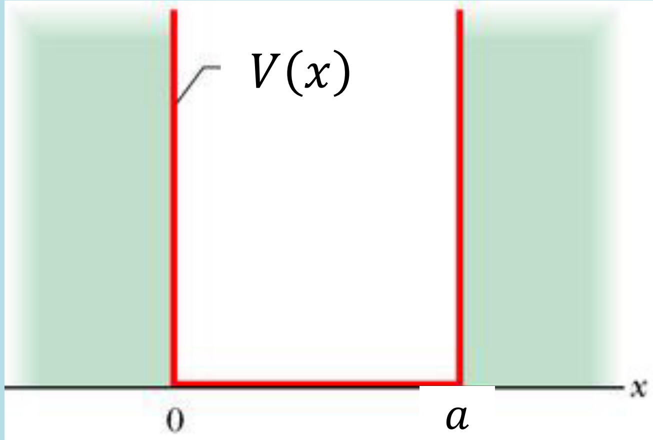
and see what the information in c_n correspond to.

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

若不需考慮邊界、離開邊界很遠，電子的狀態如何描述：

How to describe electron wave if boundary is far away and can be ignored.

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。This limit is not very convenient.

It does not have the displace symmetry of an infinite space.

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

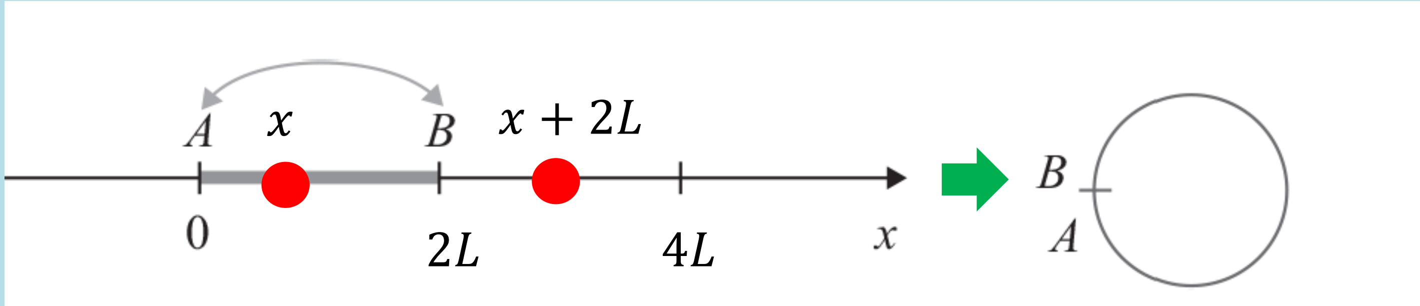
無限大無邊界的空間，可以平移而不產生可測量的物理結果，稱平移對稱。

This symmetry makes the solutions very simple and general.

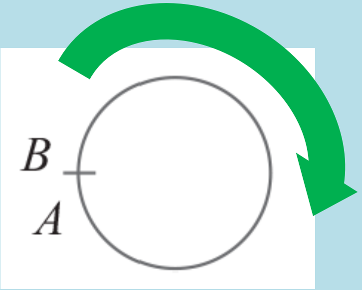
It’s better to use a boundary condition keeping this symmetry during limiting process.

The simplest one is Periodic Boundary Condition.

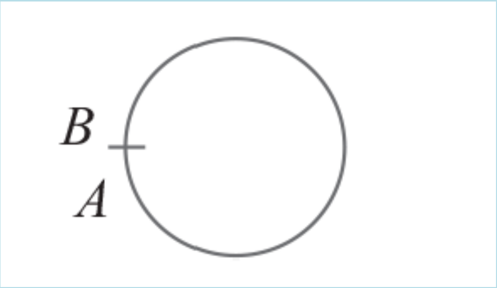
$f(x) = f(x + 2L)$ identify all $x + 2L$ with x.



The space is the same after displacement.



Function f and all its derivatives are periodic. $f'(x) = f'(x + 2L)$



$L \to \infty$

Free particle in a circle 圓周上的自由粒子

Specific Heat of Solids: Boltzmann, Einstein, and Debye

2

Generalizing to the three-dimensional case,

$$E_{n_x,n_y,n_z} = \hbar\omega[(n_x + 1/2) + (n_y + 1/2) + (n_z + 1/2)]$$

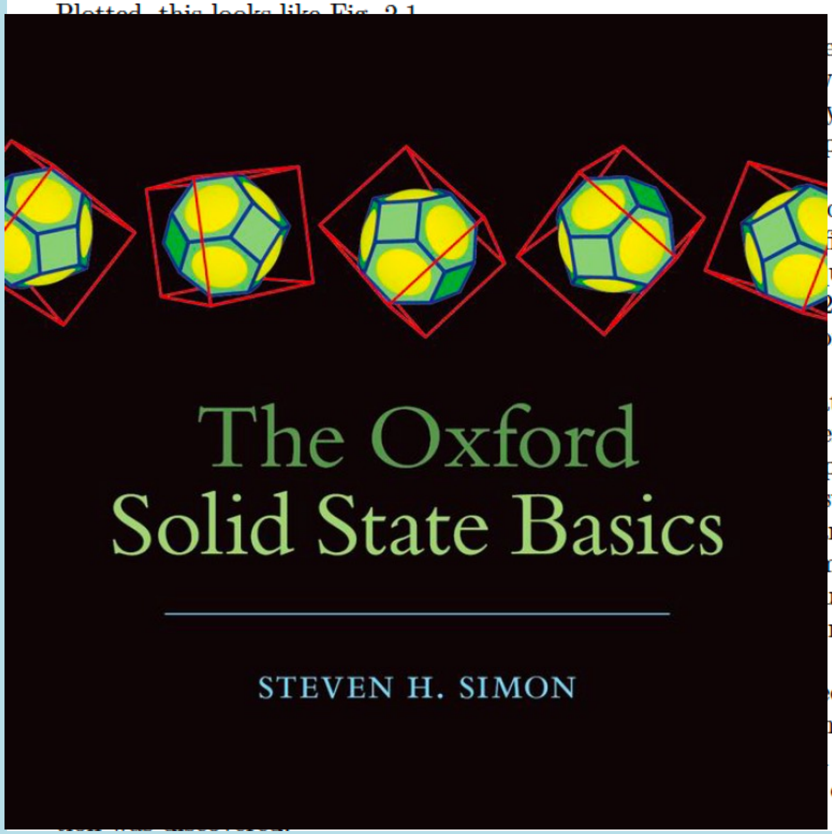
and

$$Z_{3D} = \sum_{n_x,n_y,n_z \geqslant 0} e^{-\beta E_{n_x,n_y,n_z}} = [Z_{1D}]^3$$

resulting in $\langle E_{3D}\rangle = 3\langle E_{1D}\rangle$, so correspondingly we obtain

$$C = 3k_B(\beta\hbar\omega)^2 \frac{e^{\beta\hbar\omega}}{(e^{\beta\hbar\omega} - 1)^2}.$$

Plotted, this looks like Fig. 2.1.



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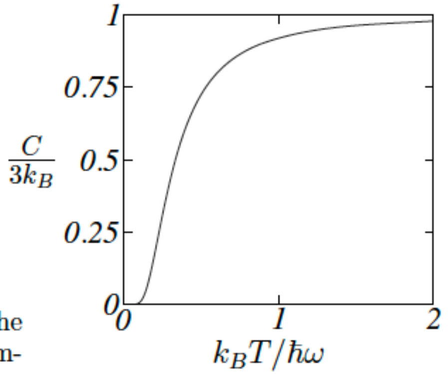


Fig. 2.1 Einstein heat capacity per atom in three dimensions.

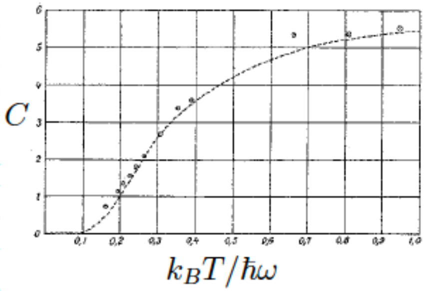
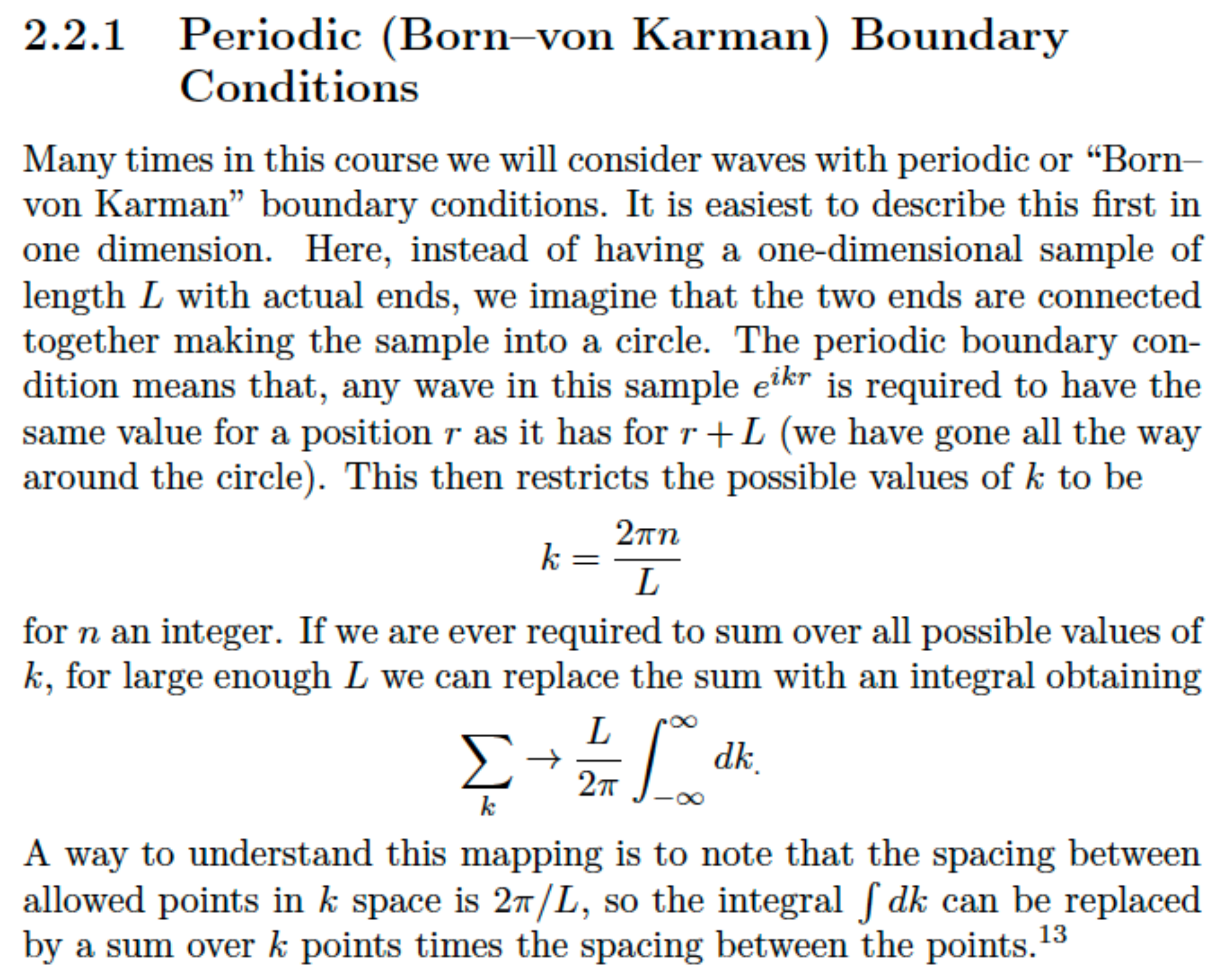


Fig. 2.2 Plot of molar heat capacity of diamond from Einstein's original paper. The fit is to the Einstein theory. The y axis is C in units of cal/(K-mol). In these units, $3R \approx 5.96$. The fitting parameter $T_{Einstein} = \hbar\omega/k_B$ is roughly 1320K. Figure from A. Einstein, *Ann. Phys.*, **22**, 180, (1907), Copyright Wiley-VCH Verlag GmbH & Co. KGaA. Reproduced with permission.



2.2.1 Periodic (Born–von Karman) Boundary Conditions

Many times in this course we will consider waves with periodic or "Born–von Karman" boundary conditions. It is easiest to describe this first in one dimension. Here, instead of having a one-dimensional sample of length L with actual ends, we imagine that the two ends are connected together making the sample into a circle. The periodic boundary condition means that, any wave in this sample e^{ikr} is required to have the same value for a position r as it has for $r + L$ (we have gone all the way around the circle). This then restricts the possible values of k to be

$$k = \frac{2\pi n}{L}$$

for n an integer. If we are ever required to sum over all possible values of k, for large enough L we can replace the sum with an integral obtaining

$$\sum_k \to \frac{L}{2\pi}\int_{-\infty}^{\infty} dk.$$

A way to understand this mapping is to note that the spacing between allowed points in k space is $2\pi/L$, so the integral $\int dk$ can be replaced by a sum over k points times the spacing between the points.[13]

In three dimensions, the story is extremely similar. For a sample of size L^3, we identify opposite ends of the sample (wrapping the sample up into a hypertorus!) so that if you go a distance L in the x, y or z direction, you get back to where you started.[14] As a result, our $\mathbf{k}$ values can only take values

$$\mathbf{k} = \frac{2\pi}{L}(n_1, n_2, n_3)$$

for integer values of n_i, so here each $\mathbf{k}$ point now occupies a volume of $(2\pi/L)^3$. Because of this discretization of values of $\mathbf{k}$, whenever we have a sum over all possible $\mathbf{k}$ values we obtain

$$\sum_{\mathbf{k}} \to \frac{L^3}{(2\pi)^3} \int \mathbf{dk}$$

with the integral over all three dimensions of $\mathbf{k}$-space (this is what we mean by the bold $\mathbf{dk}$). One might think that wrapping the sample up into a hypertorus is very unnatural compared to considering a system with real boundary conditions. However, these boundary conditions tend to simplify calculations quite a bit, and most physical quantities you might measure could be measured far from the boundaries of the sample anyway and would then be independent of what you do with the boundary conditions.

2.2.2 Debye's Calculation Following Planck

Debye decided that the oscillation modes of a solid were waves with frequencies $\omega(\mathbf{k}) = v|\mathbf{k}|$ with v the sound velocity—and for each $\mathbf{k}$ there should be three possible oscillation modes, one for each direction of

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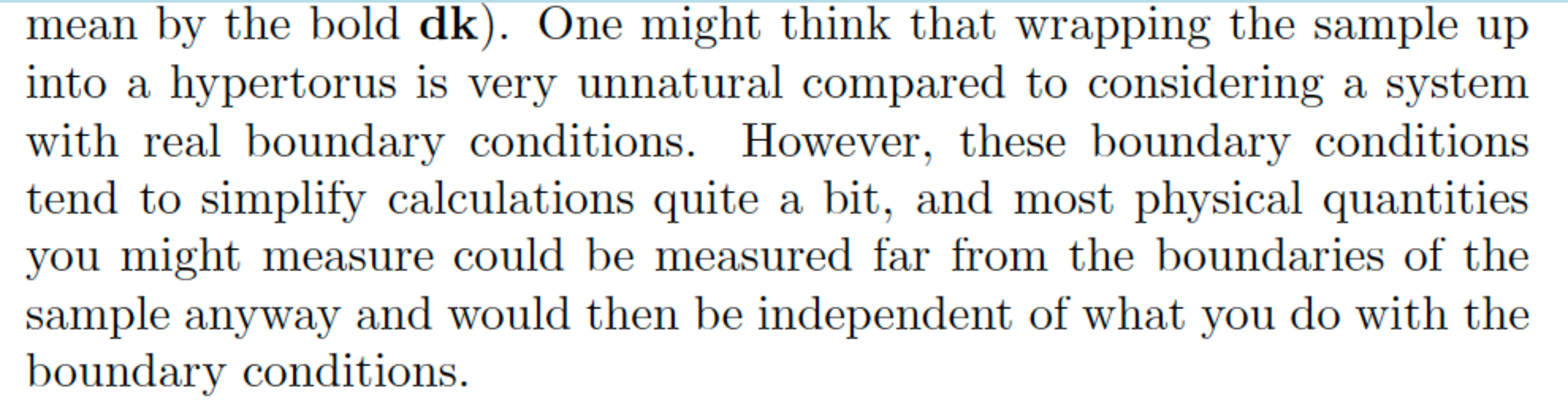
[13] In your previous courses you may have used particle-in-a-box boundary conditions where instead of plane waves $e^{i2\pi nr/L}$ you used particle in a box wavefunctions of the form $\sin(n\pi r/L)$. This gives you instead

$$\sum_k \to \frac{L}{\pi}\int_0^\infty dk$$

which will inevitably result in the same physical answers as for the periodic boundary condition case. All calculations can be done either way, but periodic Born–von Karman boundary conditions are almost always simpler.

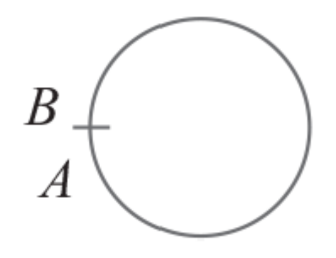
[14] Such boundary conditions are very popular in video games, such as the classic time-wasting game of my youth, *Asteroids* (you can find it online). It may also be possible that our universe has such boundary conditions—a notion known as the *doughnut universe*. Data collected by Cosmic Microwave Background Explorer (led by Nobel Laureates John Mather and George Smoot) and its successor the Wilkinson Microwave Anisotropy Probe appear consistent with this structure.



mean by the bold **dk**). One might think that wrapping the sample up into a hypertorus is very unnatural compared to considering a system with real boundary conditions. However, these boundary conditions tend to simplify calculations quite a bit, and most physical quantities you might measure could be measured far from the boundaries of the sample anyway and would then be independent of what you do with the boundary conditions.

空間部分微分方程式，或稱本徵函數方程式：

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



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

加上週期性條件，這是Sturm-Liouville Problem. 之前證明的正交與展開定理適用。

週期性條件很容易被滿足：

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

只要： $kL = n\pi$ 相角差會是$2n\pi$，即可滿足週期性條件！

這就是滿足週期性條件的自由空間電子波函數的解：

These are called the eigenfunctions in the Sturm-Liouville Problem.

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

能量、也就是本徵值，等於：

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

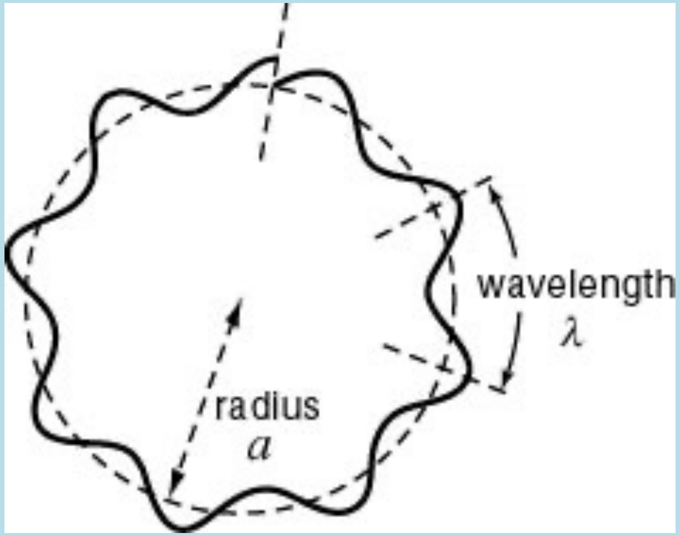
週期性自由空間的電子定態：

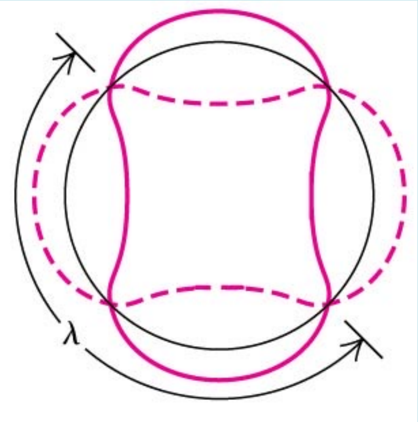
$$\Psi(x,t) = \left(Ae^{ik_nx} + Be^{-ik_nx}\right)e^{-i\frac{E_n}{\hbar}t}$$

以上的解的實數部其實就是圓形軌道上德布羅意波。

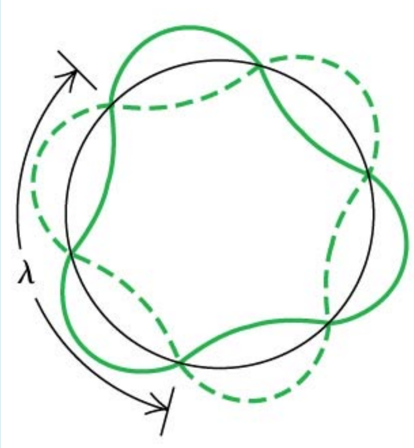
將原子中的電子波放在有限的圓形軌道上，波函數在圓周上必須一致，

圓周必須是波長的整數倍值，因此電子的軌道不能任意！

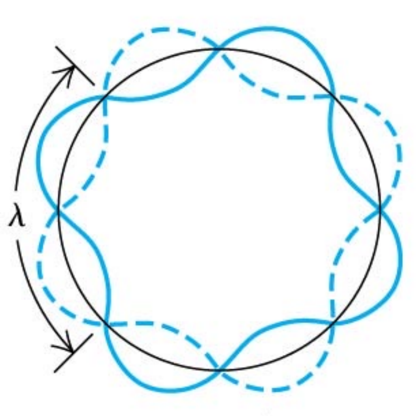




$n = 2$



$n = 3$



$n = 4$

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$$\frac{2\pi r}{\lambda} = n$$

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

週期性條件


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u_n還可以寫成週期性 Sine與Cosine函數，這是組成傅立葉級數的成分。

$$u_n(x) = Ae^{i\frac{n\pi}{L}x} + Be^{-i\frac{n\pi}{L}x} = C\sin\frac{n\pi}{L}x + D\cos\frac{n\pi}{L}x$$

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：
$$x' = \frac{n\pi}{L}x$$

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

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

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

Jean-Baptiste Joseph Fourier

1768-1830

週期性自由電子$u_n(x)$是完備的，任一週期函數可以分解成$u_n(x)$的級數和！

Method of eigenfunction expansion

將$t = 0$時的波函數，即起始條件，對定態解展開如下：

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

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

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

u_n彼此正交，係數a_n可以很容易計算：

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

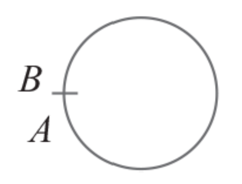
$t = 0$時此狀態可以視為定態u_n的如上疊加，

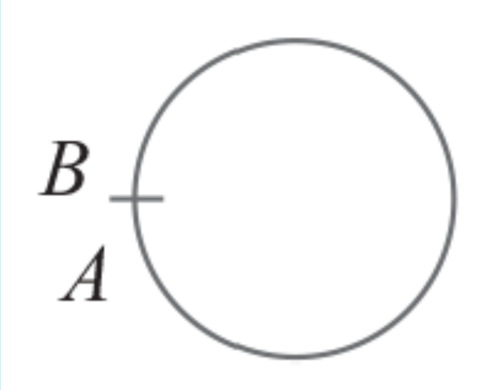
接著定態隨時間個自演化，位能下薛丁格方程式要求u_n乘上$e^{-i\frac{E_n}{\hbar}t}$。

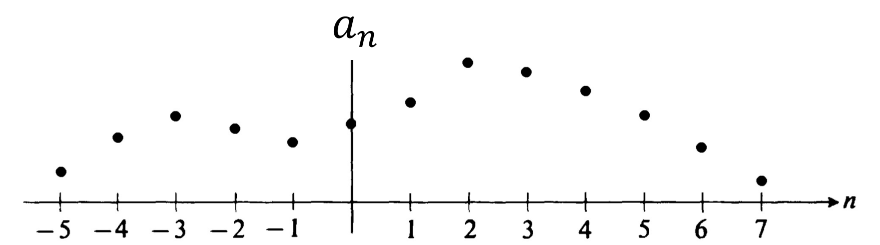
乘完之後依同樣方式疊加，整個波函數也就滿足薛丁格波方程式。

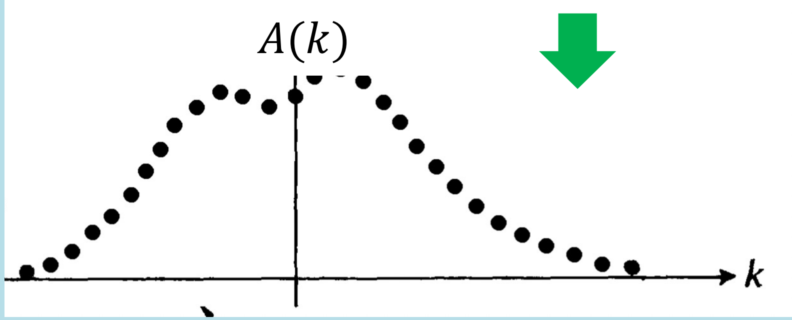
$$\Psi(x,t) = \sum_{n=-\infty}^{\infty} a_n u_n(x) e^{-i\frac{E_n}{\hbar}t}$$

現在讓空間大小趨近無限大$L \to \infty$，









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

離散可數的角波數k_n近似趨近連續變數角波數k。

$$u_n = e^{ik_n x} \to e^{ikx}$$

u_n成為角波數k的指數函數。

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$A(k)$。

$$a_n \to A(k)$$

而級數近似趨近函數積分：

$$\sum_{n=-\infty}^{\infty} \to \int_{-\infty}^{\infty} dk$$

$$\psi(x) = \sum_{n=-\infty}^{\infty} a_n e^{i\frac{n\pi}{L}x} = \sum_{n=-\infty}^{\infty} a_n e^{ik_n x}$$

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

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

更細緻的推導：

$$\Delta n = 1$$

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

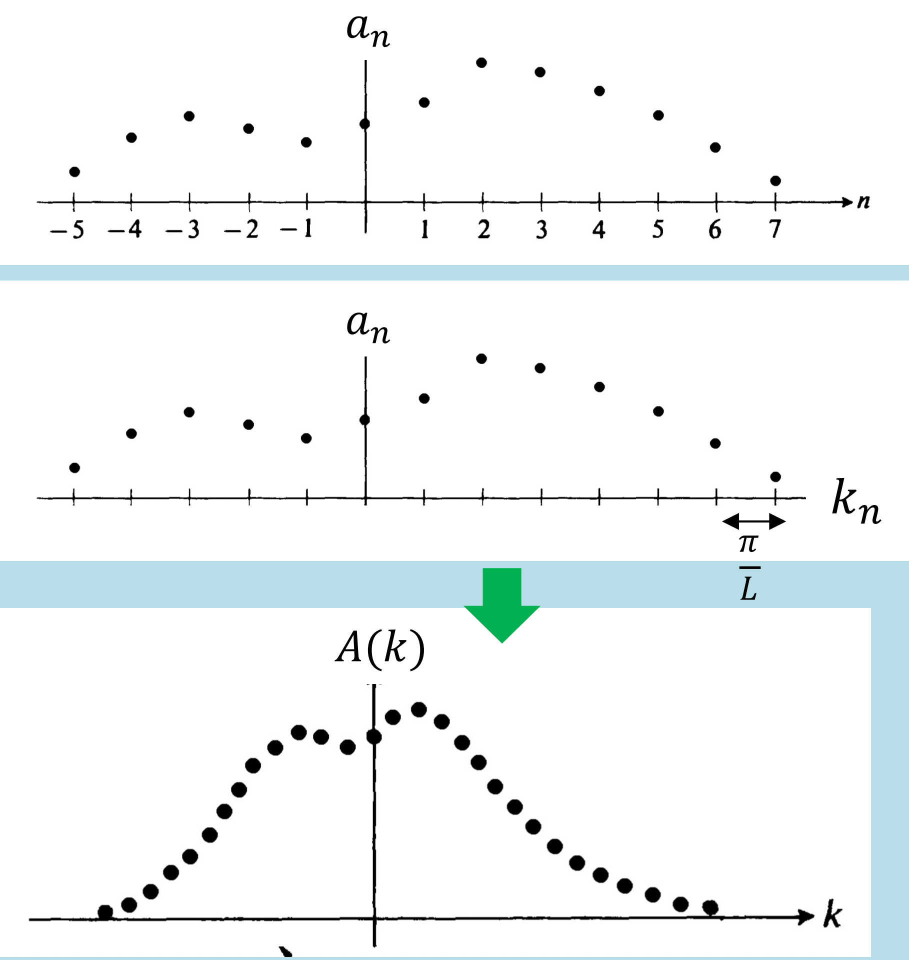
重新定義係數：

$$\frac{L}{\pi}a_n \equiv \frac{1}{\sqrt{2\pi}}A(k_n)$$

$$\psi(x) = \frac{1}{\sqrt{2\pi}}\sum_{n=-\infty}^{\infty} A(k_n)e^{ik_n x}\Delta k_n$$

$$L \to \infty \qquad k_n \to k$$

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



u_n彼此正交，係數a_n可以很容易計算：

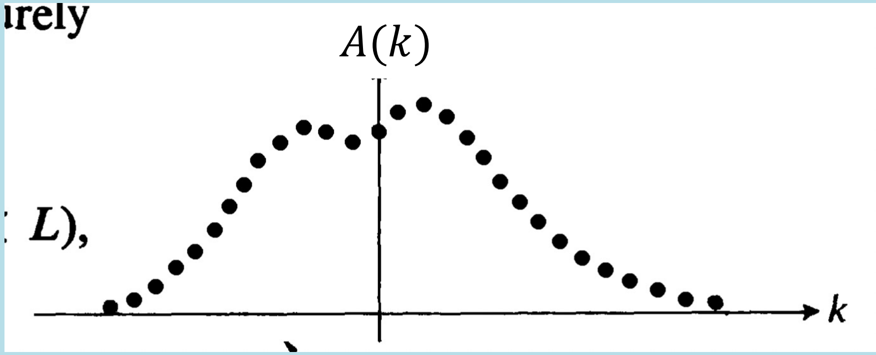
$$a_n = \frac{1}{2L}\int_{-L}^{L} dx\, e^{-i\frac{n\pi}{L}x}\psi(x) = \frac{1}{2L}\int_{-L}^{L} dx\, e^{-ik_n x}\psi(x)$$

新的係數：$A(k_n)$

$$A(k_n) = \sqrt{2\pi}\,\frac{L}{\pi}a_n = \frac{1}{\sqrt{2\pi}}\int_{-L}^{L} dx\, e^{-ik_n x}\psi(x)$$

$\downarrow$ $L \to \infty$ $k_n \to k$

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



以$A(k)$為配重係數，自定態e^{ikx}疊加出狀態函數$\psi(x)$。

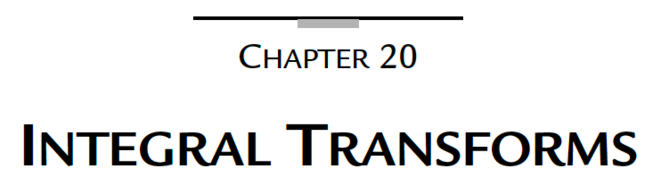
$$\psi(x)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}dk\,A(k)e^{ikx}$$

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

由$\psi(x)$也可以算出$A(k)$：

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

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



CHAPTER 20

INTEGRAL TRANSFORMS

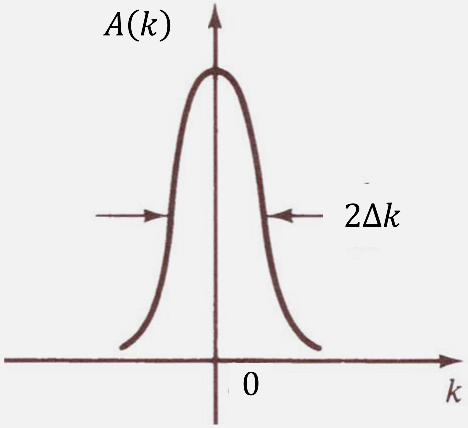
一個函數經過一個積分變換得到另一個函數，

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

波包 Wave Packet

考慮一高斯分佈Gaussian form $A(k)$：

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



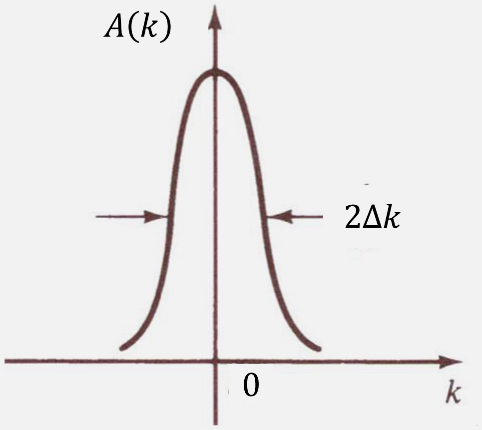
這表示是以為$k = 0$中心，形成一離開此值就快速降低的分佈

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

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

已知高斯函數的無限積分：

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



因此要將指數湊成平方：

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

$$= \int_{-\infty}^{\infty} e^{-\frac{x^2}{2\alpha}} \cdot e^{-\frac{\alpha}{2}\left(k^2 - 2\frac{ix}{\alpha}k - \frac{x^2}{\alpha^2}\right)} \cdot dk'$$

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

$$= e^{-\frac{x^2}{2\alpha}} \int_{-\infty}^{\infty} e^{-\frac{\alpha k'^2}{2}} \cdot dk'$$

$$= \sqrt{\frac{2\pi}{\alpha}}\, e^{-\frac{x^2}{2\alpha}}$$

積分已經與x無關了！就是一個常數，可以計算等於 $\sqrt{\frac{2\pi}{\alpha}}$。

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

先平方：

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

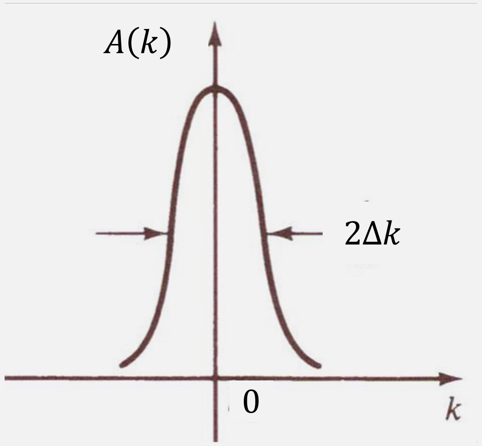
換極座標：

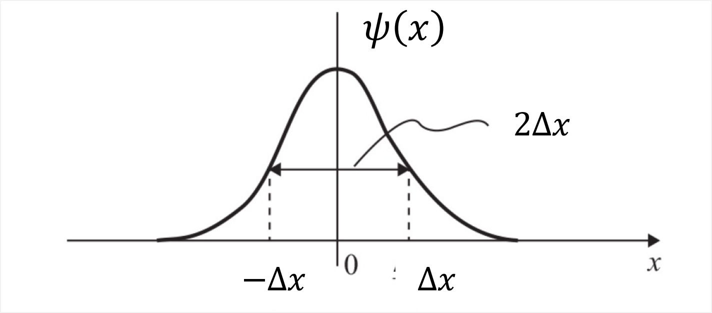
$$= \int_{0}^{2\pi} \int_{0}^{\infty} rdr \cdot d\theta \cdot e^{-ar^2} = 2\pi \int_{0}^{\infty} rdr \cdot e^{-ar^2} = \pi \int_{0}^{\infty} dr^2 \cdot e^{-ar^2} = \frac{\pi}{a}$$

開根號：

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

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





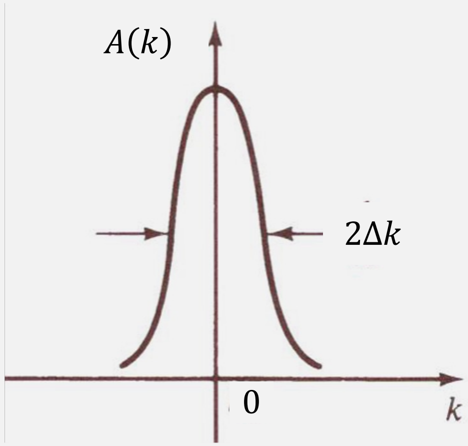
$\psi(x)$為以原點為中心，寬度由α決定的packet內。稱為波包Wave Packet。

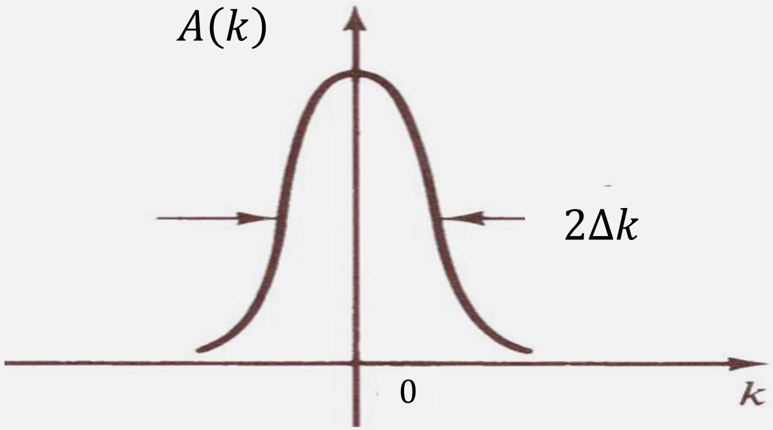
$A(k)$與$\psi(x)$都是高斯分佈，高斯分佈的傅立葉變換也是高斯分佈！

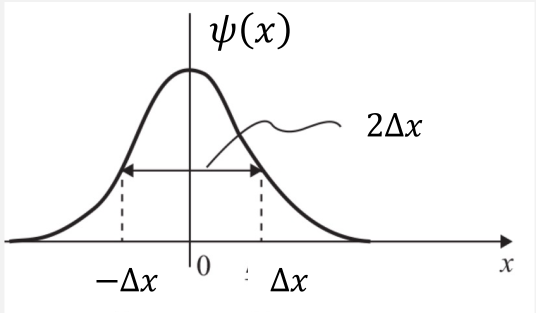
若取極值的e^{-1}左右位置為寬度： 寬度大約是$\Delta k \sim \sqrt{2}/\sqrt{\alpha}$，$\Delta x = \sqrt{2}\sqrt{\alpha}$ 。

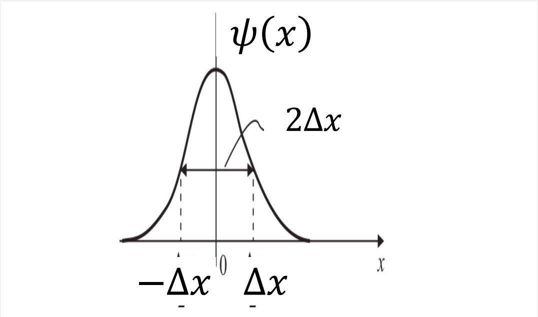
$$\Delta x \cdot \Delta k = 2$$

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





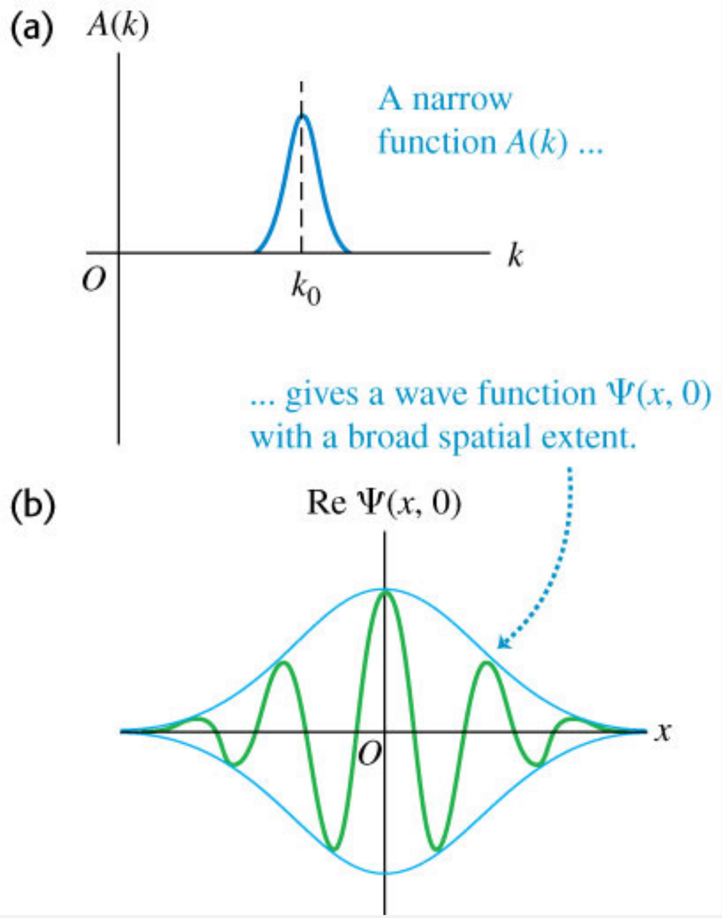




角波數***k***範圍越寬，製造出的波包的空間***x***範圍就可以越窄！

若$A(k)$高斯分佈的中心在 $k = k_0$:

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



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

$$= C\sqrt{\frac{2\pi}{\alpha}}\left(e^{-\frac{x^2}{2\alpha}}\cos k_0x + ie^{-\frac{x^2}{2\alpha}}\sin k_0x\right)$$

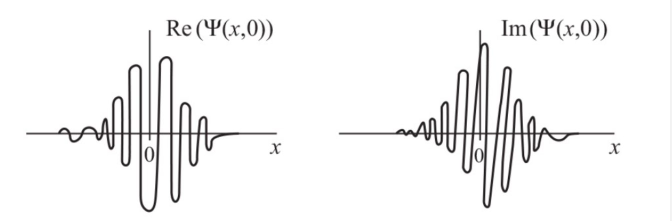
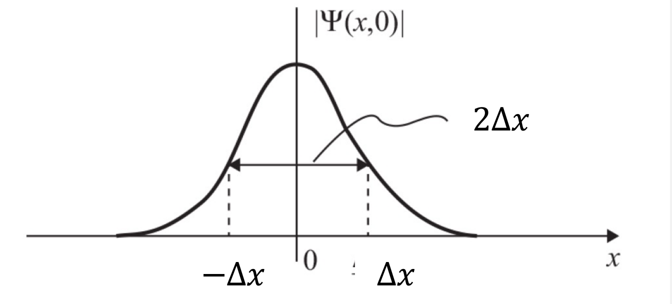


Figure 4.2
The real and imaginary parts of Ψ(x, 0).

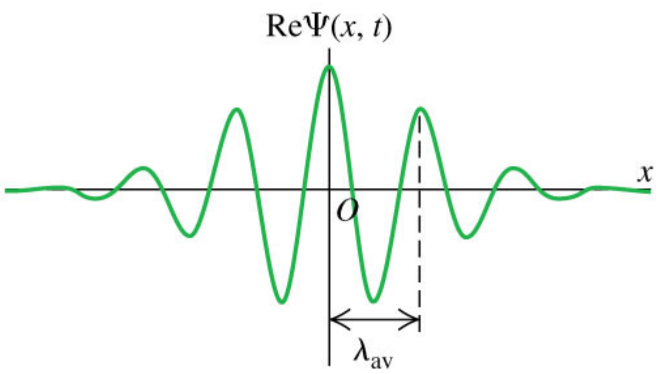


在時間為零，波函數是一類似自由電子波e^{ik_0x}的振盪函數，乘上一高斯函數。

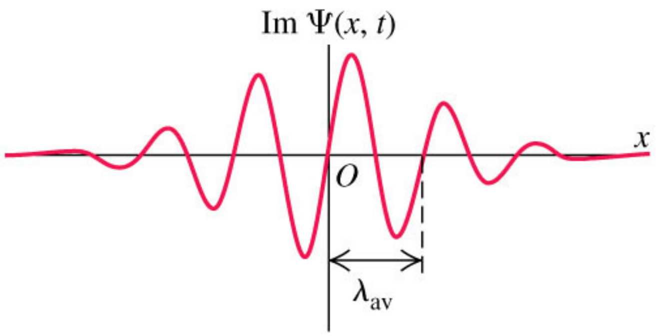
高斯函數 $e^{-\frac{x^2}{2\alpha}}$ 決定了振盪的振幅，也就是波強度：$|\Psi(x,0)|$ 。

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。

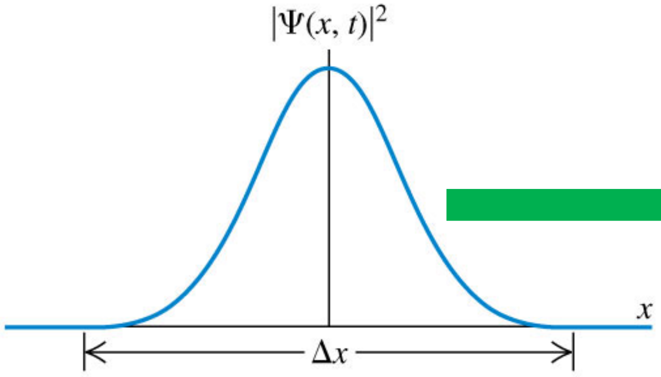
(a) Real part of the wave function at time *t*



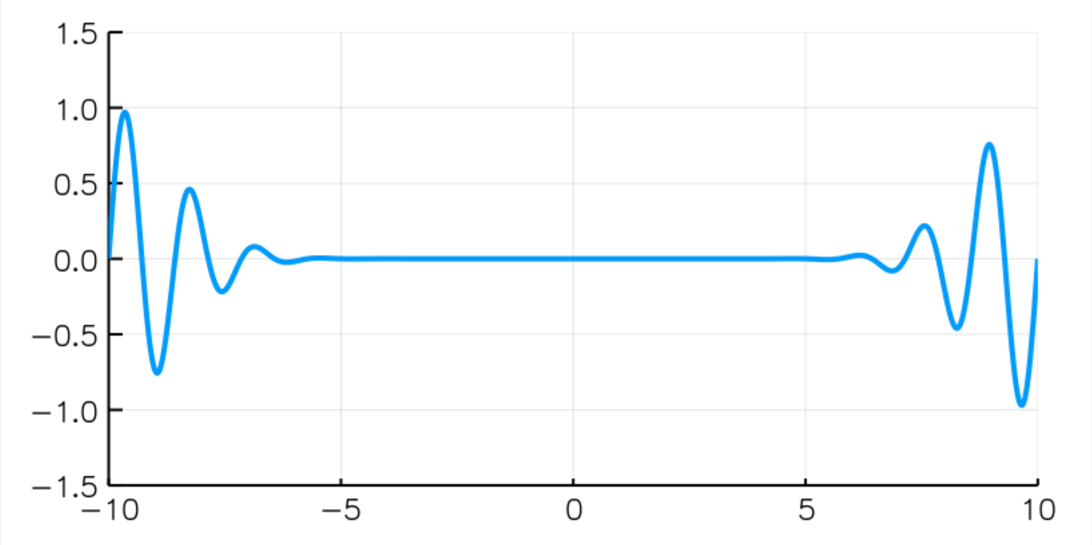
(b) Imaginary part of the wave function at time *t*

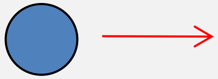


(c) Probability distribution function at time *t*

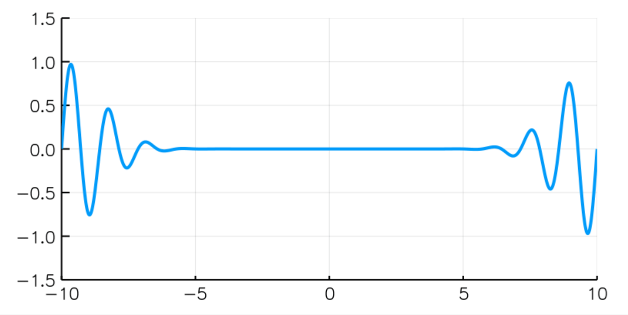


波包會隨時間移動嗎？其實答案非常簡單！





$$\Psi(x,t) \sim e^{i\left[k_0 x-\frac{\hbar}{2m}k_0^2 t\right]} e^{-\frac{(x-v_g t)^2}{2(\alpha+i\beta t)}}$$



此波包的中心點為$v_g t$，位置隨時間移動，速度為 v_g 。

對於自由電子波，群速度v_g可以算出來：

$$v_g = \left(\frac{\partial \omega}{\partial k}\right)_{k_0} = \left(\frac{\partial \frac{\hbar}{2m}k^2}{\partial k}\right)_{k_0} = \frac{\hbar}{m}k_0 = \frac{p}{m}$$

妙的是波包移動的速度不是波速，而是群速度！恰等於古典電粒子的速度！

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

以$A(k)$為配重係數，自定態e^{ikx}疊加出狀態函數$\psi(x)$。

$A(k)$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。 $p = \hbar k$

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

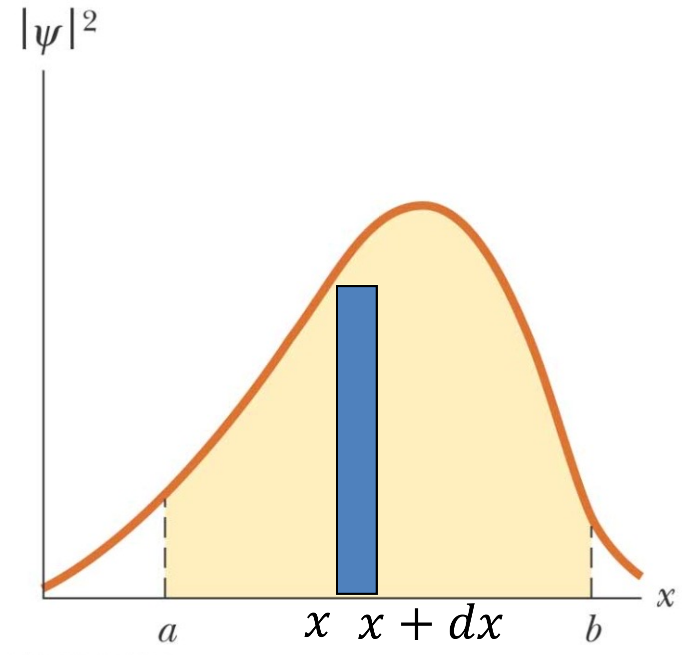
$e^{ipx/\hbar}$是動量為p的自由電子波函數，

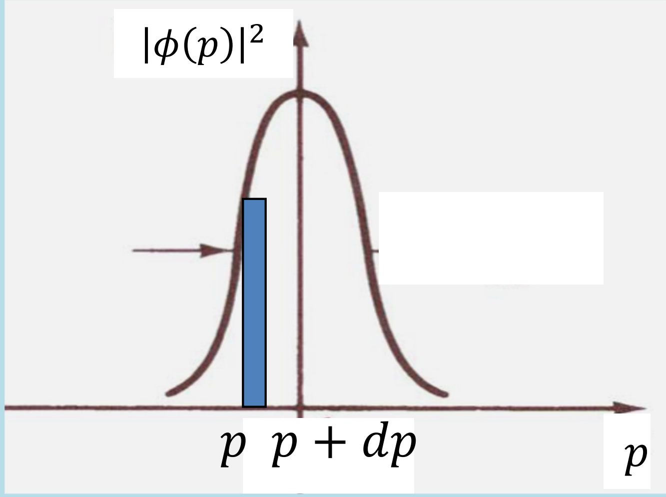
因此$\phi(p)$是疊加時，動量為p的配重。可稱為動量空間的波函數。

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：

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

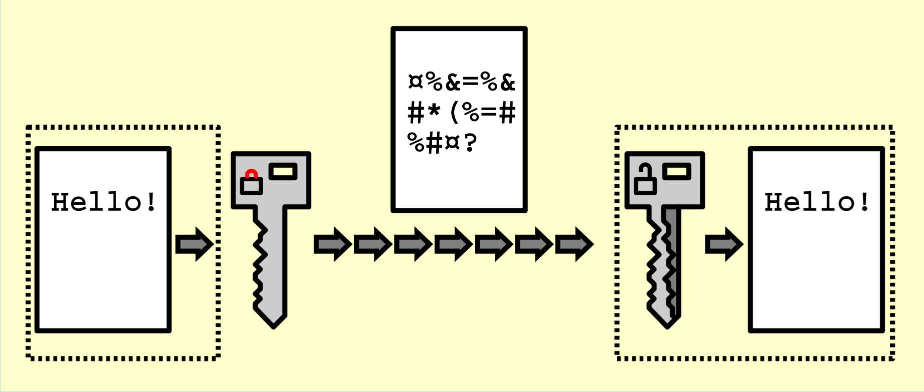
動量空間波函數$\phi(p)$與波函數$\psi(x)$互為傅立葉變換：

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

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

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

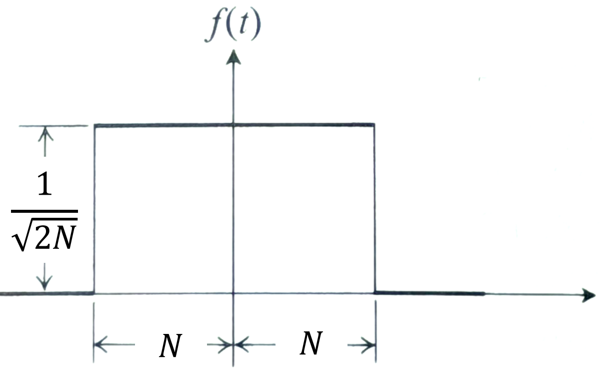
有了$\phi(p)$就能算出$\psi(x)$，反之亦然！有點像Encryption加密。



1. Consider a packet-like state :

$$\psi(x) = \frac{1}{\sqrt{2N}} \qquad -N \le x \le N$$

$$= 0 \qquad x > N, x < N$$

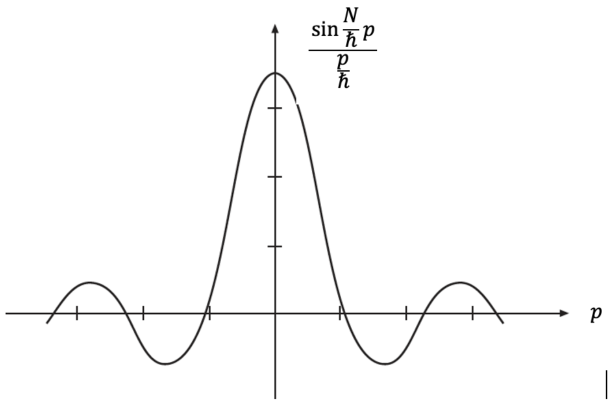


Calculate the Fourier Transform:

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

Prove that

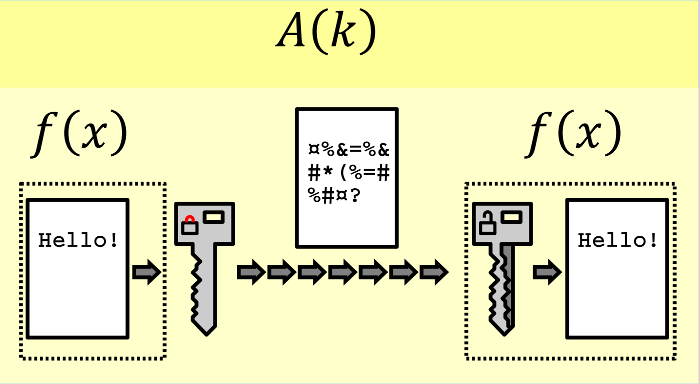
$$\phi(p) = \frac{1}{\sqrt{\pi N\hbar}} \frac{\sin \frac{N}{\hbar} p}{\frac{p}{\hbar}}$$



函數$A(k)$為函數$f(x)$的傅立葉變換：

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

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



計算函數微分的變換：

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

$$f(x) \to 0, x \to \pm\infty$$

函數微分的變換，只是乘上ik。兩次微分的變換， 只是乘上$(ik)^2$。

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

$$\mathcal{F}\{f''(x)\} = ik \cdot \mathcal{F}\left\{f'^{(x)}\right\} = (ik)^2 \cdot \mathcal{F}\{f(x)\}$$

此結果可以推廣為：

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

一函數n次微分的傅立葉變換， 等於原函數傅立葉變換乘上$(-ik)^n$。

Now we apply Fourier Transformation to solve a differential equation.

This is the equation for General forced oscillation.

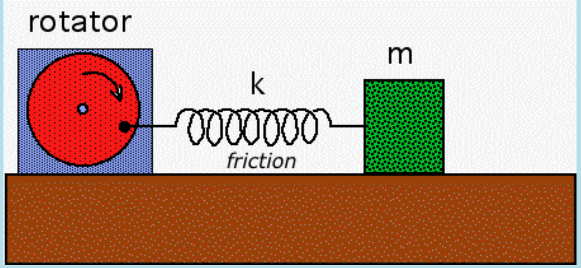
The position $x(t)$ is the function (instead of $f(x)$) we want to discuss and solve.

$$\frac{d^2x}{dt^2}+\frac{b}{m}\frac{dx}{dt}+\omega^2 x=\frac{F_0}{m}\cos\omega_D t$$

$$\Big\downarrow$$

$$\frac{d^2x}{dt^2}+2\alpha\frac{dx}{dt}+\omega_0^2 x=f(t)$$

General forced oscillation



We define Fourier Transformations for $f(t)$ and $x(t)$, with $x \rightarrow t, k \rightarrow -\omega$

Here we will need to substitute t for x and $-\omega$ for k.

Conventionally, for time Fourier transformation, there is a negative sign for ω.

$$F(\omega) \equiv \mathcal{F}\{f(t)\} = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} f(t)\cdot e^{i\omega t}\cdot dt \quad \Longleftrightarrow \quad A(k) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dx\, \psi(x) e^{-ikx}$$

$$A(\omega) \equiv \mathcal{F}\{x(t)\} = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} x(t)\cdot e^{i\omega t}\cdot dt$$

$$\frac{d^2x}{dt^2} + 2\alpha\frac{dx}{dt} + \omega_0^2 x = f(t)$$ General forced oscillation

Taking a Fourier Transformation on the whole differential equation:

$$A(\omega) \equiv \mathcal{F}\{x(t)\}$$

$$F(\omega) \equiv \mathcal{F}\{f(t)\}$$

$$A(\omega) \equiv \mathcal{F}\{x(t)\}$$

$$\mathcal{F}\{x'(t)\} = (-i\omega)A(\omega)$$

$$\mathcal{F}\{x''(t)\} = (-i\omega)^2 A(\omega)$$

$$(-i\omega)^2 A(\omega) + 2\alpha(-i\omega)^1 A(\omega) + \omega_0^2 A(\omega) = F(\omega)$$

Again, the differential equation is transformed into a algebraic equation for $A(\omega)$.

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

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

Taking the inverse Fourier Transformation of $A(\omega)$, we solved the ODE.

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

How to do the integral? Complex analysis.

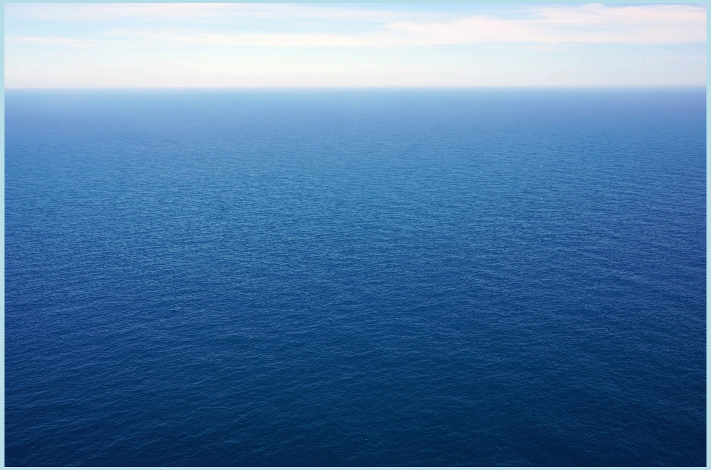
Delta Function - Distribution

Arfken p75-79

取無限大圓周極限，我們可以利用Sturm-Liouville Problem得到的結果：

我們也可以粗魯的直接討論無邊界條件的無限大空間：

空間部分微分方程式依舊相同：



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

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

$$k \equiv \sqrt{\frac{2mE}{\hbar^2}}$$

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

若無邊界條件，k可以是任意正值，$0 < k < \infty$。

第二項可以寫成負值的k： $-\infty < k < 0$。

無邊界條件的無限大空間內的定態狀態函數：

$$\psi(x) = Ae^{ikx}, -\infty < k < \infty$$

能量、也就是本徵值，等於：

$$E(k) = \frac{\hbar^2 k^2}{2m}$$

自由空間的電子定態：

$$\Psi(x,t) = Ae^{ikx}e^{-i\frac{E(k)}{\hbar}t}$$

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

依據$A(k)$為配重係數，以e^{ikx}疊加出狀態函數$\psi(x)$。

此疊加自然也是定態方程式的解！

我們從無限大圓周極限，發現由$\psi(x)$也可以算出$A(k)$：

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

從數學上看$A(k)$就是$\psi(x)$的傅立葉積分變換Fourier Transform。

這樣的$A(k)$作反傅立葉變換真能得到$\psi(x)$嗎？

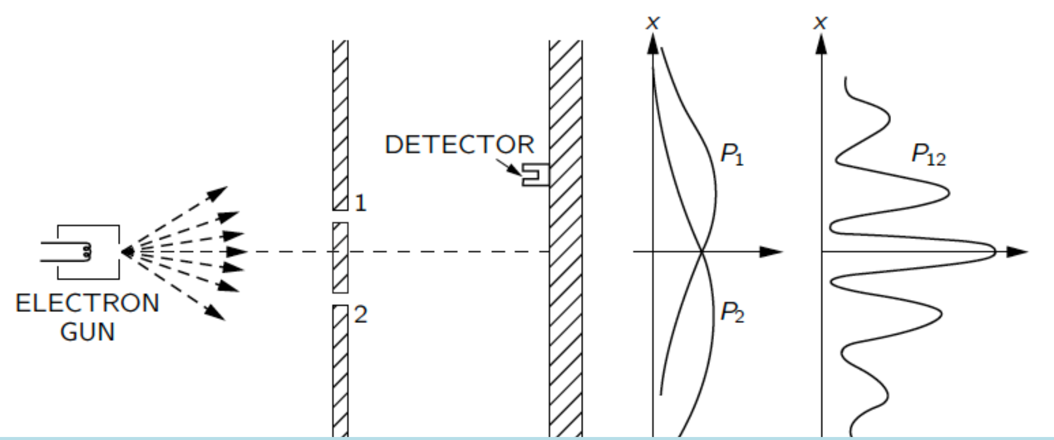
$$\psi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk\, A(k) e^{ikx}$$

如果不利用無限大圓周極限，能不能直接從數學找到計算方法？

傅立葉變換的數學方法通常會用一個新的技巧，稱為Delta Function.

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！

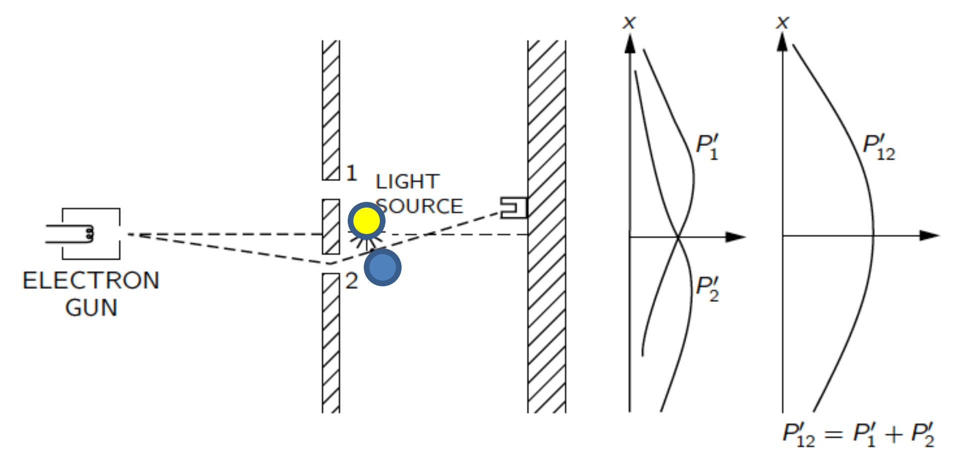


波狀的態

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

在狹縫屏幕被觀測位置後，電子像粒子，有特定的位置，

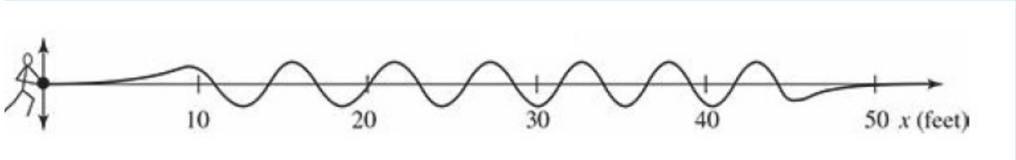
但被光子隨機撞擊改變動量，原本動量的確定性已消失。

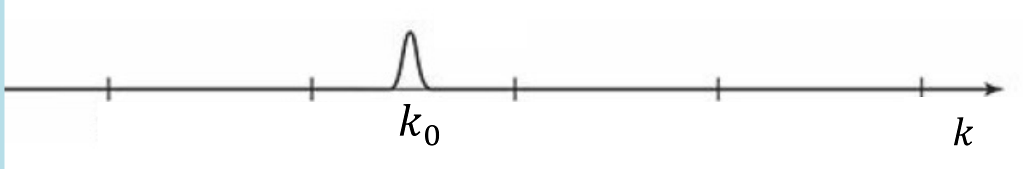


粒子狀的態

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

波狀的態的波函數就是自由電子波：Ae^{ik_0x}。

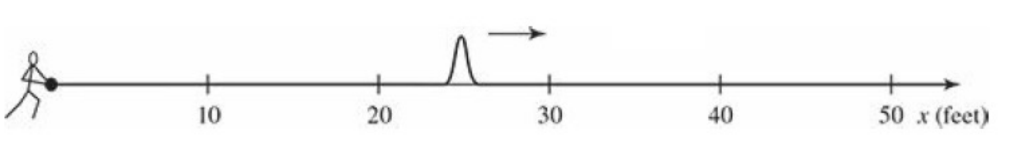


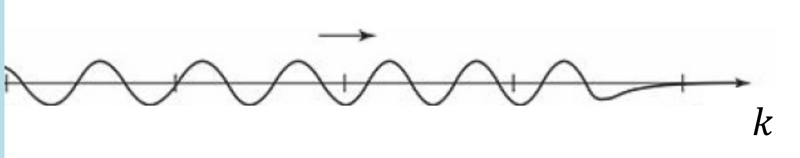


正弦波波長特定，動量特定：$\Delta p = 0$

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：$\Delta x \to \infty$

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

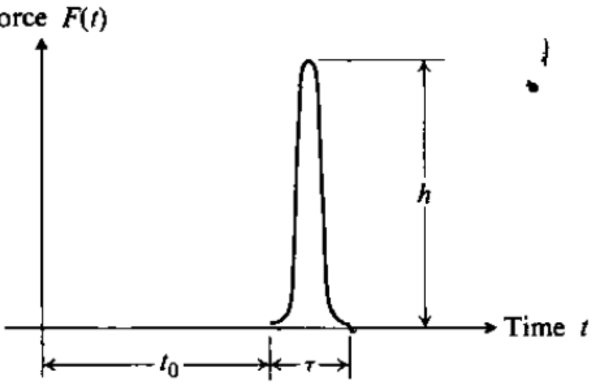


Figure 6.1

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

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

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

瞬間的衝擊！

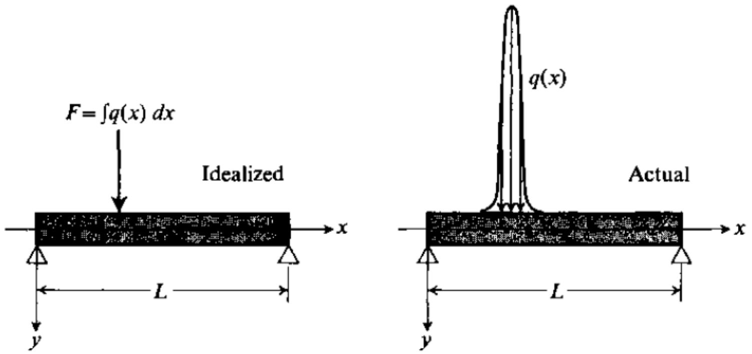


Figure 6.2

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.

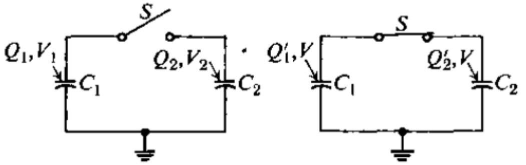
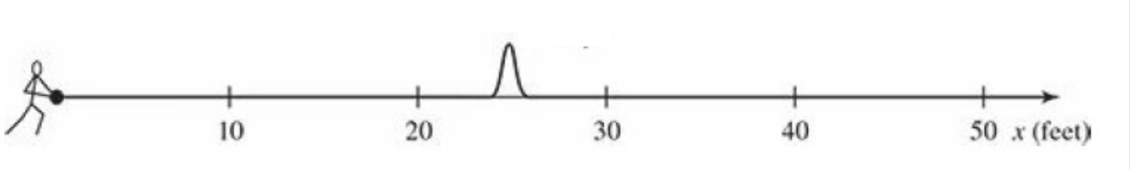


Figure 6.3

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



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x_0有值： $\psi(x) \equiv \delta(x - x_0)$

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

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

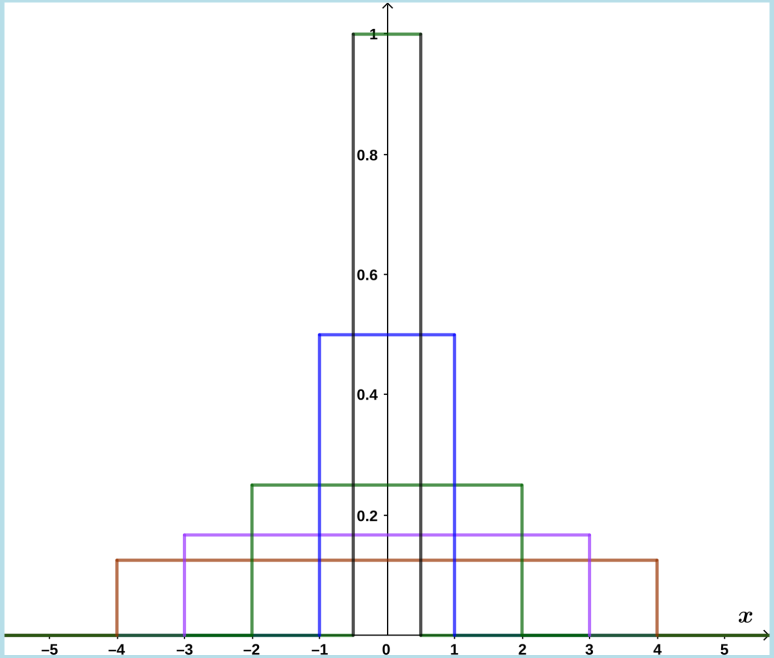
我們期待脈衝的總衝量是固定的，因此設定$\delta(x)$的積分等於1。

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

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

$\delta(x)$ 定義為以下函數取極限$\varepsilon \to 0$：

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



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！

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

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

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

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

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

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

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

$\delta(x)$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 $\delta(x^2)$.

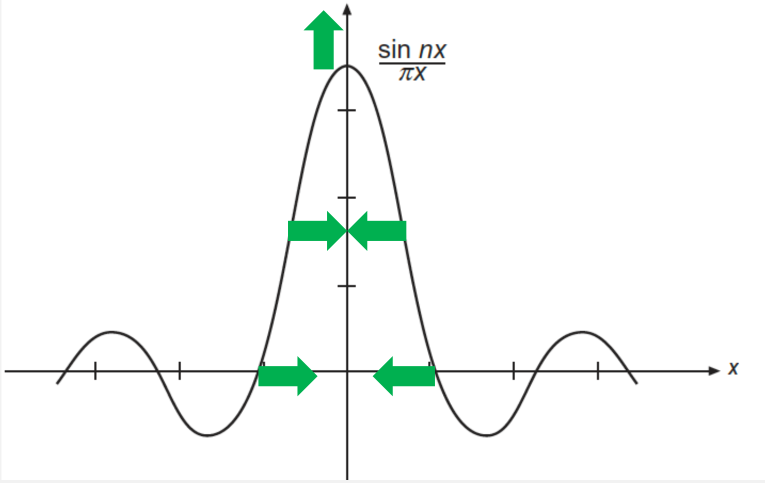
Delta Function $\delta(x)$顯然不是一個正常函數，而是極限的結果。

除了上一頁的定義，它有許多極限表示法。

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

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：

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

這裏得到一非常有用的公式，稱為$\delta(x)$的積分表現。

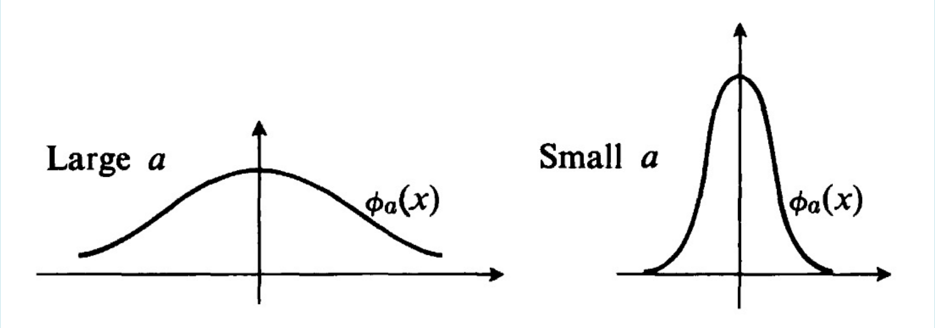
$$\int_{-\infty}^{\infty} e^{ikx} \cdot dk = 2\pi\delta(x)$$

我們可以用極窄的波包來近似：

$$\sqrt{\frac{1}{2\pi\alpha}}\,e^{-\frac{x^2}{2\alpha}} \xrightarrow[\alpha\to 0]{} \delta(x)$$

注意：

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



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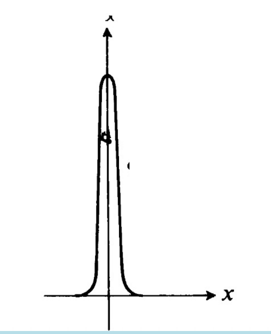


另一方面，波包可以展開為高斯函數與平面波的積分：

$$\sqrt{\frac{1}{2\pi\alpha}}\,e^{-\frac{x^2}{2\alpha}} = \int_{-\infty}^{\infty} e^{-\alpha k^2/2}\cdot e^{ikx}\cdot dk \quad \xrightarrow[\alpha\to 0]{} \int_{-\infty}^{\infty} e^{ikx}\cdot dk$$

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$\delta(x)$。

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$p'=p$。

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

Fourier Transformation 計算是的數學推導：

將此式運用於動量空間的波函數：

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

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

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

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

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

交換積分順序！

$\phi(p)$可以由$\psi(x)$得到的具體計算式：

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

動量空間波函數$\phi(p)$與波函數$\psi(x)$互為傅立葉變換：

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

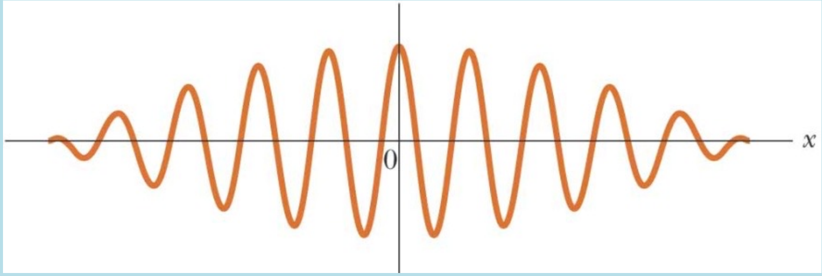
$\Psi(x,0)$就是$\phi(p)$的反傅立葉變換Inverse Fourier Transform：

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

期望值 Expectation Value

函數$\psi(x)$代表一個粒子的狀態。

$|\psi(x)|^2$代表在測量位置時結果是x的機率。

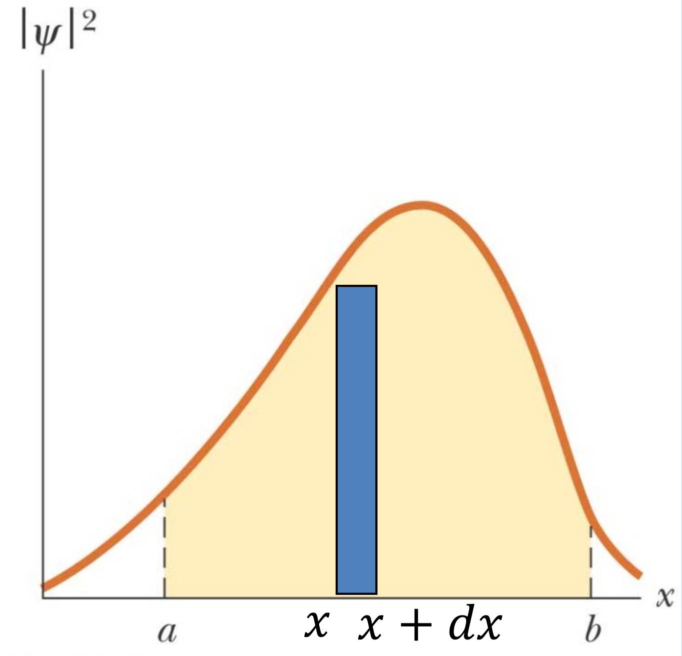


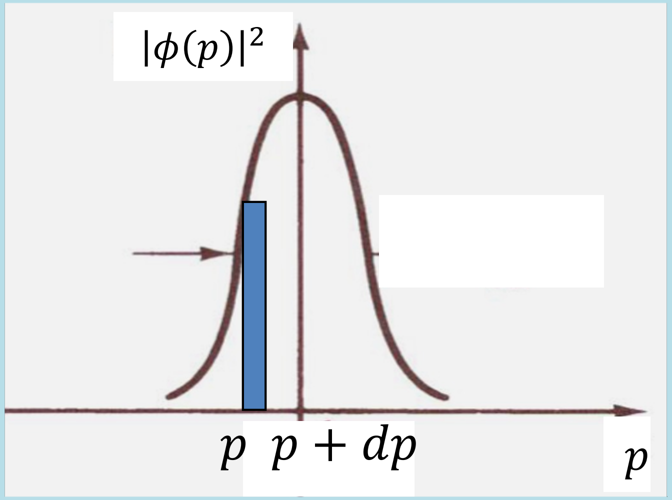
那如何預測對這個狀態、其他物理量例如動量、能量的測量？

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：

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





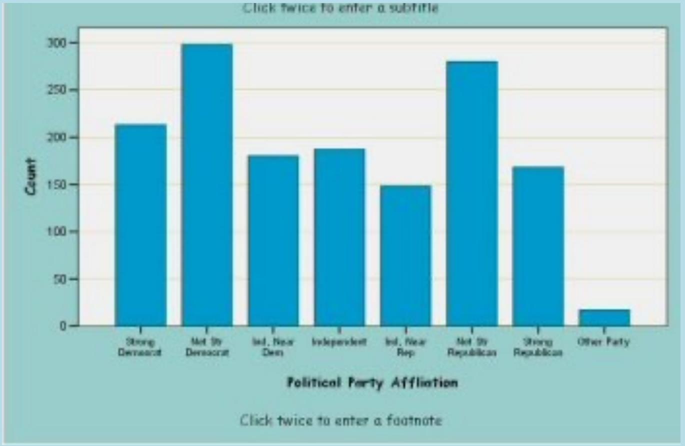
動量測量結果在p與$p + dp$之間的機率，可以寫成：

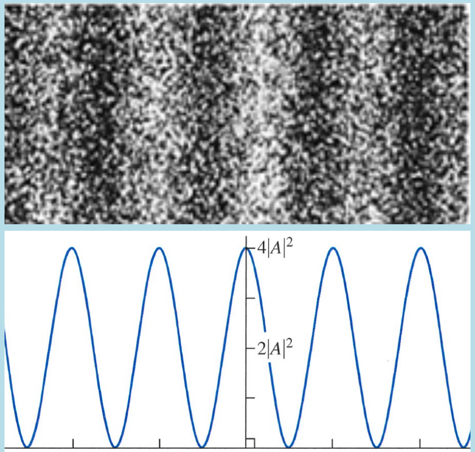
$$|\phi(p)|^2 \cdot dp = \phi^*(p) \cdot \phi(p) \cdot dp$$

以上假設可以等價用期望值來表示，那就更能直接推廣到其他物理量的測量！

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。

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

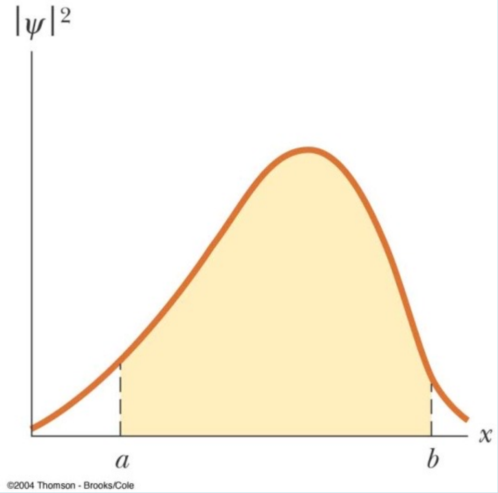
P_i是測量得到Q_i的機率

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

位置的期望值即是以機率為權重對位置求和：

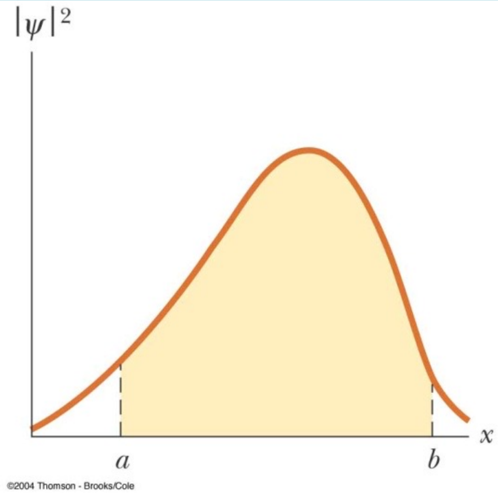
位置為連續變數，因此需做積分。注意$|\psi(x)|^2$可以寫成$\psi^*(x)\psi(x)$。

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



有了位置期望值的計算式：

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



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任何位置函數、比如位能的期望值就可以用類似方式寫下。

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

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

我們也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。

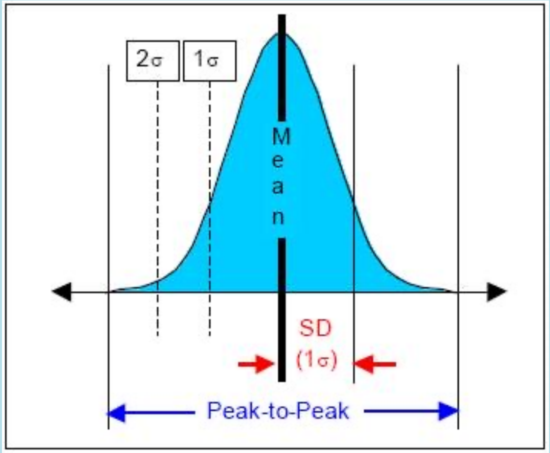
$$(\Delta x)^2 \equiv \langle (x - \langle x \rangle)^2 \rangle$$

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：

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



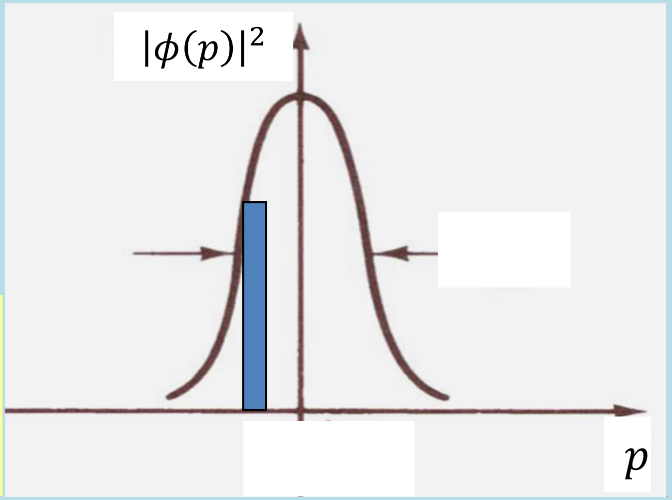
位置的不確定性Δx，現在可以精確定義與計算了。

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

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：

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

$$\left\langle \frac{p^2}{2m} \right\rangle = \int_{-\infty}^{\infty} dp \cdot \phi^*(p) \cdot \frac{p^2}{2m} \cdot \phi(p)$$

那能量的期望值可以如下記算，但兩個項用不同的波函數，不是很方便：

$$\left\langle V(x) + \frac{p^2}{2m} \right\rangle = \int_{-\infty}^{\infty} dx \cdot \psi^*(x) V(x) \psi(x) \int_{-\infty}^{\infty} dp \cdot \phi^*(p) \frac{p^2}{2m} \phi(p)$$

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。

我可以用位置空間波函數$\psi(x)$來算動量期望值嗎？

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

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

dp積分先作

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

$\frac{\hbar}{i}\frac{\partial}{\partial x}$微分可以產生$p$！

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

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

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

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

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

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：

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

例如動能的期望值$\langle KE\rangle$：

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

如此能量的期望值可以很簡潔：

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

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，何不假設對應的量子物理量的期望值都可以寫成.....

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

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，

將"波函數的空間微分"運算，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 $\hat{x}$ ！

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

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：

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

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！

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

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。

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

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

薛丁格方程式的左手邊其實就是能量算子，

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

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

能量翻譯為時間微分運算

可以簡寫為：

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

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。

與時間無關的薛丁格方程式也可以以$\hat{H}$運算子表述：

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V(x)\right]\psi_E(x)=E\psi_E(x)$$

左邊就是量子力學中對應的Hamiltan運算子：

$$\left[\frac{\hat{p}^2}{2m}+V(\hat{x})\right]\psi_E=E\psi_E$$

定態解ψ_E滿足的與時間無關的薛丁格方程式可以寫成：

$$\hat{H}\psi_E=E\psi_E$$

數學上這個關係稱為運算子$\hat{H}$的本徵函數問題！

定態的ψ_E是$\hat{H}$的本徵函數 Eigenfunction！

對應的本徵值Eigenvalue為E。

$$\hat{H}\psi_E = E\psi_E$$

能量的本徵函數，之前稱為定態，有很多重要的性質！ $\hat{H}\psi_E = E\psi_E$

計算處於定態ψ_E的電子的$\hat{H}$的期望值：$\langle\hat{H}\rangle$

$$\langle H\rangle = \int_{-\infty}^{\infty} dx \cdot \psi_E^*(x) \cdot \hat{H}\psi_E(x) = \int_{-\infty}^{\infty} dx \cdot \psi_E^*(x) \cdot E\psi_E(x)$$

$$= E\int_{-\infty}^{\infty} dx \cdot \psi_E^*(x) \cdot \psi_E(x) = E$$

$$\langle\hat{H}\rangle = E$$

本徵函數$\psi_E(x)$描述的定態的能量的期望值就是本徵值E。不意外！

定態可分解之解的空間部分，$\psi_E(x)$中的常數E就是能量的期望值！

計算本徵函數u_n描述的電子狀態的能量測量不確定性：ΔH。

$$(\Delta H)^2 \equiv \left\langle \left(\hat{H} - \langle \hat{H} \rangle\right)^2 \right\rangle = \left\langle \hat{H}^2 - 2\langle \hat{H} \rangle \hat{H} + \langle \hat{H} \rangle^2 \right\rangle = \langle \hat{H}^2 \rangle - \langle \hat{H} \rangle^2 = \langle \hat{H}^2 \rangle - E^2$$

$$\langle \hat{H}^2 \rangle = \int_{-\infty}^{\infty} dx\, \psi_E^*(x) \cdot \hat{H}\hat{H}\psi_E(x) = \int_{-\infty}^{\infty} dx\, \psi_E^*(x) \cdot \hat{H}E\psi_E(x) =$$

$$= E \int_{-\infty}^{\infty} dx\, \psi_E^*(x) \cdot \hat{H}\psi_E(x) = E^2$$

$$\Delta H = 0$$

處於定態ψ_E的電子，能量的測量值為E，而且完全沒有不確定性！

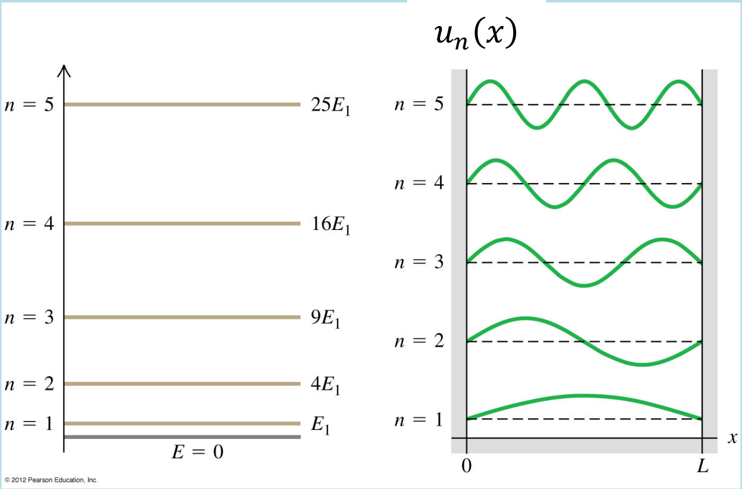
可以說定態ψ_E就是具有確定能量測量值E的狀態。

若是束縛態，如位能井，

$\hat{H}$的本徵函數是可以量子數n來數的：

$$\hat{H}u_n(x) = E_n u_n(x)$$

$$\langle \hat{H} \rangle = E_n \qquad \Delta H = 0$$



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處於定態u_n的電子，能量的測量值為E_n，完全沒有不確定性！

事實上，只有定態u_n是能量測量無不確定性的狀態。

現在考慮，對任一狀態$\psi(x)$作能量的測量，若所得到的結果是某值，

剛測量完時，立刻再作一次能量測量，結果必須還是同樣的值，無不確定性。

可見第一次剛測量完後$\Delta H = 0$，此時電子一定存在於某一能量本徵態u_n！

那麼、第一次測得的能量結果一定只能是某一本徵值E_n！u_n對應的E_n！

驚人的：任意能量測量結果只能是能量算子的某一本徵值E_n，不會測到其他值。

在束縛態中，任意電子的能量測量的確是量子化的！不是只適用於定態。

解能量算子本徵值、是在決定測量能量時會得到什麼結果：只會是E_n其中之一。

計算在狀態ψ下，能量的期望值：

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

$$\int_{-\infty}^{\infty} dx \cdot \psi^*(x) \cdot \hat{H} \cdot \sum_n [c_n u_n(x)]$$

$$= \int_{-\infty}^{\infty} dx \cdot \psi^*(x) \cdot \sum_n [c_n \cdot \hat{H} u_n(x)]$$

$$= \sum_n E_n c_n \int_{-\infty}^{\infty} dx \cdot \psi^*(x) u_n(x)$$

$$= \sum_n E_n c_n c_n^* = \sum_n E_n \cdot |c_n|^2$$

$$\langle H\rangle = \sum_n E_n \cdot |c_n|^2$$

$$\psi(x) = \sum_a c_n u_n(x)$$

$$\hat{H} u_n(x) = E_n u_n(x)$$

$$c_n = \int_0^a dx \cdot u_n^*(x)\psi(x)$$

狀態函數$\psi(x)$的展開分量的物理意義

$$\langle H\rangle = \sum_n E_n \cdot |c_n|^2$$

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

P_i是測量得到Q_i的機率

任意能量測量結果只能是能量算子的某一本徵值E_n，

可見$|c_n|^2$就是測量能量時，得到結果是E_n的機率！

Measurement Theorem 測量定理

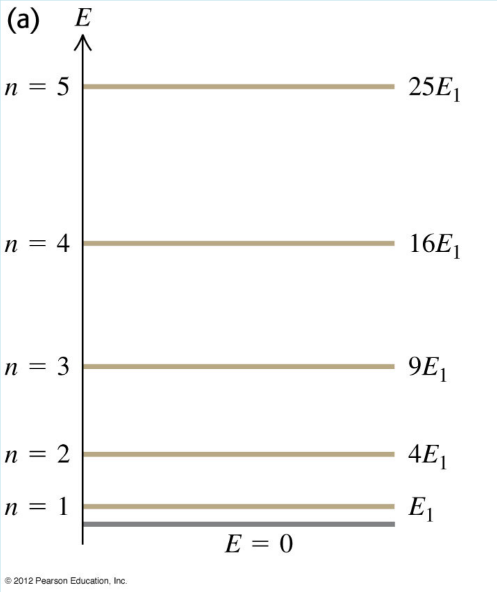
測量能量時，得到結果只能是E_n其中之一！

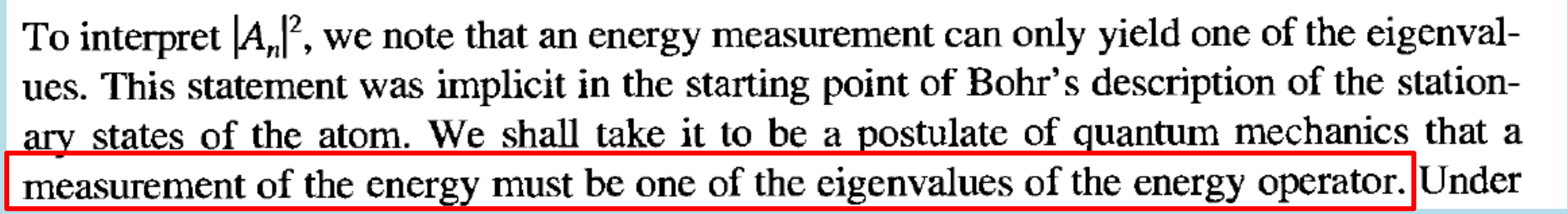
真是如此，那機率總和必須等於1！

$$1=\int_{-\infty}^{\infty} dx\cdot\psi^*(x)\,\psi(x)=\int_{-\infty}^{\infty} dx\cdot\psi^*(x)\cdot\sum_n\left[c_n u_n(x)\right]$$

$$=\sum_n c_n\int_{-\infty}^{\infty} dx\cdot\psi^*(x)u_n(x)=\sum_n c_n c_n^*=\sum_n |c_n|^2$$

$$\sum_n |c_n|^2=1$$

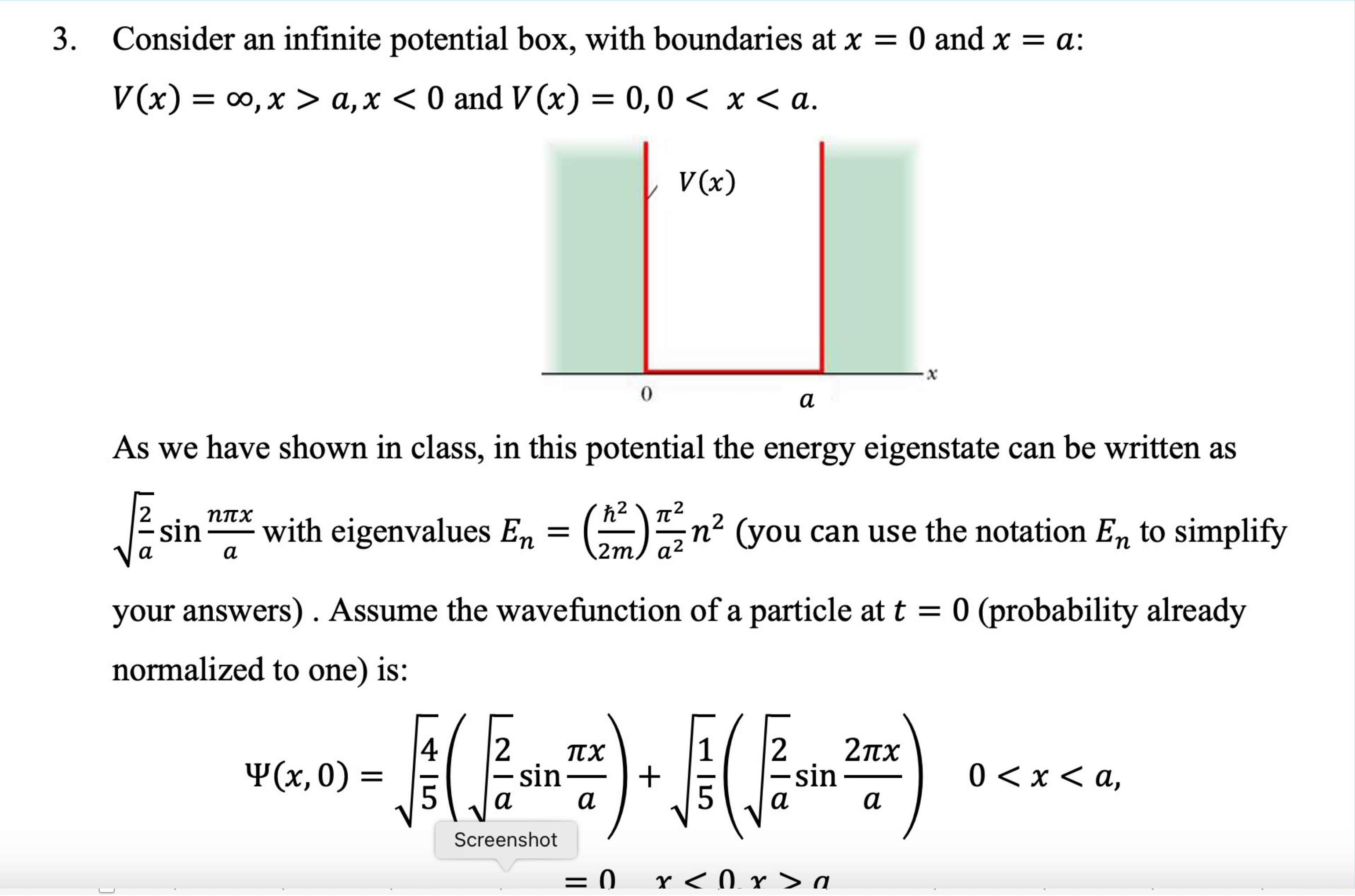




To interpret $|A_n|^2$, we note that an energy measurement can only yield one of the eigenvalues. This statement was implicit in the starting point of Bohr's description of the stationary states of the atom. We shall take it to be a postulate of quantum mechanics that a measurement of the energy must be one of the eigenvalues of the energy operator. Under

果然沒有遺漏，再次確認對能量的測量結果只能是本徵值E_n其中之一。

如果還會測到其他值，總機率就要超過1了！



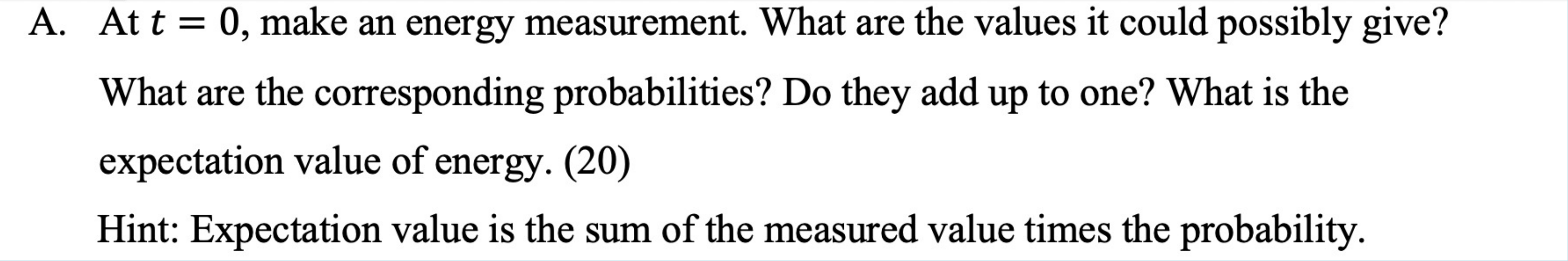
3. Consider an infinite potential box, with boundaries at $x = 0$ and $x = a$:

$V(x) = \infty, x > a, x < 0$ and $V(x) = 0, 0 < x < a$.

As we have shown in class, in this potential the energy eigenstate can be written as $\sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a}$ with eigenvalues $E_n = \left(\frac{\hbar^2}{2m}\right)\frac{\pi^2}{a^2} n^2$ (you can use the notation E_n to simplify your answers) . Assume the wavefunction of a particle at $t = 0$ (probability already normalized to one) is:

$$\Psi(x, 0) = \sqrt{\frac{4}{5}}\left(\sqrt{\frac{2}{a}} \sin \frac{\pi x}{a}\right) + \sqrt{\frac{1}{5}}\left(\sqrt{\frac{2}{a}} \sin \frac{2\pi x}{a}\right) \qquad 0 < x < a,$$

$$= 0 \qquad x < 0, x > a$$



A. At $t = 0$, make an energy measurement. What are the values it could possibly give? What are the corresponding probabilities? Do they add up to one? What is the expectation value of energy. (20)

Hint: Expectation value is the sum of the measured value times the probability.

$$\Psi(x,0)=\sqrt{\frac{4}{5}}\left(\sqrt{\frac{2}{a}}\sin\frac{\pi x}{a}\right)+\sqrt{\frac{1}{5}}\left(\sqrt{\frac{2}{a}}\sin\frac{2\pi x}{a}\right)\qquad 0<x<a,$$

$$=\sqrt{\frac{4}{5}}u_1(x)+\sqrt{\frac{1}{5}}u_2(x)$$

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

$$=\int_{-\infty}^{\infty}dx\cdot\psi^*(x)\cdot\hat{H}\cdot\left[\sqrt{\frac{4}{5}}u_1(x)+\sqrt{\frac{1}{5}}u_2(x)\right]$$

$$=\int_{-\infty}^{\infty}dx\cdot\left[\sqrt{\frac{4}{5}}u_1(x)+\sqrt{\frac{1}{5}}u_2(x)\right]\cdot\left[\sqrt{\frac{4}{5}}E_1u_1(x)+\sqrt{\frac{1}{5}}E_2u_2(x)\right]$$

$$=\frac{4}{5}E_1+\frac{1}{5}E_2=|c_1|^2E_1+|c_2|^2E_2$$

$$\frac{4}{5}+\frac{1}{5}=1$$

測量結果 機率

對任一狀態$\psi(x)$作能量的測量，若所得到的結果是某一E_n，

剛測量完時$\Delta H = 0$，此時電子一定存在於能量本徵態u_n！

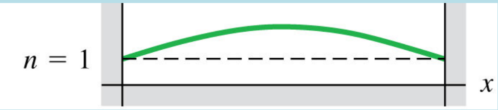
可見測量使粒子的狀態由$\psi(x)$瞬間崩潰變成了$u_n(x)$。

$$\psi(x) \xrightarrow[\hat{H}\to E_n]{} u_n(x)$$

在非本徵態$\psi(x)$，測量結果不會是確定的！崩潰變成的態也就不確定。

$\mathrm{E} = \mathrm{E}_1$

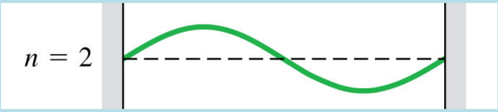
$P_1 \sim \frac{4}{5}$



$$\psi(x) = \sqrt{\frac{4}{5}}\left(\sqrt{\frac{2}{a}}\sin\frac{\pi x}{a}\right) + \sqrt{\frac{1}{5}}\left(\sqrt{\frac{2}{a}}\sin\frac{2\pi x}{a}\right)$$

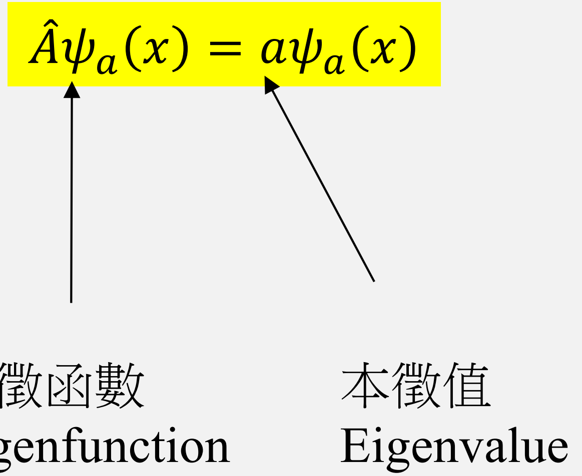
$E = E_2$

$P_2 \sim \frac{1}{5}$



這個結果不只適用於能量，對任何測量物理量如位置、動量、角動量都成立。

這個本徵函數、本徵值與測量的關係可以推廣到其他的物理量$\hat{A}$：



$$\hat{A}\psi_a(x) = a\psi_a(x)$$

本徵函數
Eigenfunction

本徵值
Eigenvalue

算子化為數 $\hat{A} \to a$

直覺上，這個關係可以解讀為：算子$\hat{A}$作用於本徵函數的效果與數一樣，

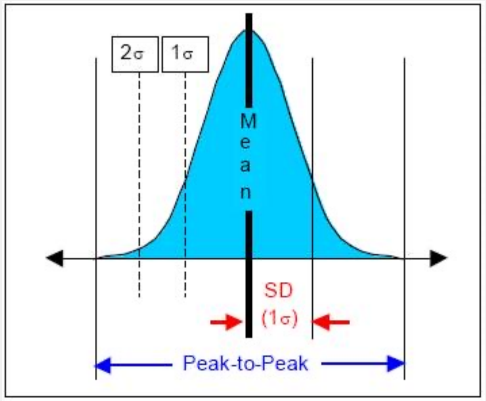
隱含：物理量$\hat{A}$測量時如古典量，也就是有確定的值。

狀態ψ_a時，該物理量算子$\hat{A}$的期望值：

$$\langle \hat{A} \rangle = \int_{-\infty}^{\infty} dx \cdot \psi_a^*(x) \cdot \hat{A}\psi_a(x) = a \int_{-\infty}^{\infty} dx \cdot \psi_a^*(x)\psi_a(x) = a$$

a值就是測量期望值。

狀態ψ_a，物理量算子$\hat{A}$的測量不準度：



$$\Delta A \equiv \left\langle \left(\hat{A} - \langle \hat{A} \rangle\right)^2 \right\rangle = \left\langle \hat{A}^2 - 2\langle \hat{A} \rangle \hat{A} + \langle \hat{A} \rangle^2 \right\rangle = \langle \hat{A}^2 \rangle - \langle \hat{A} \rangle^2$$

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

$$= a \int_{-\infty}^{\infty} dx \cdot \psi_a^*(x) \cdot \hat{A}\psi_a(x) = a^2 \cdot \int_{-\infty}^{\infty} dx \cdot \psi_a^*(x)\psi_a(x) = a^2$$

$$\Delta A = 0$$

物理量算子$\hat{A}$的本徵態，測量該量的期望值即為本徵值a，不準度為零。

對一物理量測量結果確定的狀態就是該物理量算子$\hat{A}$的本徵態ψ_a。

Measurement Theorem Again

$$\psi(x) = \sum_a c_a \cdot \psi_a(x)$$

$$\langle A\rangle = \int_{-\infty}^{\infty} dx \cdot \psi^*(x) \cdot \hat{A}\psi(x) = \int_{-\infty}^{\infty} dx \cdot \sum_b [c_b \cdot \psi_b(x)]^* \cdot \hat{A} \cdot \sum_a [c_a \cdot \psi_a(x)]$$
$$= \int_{-\infty}^{\infty} dx \cdot \sum_b [c_b \cdot \psi_b(x)]^* \cdot \sum_a a \cdot [c_a \cdot \psi_a(x)] = \sum_a \sum_b a \cdot c_b^* \cdot c_a \cdot \int_{-\infty}^{\infty} dx \cdot \psi_b(x)^* \cdot \psi_a(x)$$
$$= \sum_a \sum_b a \cdot c_b^* \cdot c_a \cdot \delta_{ba} = \sum_a a \cdot |c_a|^2$$

$|c_a|^2$是測量$\hat{A}$時得到結果是 a 的機率！

狀態函數ψ沿$\psi_a(x)$的分量 c_a = $\hat{A}$測量得到結果是 a 的振幅。

此測量使粒子的狀態由 $\psi(x)$ 瞬間崩潰成了ψ_a： $\psi(x) \xrightarrow[\hat{A}\to a]{} \psi_a(x)$

$\psi(x)$

在不同的狀態下，測量結果的機率不同！

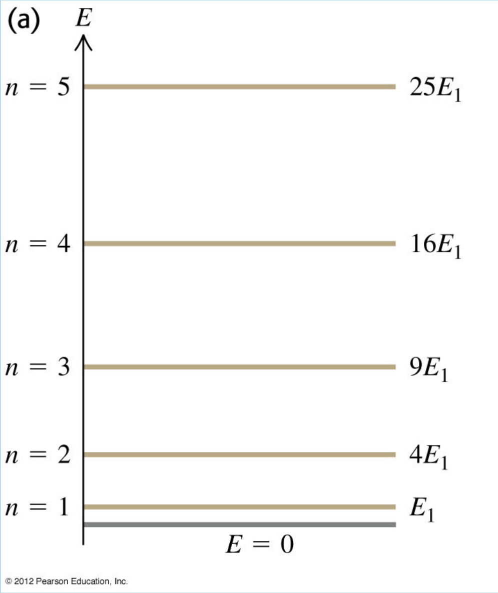
$|c_n|^2, n = 1,2,3 \cdots$

但可能的測量結果卻一樣！

$\hat{A}$

測量、算子是很有個性的！

由它來決定測量的結果有哪些可能！



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算子有它的堅持！

解一個物理量算子的eigenfunction、是在決定你測量此量時會得到什麼結果。

決定得到某eigenvalue時，粒子的狀態會崩潰為何種狀態(eigenfunction)。

自然的猜測：若以某算子的本徵函數ψ_a展開一個狀態函數$\psi(x)$，

$$\psi(x) = \sum_a c_a \cdot \psi_a(x)$$

分量$|c_n|^2$就是在$\psi(x)$狀態，測量此算子時得到結果是a的機率！

之前曾大膽假設，電子在狀態$\psi(x)$測量動量時，得到某p的機率，

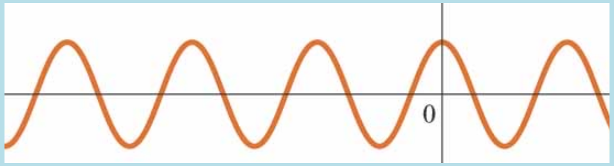
即是$\psi(x)$的傅立葉變換$\phi(p)$的絕對值平方：$|\phi(p)|^2$。

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

$\phi(p)$就是以動量的本徵函數：自由電子波，作展開的分量！

對於自由粒子波狀的態，動量是確定的（但位置測量不確定）：

$$u_p(x) = e^{i\frac{p}{\hbar}x}$$



這果然如預期是動量算子的本徵函數：

$$\hat{p}u_p(x) = -i\hbar\frac{d}{dx}e^{i\frac{p}{\hbar}x} = p\cdot u_p(x)$$

$$\Delta p = 0$$

剛剛作完位置測量的粒子，設其位置為 x_0，則其波函數只有在此處不為零！

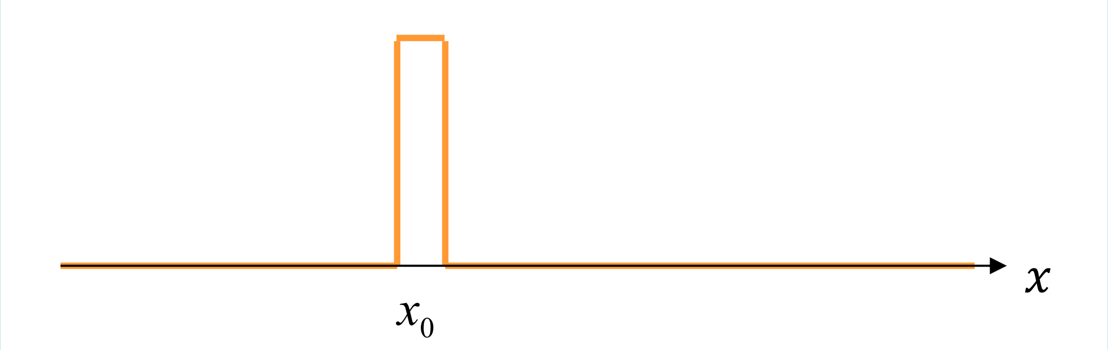
波函數是一個delta function！

$$u_{x_0} = \delta(x - x_0)$$

這是位置算子$\hat{x}$的本徵函數：

$$\hat{x}u_{x_0} = x\cdot\delta(x - x_0) = x_0\cdot\delta(x - x_0) = x_0\cdot u_{x_0}$$

$$\Delta x = 0$$



量子力學的原則完整版

某瞬間時刻的狀態 ⟶ 狀態函數 $\psi(x)$

可測量的物理量 ⟶ 算子 $\hat{A}$ 基本上 Sturm-Liouville 算子

例如位置算子為乘上位置座標，動量算子為對座標微分：$\hat{x} \equiv x, \hat{p} \equiv -i\hbar\dfrac{d}{dx}$

有古典對應的物理量，就直接將位置算子及動量算子代入同樣的數學形式：

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

就得到量子力學中對應的算子。

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

把對應的算子放入此式，就可得到測量期望值。

對一物理量A測量，結果完全確定的狀態：$\hat{A}\psi_a(x) = a\psi_a(x)$

就是該物理量對應算子$\hat{A}$的本徵函數$\psi_a(x)$，本徵值a就是測量結果。

任一物理量測量結果只能是算子某一本徵值a，不會測到其他值。

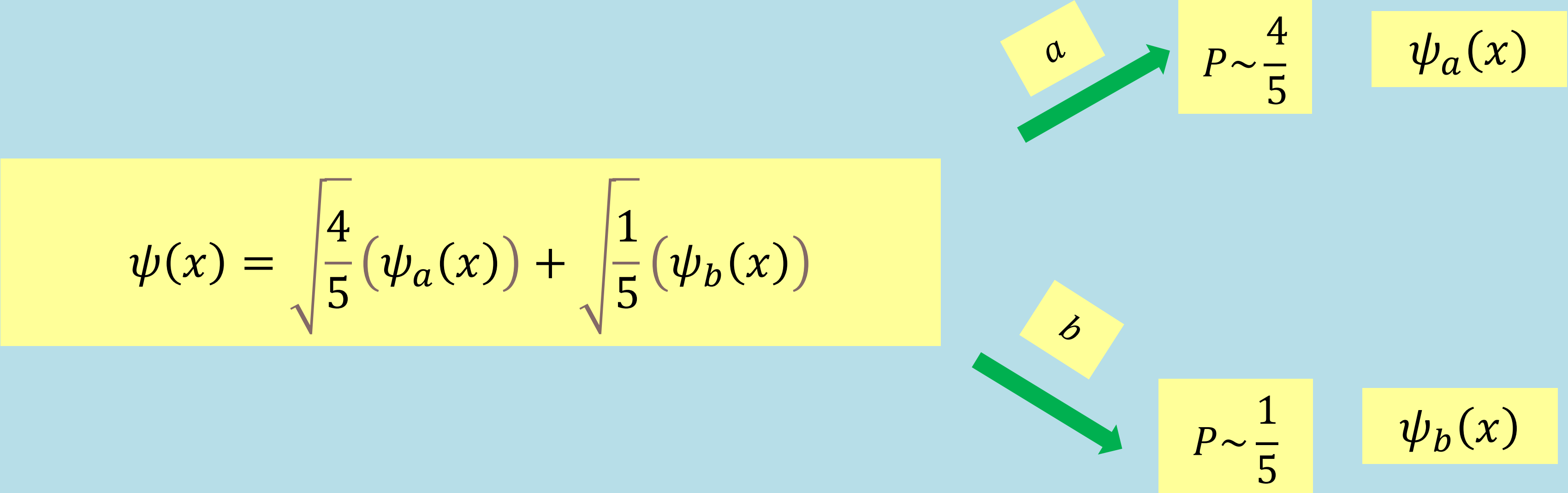
$|c_a|^2$是在狀態$\psi(x) = \sum_a c_a\psi_a(x)$ 測量$\hat{A}$時得到結果是a的機率！

對任一狀態$\psi_a(x)$作測量，若所得到的結果是某一本徵值a。

測量使粒子的狀態由$\psi(x)$瞬間崩潰變成了$\psi_a(x)$。

$$\boxed{\psi(x) \xrightarrow[\hat{A}\to a]{} \psi_a(x)}$$

在非本徵狀態$\psi(x)$，測量結果不會是確定的！崩潰變成的態也就不確定。



$$\psi(x) = \sqrt{\frac{4}{5}}\left(\psi_a(x)\right) + \sqrt{\frac{1}{5}}\left(\psi_b(x)\right)$$

$P \sim \frac{4}{5}$

$\psi_a(x)$

$P \sim \frac{1}{5}$

$\psi_b(x)$