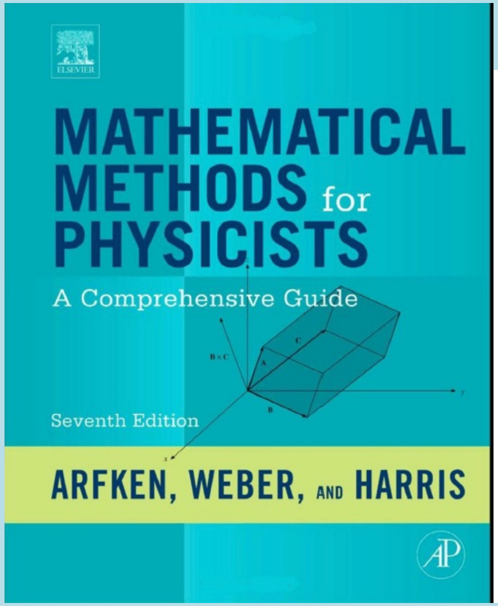
與時間無關的薛丁格方程式並不是波方程式，而是$\hat{H}$的本徵函數方程式！



CHAPTER 6

EIGENVALUE PROBLEMS

特徵值、本徵值

6.1 EIGENVALUE EQUATIONS 線性算子具有本徵函數 eigenfunction。

Many important problems in physics can be cast as equations of the generic form

$$A\psi = \lambda\psi, \tag{6.1}$$

where A is a linear operator whose domain and range is a Hilbert space, ψ is a function in the space, and λ is a constant. The operator A is known, but both ψ and λ are unknown, and the task at hand is to solve Eq. (6.1). Because the solutions to an equation of this type yield functions ψ that are unchanged by the operator (except for multiplication by a scale factor λ), they are termed **eigenvalue equations**: **Eigen** is German for "[its] own." A function ψ that solves an eigenvalue equation is called an **eigenfunction**, and the value of λ that goes with an eigenfunction is called an **eigenvalue**.

To see why eigenvalue equations are common in physics, let's cite a few examples:

1. The resonant standing waves of a vibrating string will be those in which the restoring force on the elements of the string (represented by $A\psi$) are proportional to their displacements ψ from equilibrium.
2. The angular momentum $\mathbf{L}$ and the angular velocity $\boldsymbol{\omega}$ of a rigid body are three-dimensional (3-D) vectors that are related by the equation

$$\mathbf{L} = \mathsf{I}\boldsymbol{\omega},$$

where I is the 3×3 moment of inertia matrix. Here the direction of $\boldsymbol{\omega}$ defines the axis of rotation, while the direction of $\mathbf{L}$ defines the axis about which angular momentum is generated. The condition that these two axes be in the same direction (thereby defining what are known as the **principal axes** of inertia) is that $\mathbf{L} = \lambda\boldsymbol{\omega}$, where λ is a proportionality constant. Combining with the formula for $\mathbf{L}$, we obtain

$$\mathsf{I}\boldsymbol{\omega} = \lambda\boldsymbol{\omega},$$

which is an eigenvalue equation in which the operator is the matrix I and the eigenfunction (then usually called an **eigenvector**) is the vector $\boldsymbol{\omega}$.
3. The time-independent Schrödinger equation in quantum mechanics is an eigenvalue equation, with A the Hamiltonian operator H, ψ a wave function and $\lambda = E$ the energy of the state represented by ψ.

定態解事實上是能量算子的eigenfunction。

動量算子$\hat{p}$定義為空間微分運算，那能量算子可以寫成：

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

$$\hat{p} \equiv -i\hbar\frac{d}{dx}$$

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

漢米爾頓、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與運算子之間的關係！

與古典力學中，這些物理量的關係一致。

薛丁格方程式就可以寫為：

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

$$\Downarrow$$

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

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。

量子力學的原則完整版

某一個瞬間時刻的狀態 $\longrightarrow$ 狀態函數 $\psi(x)$

物理量測量 $\longrightarrow$ 運算子 $\hat{A}$

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

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：

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

就得到量子力學對應的算子。

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

把對應算子放入此式就可得到測量期望值。

對一物理量$\hat{A}$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。

以上原則對每一個時間的瞬間都成立！

瞬間狀態隨時間演化 $\longrightarrow$ 波函數 $\Psi(x,t)$

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

狀態函數隨時間的演化由漢米爾頓量來負責！

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：

固定能量解ψ_E滿足與時間無關的薛丁格方程式可以寫成：

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

也就是：

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

Many important problems in physics can be cast as equations of the generic form

$$A\psi=\lambda\psi, \tag{6.1}$$

where A is a linear operator whose domain and range is a Hilbert space, ψ is a function in the space, and λ is a constant. The operator A is known, but both ψ and λ are unknown,

數學上這個關係稱為運算子$\hat{H}$的本徵函數問題！

原來，與時間無關的薛丁格方程式並不是波方程式，而是$\hat{H}$的本徵函數方程式！

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！

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。

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

$$= \left\langle \hat{H}^2 - 2\langle \hat{H} \rangle \hat{H} + \langle \hat{H} \rangle^2 \right\rangle = \langle \hat{H}^2 \rangle - 2\langle \hat{H} \rangle^2 + \langle \hat{H} \rangle^2 = \langle \hat{H}^2 \rangle - \langle \hat{H} \rangle^2$$

$$= \int_{-\infty}^{\infty} dx\, \psi_E^*(x) \cdot \hat{H}^2 \psi_E(x) - E^2 = E \int_{-\infty}^{\infty} dx\, \psi_E^*(x) \cdot \hat{H} \psi_E(x) - E^2 = E^2 - E^2 = 0$$

處於定態ψ_E的電子，能量的測量值為E，完全沒有不確定性！ $\Delta H = 0$

可以說定態ψ_E是具有特定確定能量的測量值為E的狀態。這是定態第三個意義。

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 $\hat{A} \rightarrow a$

直覺上，這個關係可以解讀為：算子作用於本徵態函數的效果與數一樣，

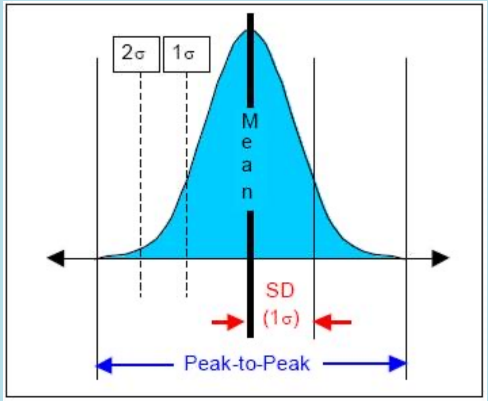
隱含：物理量$\hat{A}$測量時如古典量，也就是有確定的值。

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：



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

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

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

$$= a^2 \cdot \int_{-\infty}^{\infty} dx \cdot \psi_a^*(x) \psi_a(x) - a^2 = a^2 - a^2 = 0$$

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。

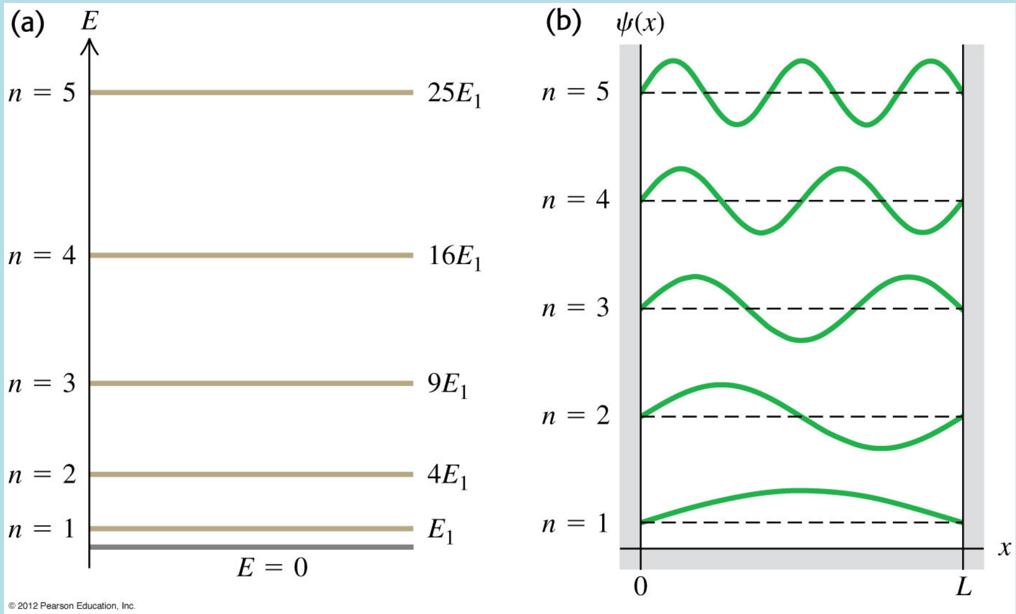
對一物理量測量結果確定的狀態就是該物理量算子$\hat{A}$的本徵態ψ_a。

以上結果適用於無限大位能井。

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

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

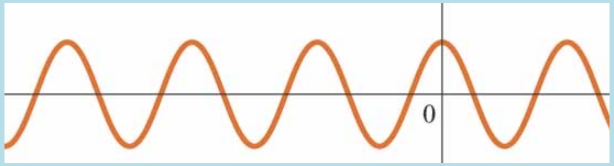
$$(\Delta H)^2 = 0$$



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！ $\Delta H = 0$

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！

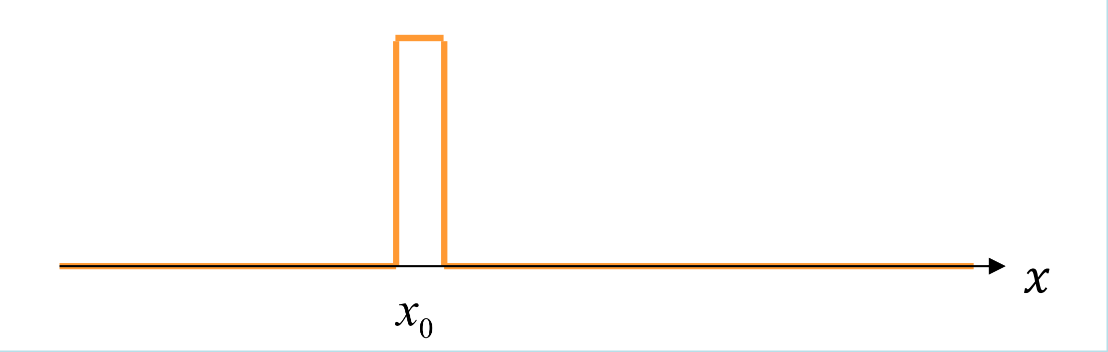
波函數是一個delta function！

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

這是位置算子$\hat{x}$的本徵函數：

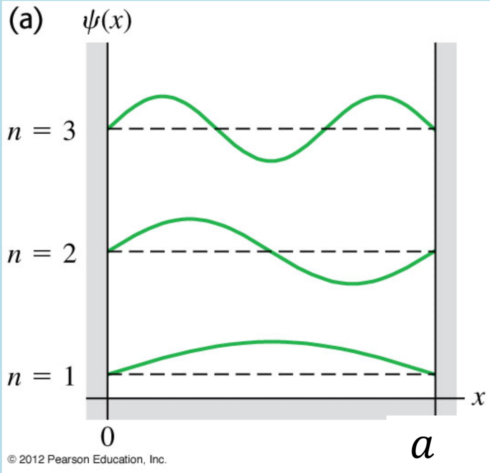
$$\hat{x}u_{x_0} = x \cdot \delta(x - x_0) = x_0 \cdot \delta(x - x_0) = x_0 \cdot u_{x_0}$$

$$\Delta x = 0$$



我們以無限位能井的能量本徵函數u_n為例，

來介紹任意算子的本徵函數普遍具有的幾個重要性質。



無限位能井的能量本徵函數u_n滿足正交定理，Orthogonality。

不同本徵值的本徵函數彼此正交！正交的意思是：

$$\int_{-\infty}^{\infty} dx \cdot u_n^*(x) u_m(x) = \delta_{mn}$$

$$\int_0^a dx\, u_n^*(x) u_m(x) = \int_0^a dx \frac{2}{a} \sin\frac{n\pi x}{a} \sin\frac{m\pi x}{a}$$

$$= \frac{1}{a}\int_0^a dx \left\{ \cos\frac{(n-m)\pi x}{a} - \cos\frac{(n+m)\pi x}{a} \right\}$$

$$= \frac{\sin(n-m)\pi}{(n-m)\pi} - \frac{\sin(n+m)\pi}{(n+m)\pi}$$

$$= 0 \qquad \text{when } n \neq m$$

$$= 1 \qquad \text{when } n = m$$ 歸一化

根據傅立葉分析，滿足邊界條件的任何函數$\psi(x)$，

都可以分解為正弦函數、也就是u_n的疊加！ 展開定理Expansion Theorem

$$\psi(x) = \sum_{n=1}^{\infty} C_n \sin\left(\frac{n\pi}{a}x\right) = \sum_{n=1}^{\infty} c_n u_n(x)$$

此展開神似向量以基底展開，讓我們沿用向量語言，把展開係數c_n稱為分量。

分量c_n可以利用u_n彼此正交的特性計算出來：

$$\int_{-\infty}^{\infty} dx \cdot u_n^*(x)\psi(x) = \int_0^a dx \cdot u_n^*(x)\left[\sum_{m=1}^{\infty} c_m u_m(x)\right]$$

代入ψ的展開。

$$= \sum_{m=1}^{\infty} c_m \int_0^a dx \cdot u_n^*(x) u_m(x) = \sum_{m=1}^{\infty} c_m \delta_{mn} = c_n$$

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

任何可行的狀態函數，都可以展開成能量的本徵函數u_n的疊加！

如同傅立葉分析，展開的分量c_n就包含原來狀態函數$\psi(x)$的所有資訊！

以上的結果與求向量的分量的方法神似：

$$\vec{a} = \sum_{n=1}^{l} a_n \hat{\imath}_n$$

幾何上，分量就是向量沿單位向量的投影。

$$a_m = \hat{\imath}_m \cdot \vec{a}$$

代數上，此式可以如下得到：

$$\hat{\imath}_m \cdot \vec{a} = \hat{\imath}_m \cdot \sum_{n=1}^{l} a_n \hat{\imath}_n$$

$$\hat{\imath}_m \cdot \hat{\imath}_n = \delta_{mn}$$

$$= \sum_{n=1}^{l} a_n (\hat{\imath}_m \cdot \hat{\imath}_n) = \sum_{n=1}^{l} a_n \delta_{mn} = a_m$$

一系列能量的本徵函數u_n滿足：

展開定理：任一狀態ψ可以u_n作展開。展開讓我們聯想到向量以基底展開：

$$\psi(x) = \sum_n [c_n \cdot u_n(x)] \quad \Rightarrow \quad \vec{a} = \sum_{m=1}^{l} a_m \hat{\imath}_m$$

正交定理：本徵函數彼此正交。這很像一組彼此正交的基底！

$$\int_{-\infty}^{\infty} dx \cdot u_m(x)^* \cdot u_n(x) = \delta_{mn} \quad \Rightarrow \quad \hat{\imath}_m \cdot \hat{\imath}_n = \delta_{mn}$$

分量c_a可以寫成態函數與本徵函數的空間積分:

$$c_n = \int_{-\infty}^{\infty} dx \cdot u_n(x)^* \cdot \psi(x) \quad \Rightarrow \quad a_m = \vec{a} \cdot \hat{\imath}_m$$

把狀態視為向量，展開與正交定理，就如同向量空間的向量分析一模一樣！

能量的本徵函數u_n形成一組完整的基底。

任一狀態函數可以此基底作展開，疊加係數c_n就如同向量對一組基底的分量。

一系列能量的本徵函數u_n滿足：

展開定理：任一狀態ψ可以u_n作展開。展開讓我們聯想到向量以基底展開：

$$\psi(x) = \sum_n [c_n \cdot u_n(x)] \quad \rightarrow \quad \vec{a} = \sum_{m=1}^{l} a_m \hat{\imath}_m$$

正交定理：本徵函數彼此正交。這很像一組彼此正交的基底！

$$\boxed{\int_{-\infty}^{\infty} dx \cdot u_m(x)^* \cdot u_n(x)} = \delta_{mn} \quad \rightarrow \quad \boxed{\hat{\imath}_m \cdot \hat{\imath}_n} = \delta_{mn}$$

分量c_a可以寫成態函數與本徵函數的空間積分:

$$c_n = \boxed{\int_{-\infty}^{\infty} dx \cdot u_n(x)^* \cdot \psi(x)} \quad \rightarrow \quad a_m = \boxed{\vec{a} \cdot \hat{\imath}_m}$$

在這對應中，最關鍵的是：我們熟悉的積分，在這向量空間內就是內積：

$$\int_{-\infty}^{\infty} dx \cdot \psi(x)^* \cdot \phi(x) \quad \rightarrow \quad \vec{a} \cdot \vec{b}$$

這一展開式提供對無限大位能井位能下薛丁格波方程式的普遍解法：

將$t = 0$時的波函數，即起始條件，對定態解u_n展開如下：

$$\Psi(x,0) = \sum_{n=1}^{\infty} c_n u_n(x)$$

根據展開定理，這永遠可以做到！

$t = 0$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$e^{-i\frac{E_n}{\hbar}t}$。

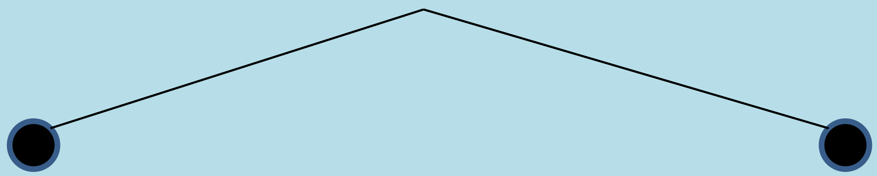
乘完之後依同樣方式疊加，整個波函數也就滿足薛丁格波方程式。

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n u_n(x) e^{-i\frac{E_n}{\hbar}t}$$

我們已經在自由薛丁格方程式用了這樣的策略！當時的正弦波就是定態。

很明顯，這個程序不只適用於無限大位能井，原則上適用於任何位能。

兩端固定的弦的任一起始條件可以用駐波模式來疊加：例如下圖：



$$\Psi(x,0) = \sin\frac{\pi}{a}x - \frac{1}{9}\sin\frac{3\pi}{a}x + \cdots$$

如果這是波函數的起始條件$\Psi(x,0)$，它可以同樣以$u_n(x)$展開。

各個定態就會各自演化後再疊加。

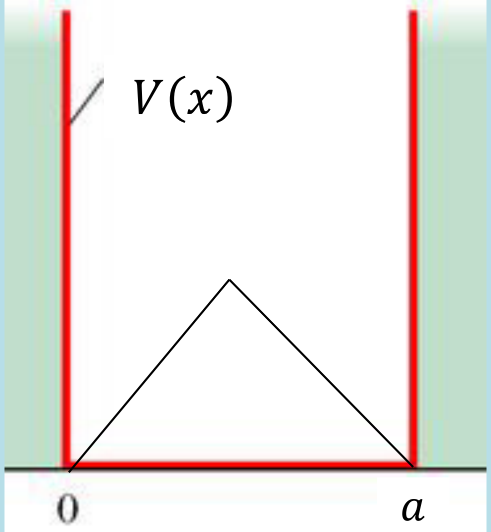
$$\Psi(x,t) \sim \sin\frac{\pi}{a}x\, e^{-i\frac{E_1}{\hbar}t} - \frac{1}{9}\sin\frac{3\pi}{a}x\, e^{-i\frac{E_3}{\hbar}t} + \cdots$$

EXAMPLE 3-5

Consider a particle in a box. Its wave function is given by

$$\psi(x) = A(x/a) \qquad 0 < x < a/2$$
$$= A(1 - x/a) \qquad a/2 < x < a$$

where $A = \sqrt{12/a}$ so as to satisfy $\int_0^a dx|\psi(x)|^2 = 1$. Calculate the probability that a measurement of the energy yields the eigenvalue E_n.



SOLUTION We want to calculate A_n in the expansion

$$A_n = \int_0^a dx\, \psi(x) \sqrt{\frac{2}{a}} \sin\frac{n\pi x}{a}$$

$$= \frac{\sqrt{24}}{a}\left[\int_0^{a/2} dx \left(\frac{x}{a}\right) \sin\frac{n\pi x}{a} + \int_{a/2}^{a} dx \left(1 - \frac{x}{a}\right) \sin\frac{n\pi x}{a}\right]$$

With the change of variables $\pi x/a = u$ in the first integral and $\pi x/a = \pi - u$ in the second integral, we get

$$A_n = \frac{\sqrt{24}}{\pi}\int_0^{\pi/2} du\, \frac{u}{\pi} \sin nu(1 - (-1)^n)$$

The A_n for n even vanish because of the last factor. The integral is easily calculated, and we get, *for n odd only,*

$$\boxed{A_n = \frac{\sqrt{24}}{\pi} 2 \frac{1}{\pi n^2}(-1)^{n+1}}$$

$$c_n \sim \frac{1}{n^2}$$

so that

$$|A_n|^2 = \frac{96}{\pi^4 n^4} \qquad \text{for } n \text{ odd}$$
$$= 0 \qquad \text{for } n \text{ even}$$

One can easily check, using the fact that $\sum_{\text{all}} n^{-4} = \pi^4/90$ and

$$\sum_{\text{all}} n^{-4} = \sum_{\text{even}} n^{-4} + \sum_{\text{odd}} n^{-4} = \sum_{\text{odd}} n^{-4} + (1/16)\sum_{\text{all}} n^{-4}$$

that the sum of all the probabilities is 1:

$$\frac{96}{\pi^4}\sum_{\text{odd}} n^{-4} = \frac{96}{\pi^4}\left(1 - \frac{1}{16}\right)\sum_{\text{all}} n^{-4} = \frac{96}{\pi^4}\cdot\frac{15}{16}\cdot\frac{\pi^4}{90} = 1$$

Example 6.3. The expanding box

As a further example, let us consider the case of a particle in the symmetric well, known somehow to be in its ground state. *Very suddenly*, at $t = 0$, the walls are pulled apart symmetrically to a new width $2b$ (where $b > a$). (This is in contrast to P5.21 where slow or adiabatic changes were discussed.)

The initial wavefunction of the particle in this new well (see Fig. 6.3 for the situation at $t = 0$), defined via

$$\psi(x,0) = \begin{cases} u_1^{(+)}(x;a) = \cos(\pi x/2a)/\sqrt{a} & \text{for } |x| < a \\ 0 & \text{for } a < |x| < b \end{cases} \tag{6.52}$$

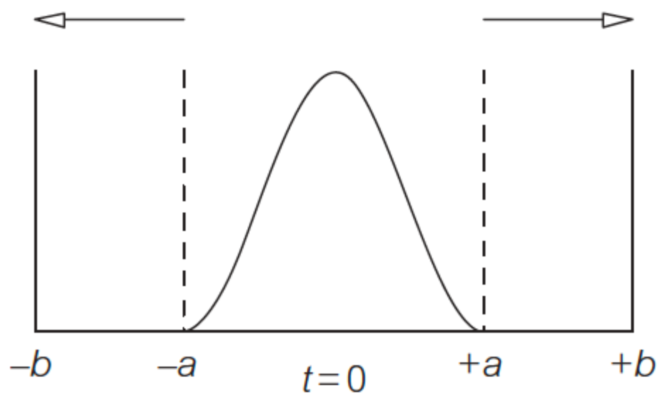


Figure 6.3. Initial state wavefunction of the "expanded well" state of Example 6.3 where the walls are suddenly moved from $\pm a$ to $\pm b$.

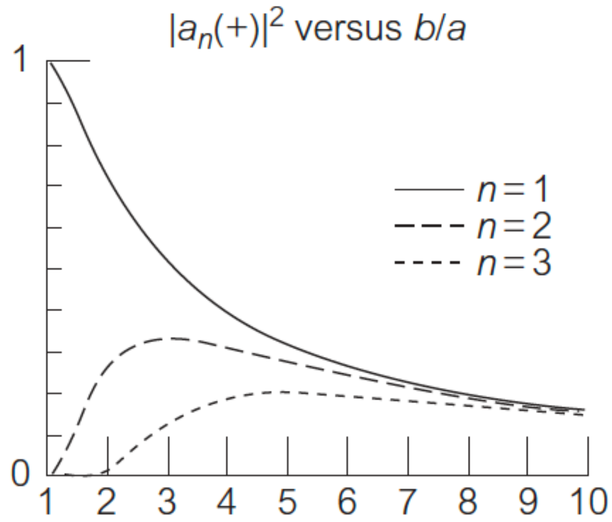


Figure 6.4. Expansion coefficients squared ($|a_n|^2$) for first three even levels versus b/a from Example 6.3.

can now be expanded in terms of the energy eigenstates of its new "universe" (the new well), that is, in terms of the $u_n^{(\pm)}(x; b)$. The result is that

$$a_n^{(-)} = 0 \qquad \text{and} \qquad a_n^{(+)} = \frac{4ab^2}{\pi\sqrt{ab}}\left(\frac{\cos((2n-1)\pi a/2b)}{(b^2-(2n-1)^2a^2)}\right) \tag{6.53}$$

Once again, the odd state expansion coefficients vanish because of symmetry considerations. We plot the probabilities of finding the particle in the ground state, and first and second excited *even* states of the new well versus b/a in Fig. 6.4; as $b/a \rightarrow 1$, only the original ground state is required.

Having once calculated the expansion coefficients for the given initial waveform, the future time-dependence of each term is dictated solely by the $\exp(-iE_n^{(\pm)}t/\hbar)$ factors. The wavefunction at later times is then given by

$$\psi(x,t) = \sum_{n=1}^{\infty} a_n^{(+)} \frac{1}{\sqrt{b}} \cos\left(\frac{(n-1/2)\pi x}{b}\right) e^{-iE_n^{(+)}(b)t/\hbar} \tag{6.54}$$

and we plot in Fig. 6.5 the resulting probability density (given by $|\psi(x,t)|^2$) for various future times. Because of the simplicity of the infinite well (specifically its energy eigenvalues), the behavior is periodic, and we plot various times during the first half-cycle only; it need not be exactly periodic in a general potential.

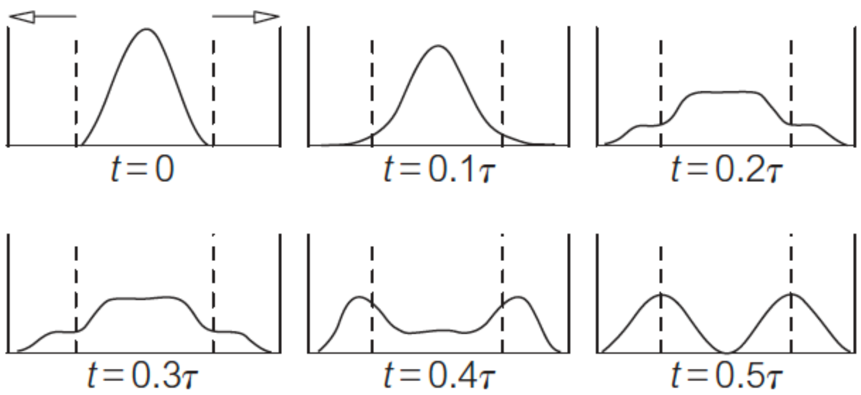


Figure 6.5. Time-development of "expanded well" system illustrated by plots of $|\psi(x,t)|^2$ versus x for various times in the first half-cycle.

例如：無限大位能井中波包隨時間的演化：將波包以u_n展開。
別忘了在位能井內，u_n就是兩個自由電子波的組合。

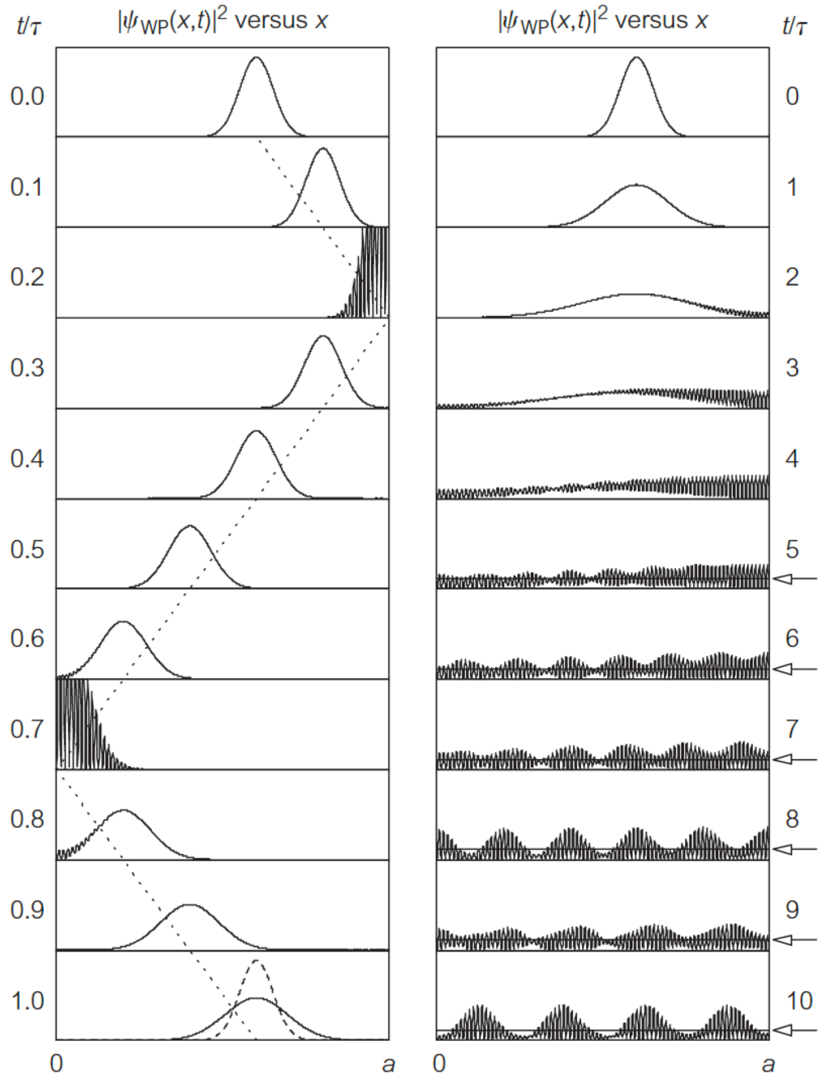


Figure 5.9. Time-development of $|\psi(x,t)|^2$ versus x for a Gaussian-like wave packet in the standard infinite well, over one classical period (left) and 10 classical periods (right); the classical periodicity and the spreading time (t_0) are chosen to be comparable. The classical trajectory is shown as the dotted line. The classical probability density, $P_{CL}(x) = 1/a$ is shown on the right as the horizontal solid line, indicated by the arrows for later times.

別忘了在位能井內，u_n就是兩個自由電子波的組合。

Motivated by the Gaussian wave packet of Section 3.2.2, we can write a solution involving stationary states of the standard infinite well given by

$$\psi_{\mathrm{WP}}(x,t) = \sum_{n=1}^{\infty} a_n u_n(x)\, e^{-iE_n t/\hbar} \tag{5.76}$$

where we choose coefficients of the form

$$a_n = e^{-((p_n-p_0)^2\alpha^2/2)}\, e^{-ip_n x_0/\hbar} \tag{5.77}$$

Here $p_n \equiv \hbar n\pi/a$ is the analog of the continuous momentum variable and $p_0 \equiv \hbar n_0\pi/a$ defines some central value of n, while this form also allows for arbitrary values of the central peak position, x_0. (For a more complete discussion, see

Example 6.4. Gaussian wave packets in the standard infinite well

While the general Gaussian wave packet discussed in Chapter 3 (especially as defined in Eqn. (3.35)) is a very useful example, it is not strictly an allowable quantum state in the standard infinite well, since it does not satisfy the boundary conditions that $\psi(0,t) = \psi(a,t) = 0$. However, for a sufficiently narrow initial wave packet, far enough from either wall, the error made in neglecting the "tails" of the Gaussian wave packet outside the well can be made arbitrarily (exponentially) small. In order to extract the expansion coefficients of a Gaussian initial state (with $b \equiv \hbar\alpha$) given by

$$\psi_{(G)}(x,0) = \frac{1}{\sqrt{b\sqrt{\pi}}}\, e^{-(x-x_0)^2/2b^2}\, e^{ip_0(x-x_0)/\hbar} \tag{6.55}$$

placed inside the standard infinite well, we require the overlap integrals

$$a_n = \int_0^a u_n(x)\, \psi_G(x,0)\, dx \tag{6.56}$$

where we again use the fact that the $u_n(x)$ are real. Since the integral is assumed to be exponentially small outside the $(0,a)$ interval, we can extend the region of integration to $(-\infty,+\infty)$ with negligible error. This is important since the resulting Gaussian integrals can be done in closed form, giving

$$a_n \approx \frac{1}{\sqrt{b\sqrt{\pi}}} \int_{-\infty}^{+\infty} \left[\sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right)\right] e^{-(x-x_0)^2/2b^2} e^{ip_0(x-x_0)/\hbar} dx$$
$$= \left(\frac{1}{2i}\right)\sqrt{\frac{4b\pi}{a\sqrt{\pi}}} \left[e^{in\pi x_0/a} e^{-b^2(p_0+n\pi\hbar/a)^2/2\hbar^2} - e^{-in\pi x_0/a} e^{-b^2(p_0-n\pi\hbar/a)^2/2\hbar^2}\right] \tag{6.57}$$

(Note that in Section 5.4.2 we used an approximate, unnormalized version of this more precise result; the plots in Fig. 5.9 were obtained using the values in Eqn. (6.57).) The general time-dependent wavefunctions, in position- and momentum-space can then be written as

$$\psi_{WP}(x,t) = \sum_{n=1}^{\infty} a_n u_n(x)\, e^{-iE_n t/\hbar} \quad \text{and} \quad \phi_{WP}(p,t) = \sum_{n=1}^{\infty} a_n \phi_n(p)\, e^{-iE_n t/\hbar} \tag{6.58}$$

and while the sums are formally infinite, the contributions are peaked about values of n for which $p_n = n\hbar\pi/a \approx p_0$. We can also make use of this connection to estimate the number of states necessary to approximate the state by noting that

$$\frac{\hbar}{2\Delta x_0} = \frac{\hbar}{\sqrt{2}b} = \Delta p = \frac{\pi\hbar}{a}\Delta n \qquad \text{or} \qquad \Delta n = \frac{a}{2\pi\,\Delta x_0} \tag{6.59}$$

so that the narrower the initial wave packet, the larger the number of states required to reproduce it faithfully.

狀態函數$\psi(x)$的展開分量的物理意義

之前曾大膽假設，電子在狀態$\Psi(x,0)$測量動量時，得到某p的機率，即是$\Psi(x,0)$的傅立葉變換$\phi(p)$的絕對值平方：$|\phi(p)|^2$。

傅立葉變換$\phi(p)$就是展開的分量！

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

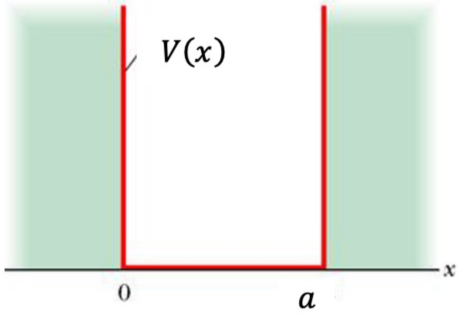
自然的猜測：對於以能量本徵函數u_n展開的狀態函數$\psi(x)$，

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

$|c_n|^2$就是在$\psi(x)$狀態，測量能量時得到結果是E_n的機率！

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.

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

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

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

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

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

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

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

測量結果 機率

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:

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

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.

解答：

A. $\Psi(x,0) = \sqrt{\frac{4}{5}}\left(\sqrt{\frac{2}{a}}\sin\frac{\pi x}{a}\right) + \sqrt{\frac{1}{5}}\left(\sqrt{\frac{2}{a}}\sin\frac{2\pi x}{a}\right) = \sqrt{\frac{4}{5}}u_1(x) + \sqrt{\frac{1}{5}}u_2(x)$. The wave function is a superposition of the eigenfunction u_1, u_2 of eigenvalues E_1, E_2, with amplitudes $c_1 = \sqrt{\frac{4}{5}}$, $c_2 = \sqrt{\frac{1}{5}}$, $c_n = 0, n > 2$. You can simply see it from the formula or use the formula $c_n = \int_{-\infty}^{\infty} dx \cdot u_n(x)^* \cdot \psi(x)$ and orthogonality theorem $\int_{-\infty}^{\infty} dx \cdot u_m(x)^* \cdot u_n(x) = \delta_{mn}$ to get it. The energy could only be E_1 or E_2. The corresponding probabilities are the square of the magnitudes c_1 and c_2: $\frac{4}{5}$ and $\frac{1}{5}$ 。

我們可以利用計算在此狀態ψ下能量的期望值來驗證以上猜測！

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

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

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

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

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

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

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

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

可見$|c_n|^2$就是測量能量時，得到結果是E_n的機率！

波函數沿本徵函數u_n的展開分量c_n，就是對$\hat{H}$測量得到結果是E_n的振幅。

Measurement Theorem 測量定理

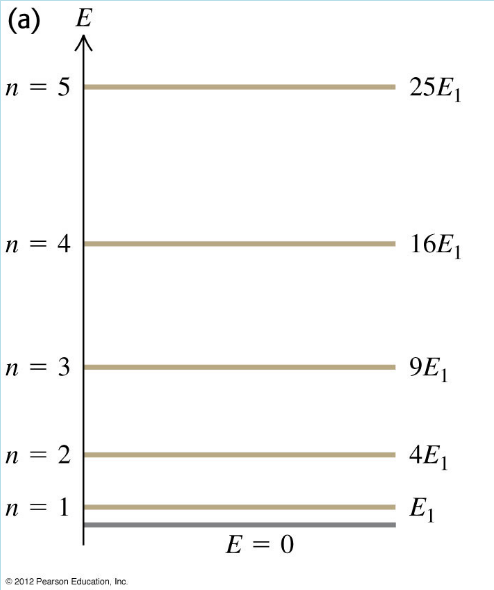
這強烈暗示測量能量時，得到結果只能是E_n其中之一！不會測到其他的值。

如果真是如此，機率總和必須等於1！

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

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

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



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

沒有遺漏，可見對能量的測量結果只能是本徵值E_n其中之一，不能是其他的值。

如果還會測到其他值，總機率就要超過1了！

到此，無限大位能井內的電子，不一定是在定態，能量的量子化完全確立！

$\psi(x)$

$\hat{\mathcal{A}}$

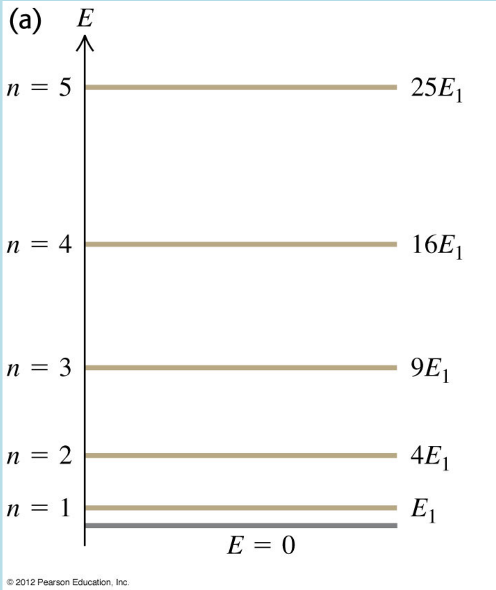
不同的狀態下，機率的分佈不同！

但可能的結果卻一樣！

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

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！



算子有它的堅持！

解eigenfunction、例如能量算子的定態，是在決定你測量時會得到什麼結果。

得到某結果時粒子的狀態會崩潰為何種狀態。

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，立刻再作一次能量的測量，結果一定確定還是E_n，

測量第一次完畢後，狀態已經不會再是結果不確定的狀態$\psi(x)$，

而是結果完全確定的本徵函數$u_n(x)$。

所以第一次的測量使粒子的狀態由$\psi(x)$瞬間崩潰變成了$u_n(x)$。

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

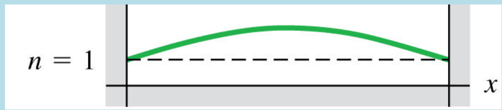
在特定狀態，每一個初次測量結果不會是確定的！

崩潰變成的態也就不確定。

$$\Psi(x,0) = \sin\frac{\pi}{a}x - \frac{1}{9}\sin\frac{3\pi}{a}x + \cdots$$

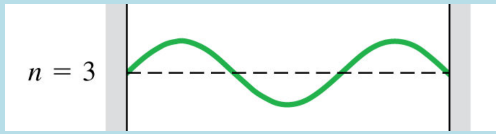
$$E = E_1 = \left(\frac{\hbar^2}{2m}\right)\frac{\pi^2}{a^2}$$

$P_1 \sim 1$



$E = E_3$

$P_3 \sim \dfrac{1}{81}$



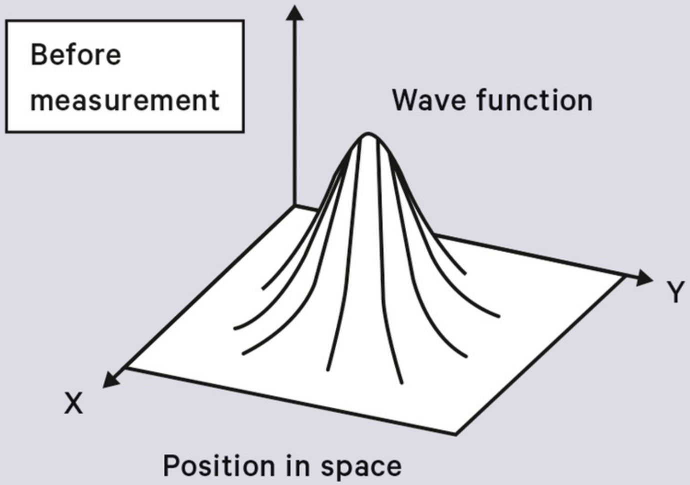
$\cdots$

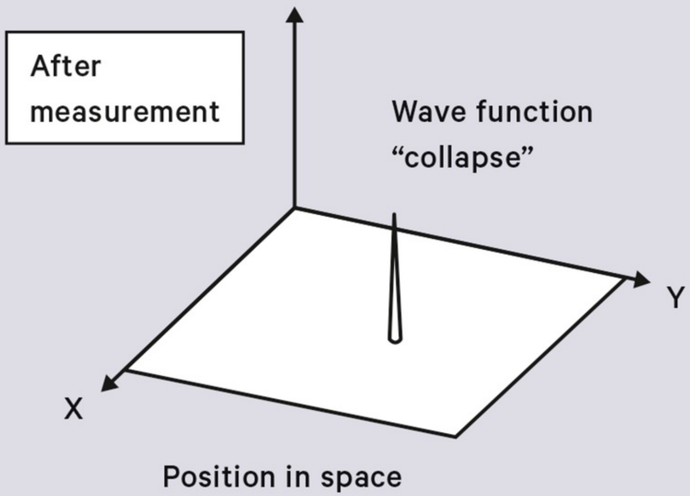
但不會測到E_{2m}。

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。

THE COPENHAGEN INTERPRETATION

The act of measurement causes all the possible positions of the wave function to collapse into a single point. What happens to the other positions? According to Hugh Everett, they split off into other worlds.

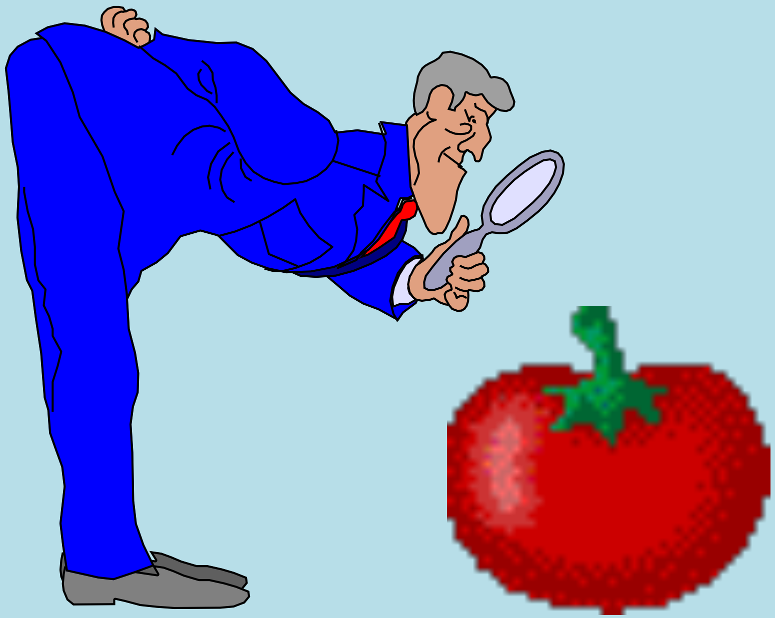




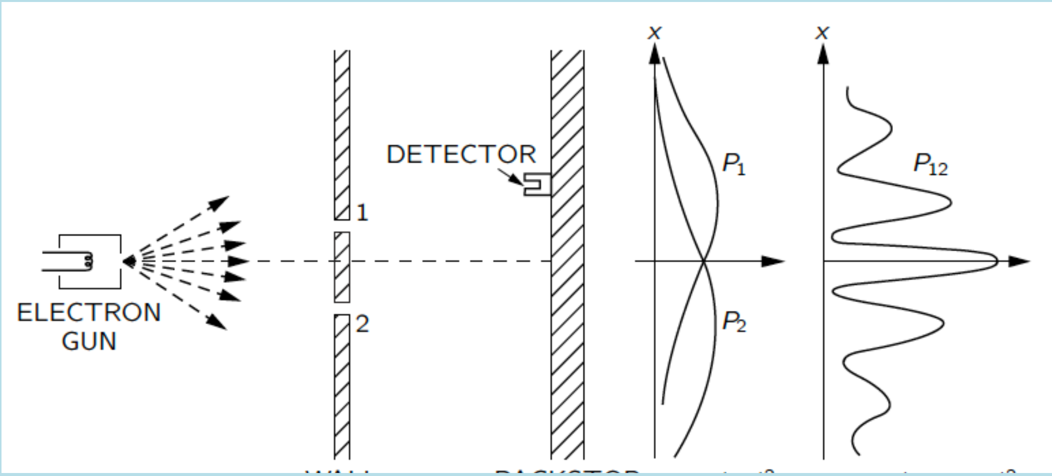
古典力學假設物體的性質如位置，是獨立於觀察的行為而客觀存在的。

看不看它都存在！

因此觀察者可以以不擾動對象的方式來觀察！



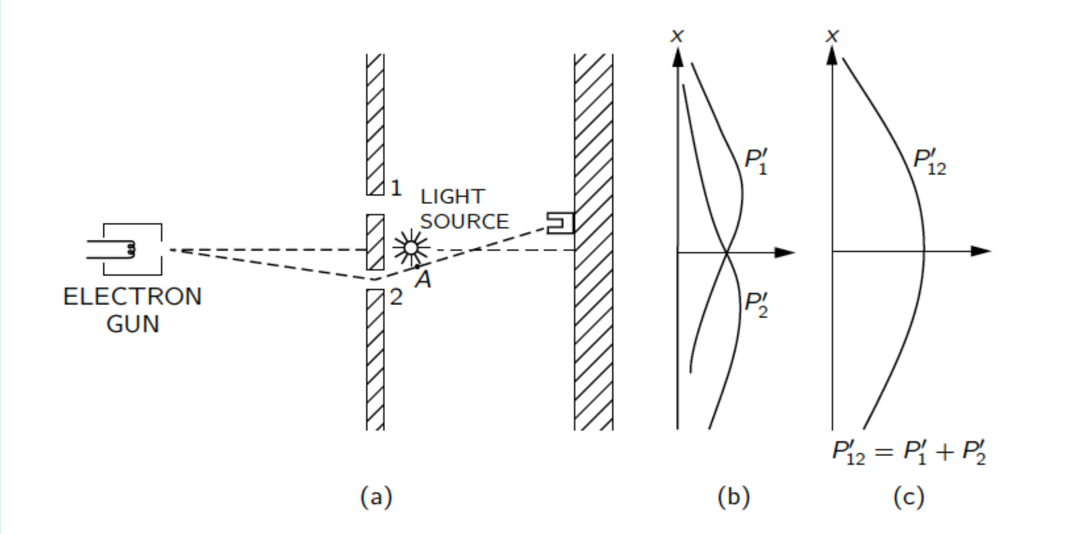
電子位置的測量：



電子在到達狹縫時沒有特定的位置可言，

但看到電子，就是對電子位置的測量！

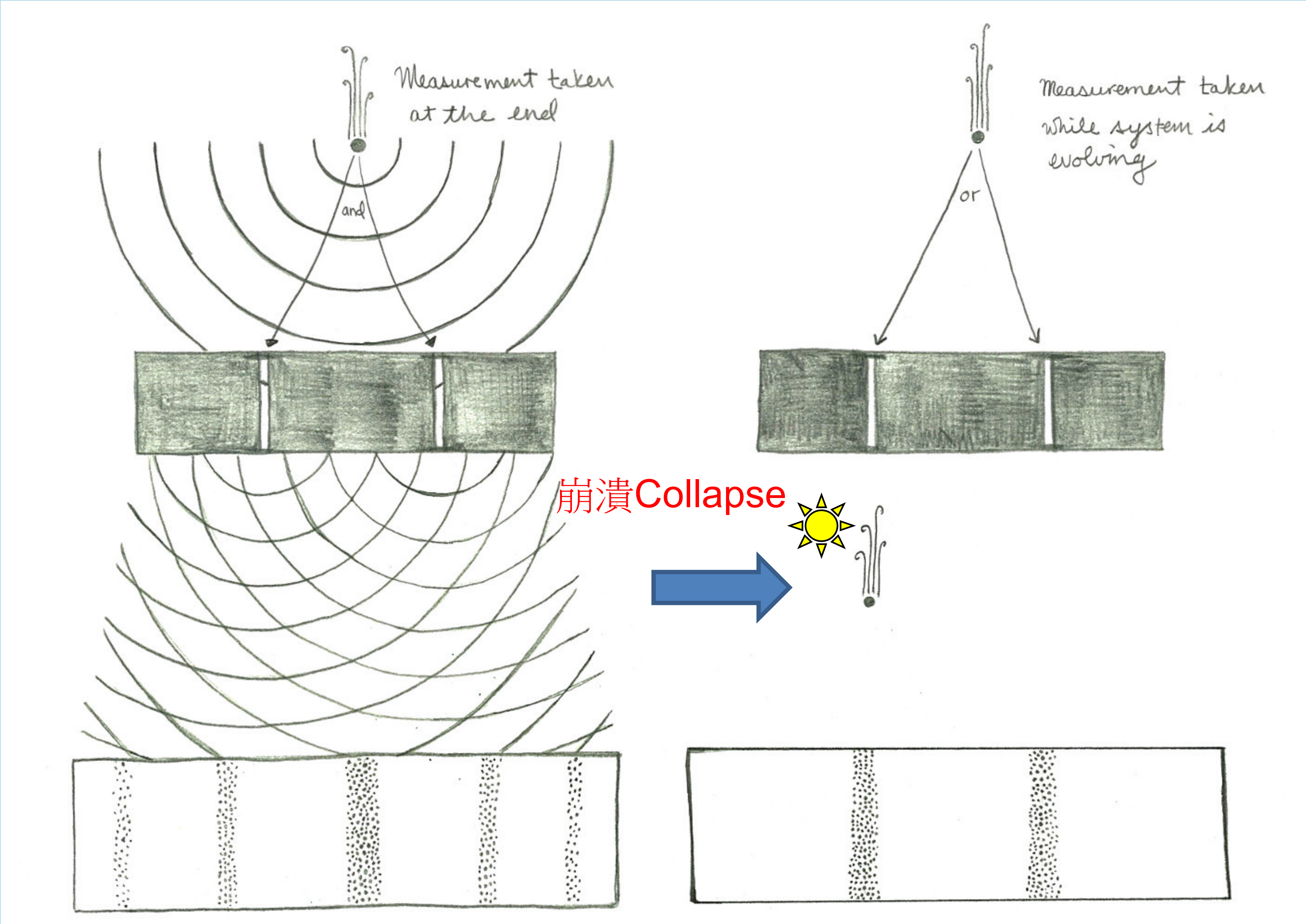
在狹縫處對位置的觀測改變了電子的狀態



剛到達狹縫的電子，並無特定位置，波狀的態： $\Delta x \to \infty, \Delta p = 0$

在狹縫剛測完位置的電子，當然有特定位置！粒子狀的態： $\Delta x = 0, \Delta p \to \infty$

以燈光對位置的測量，強迫電子由波狀的態崩潰為粒子狀的態。

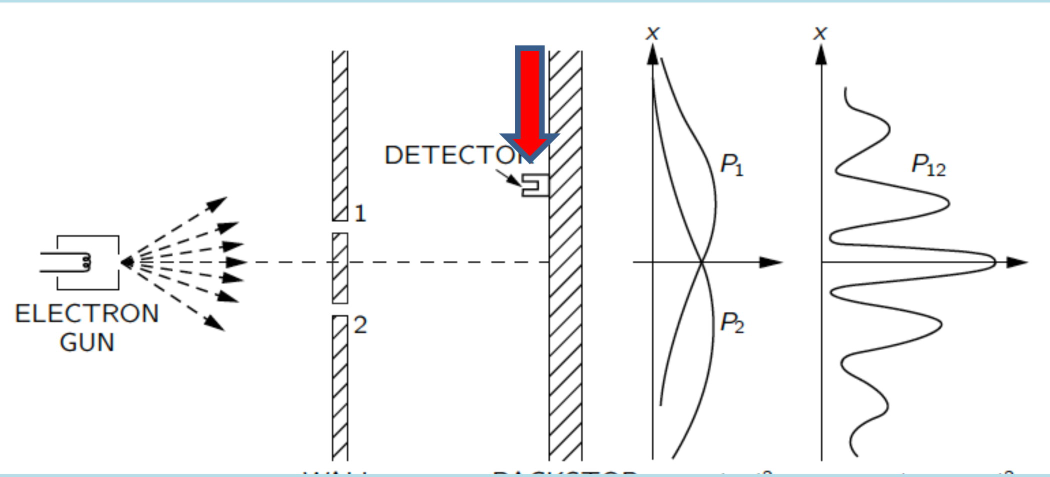

Measurement taken at the end
and
Measurement taken while system is evolving
or
崩潰Collapse

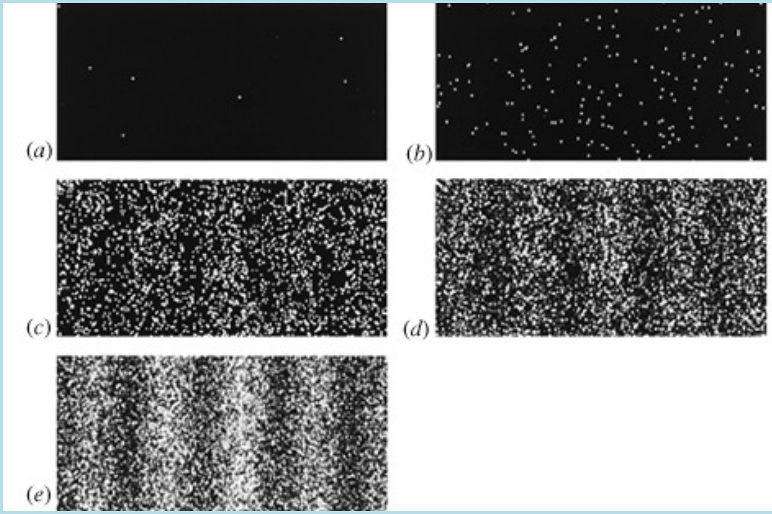
這也是標準干涉實驗中（未在狹縫處測位置）發生於觀察屏幕的狀況：

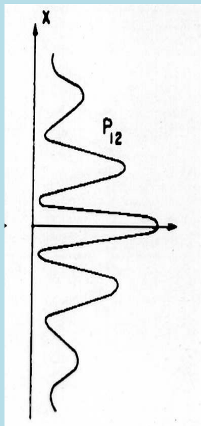
觀察屏幕即是對位置的測量

觀察屏幕強迫電子崩潰為粒子狀的態，

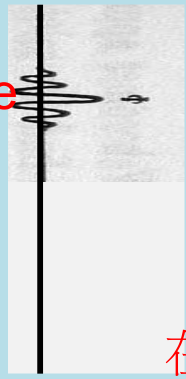
崩潰為特定位置的粒子態的機率即是波函數的強度！



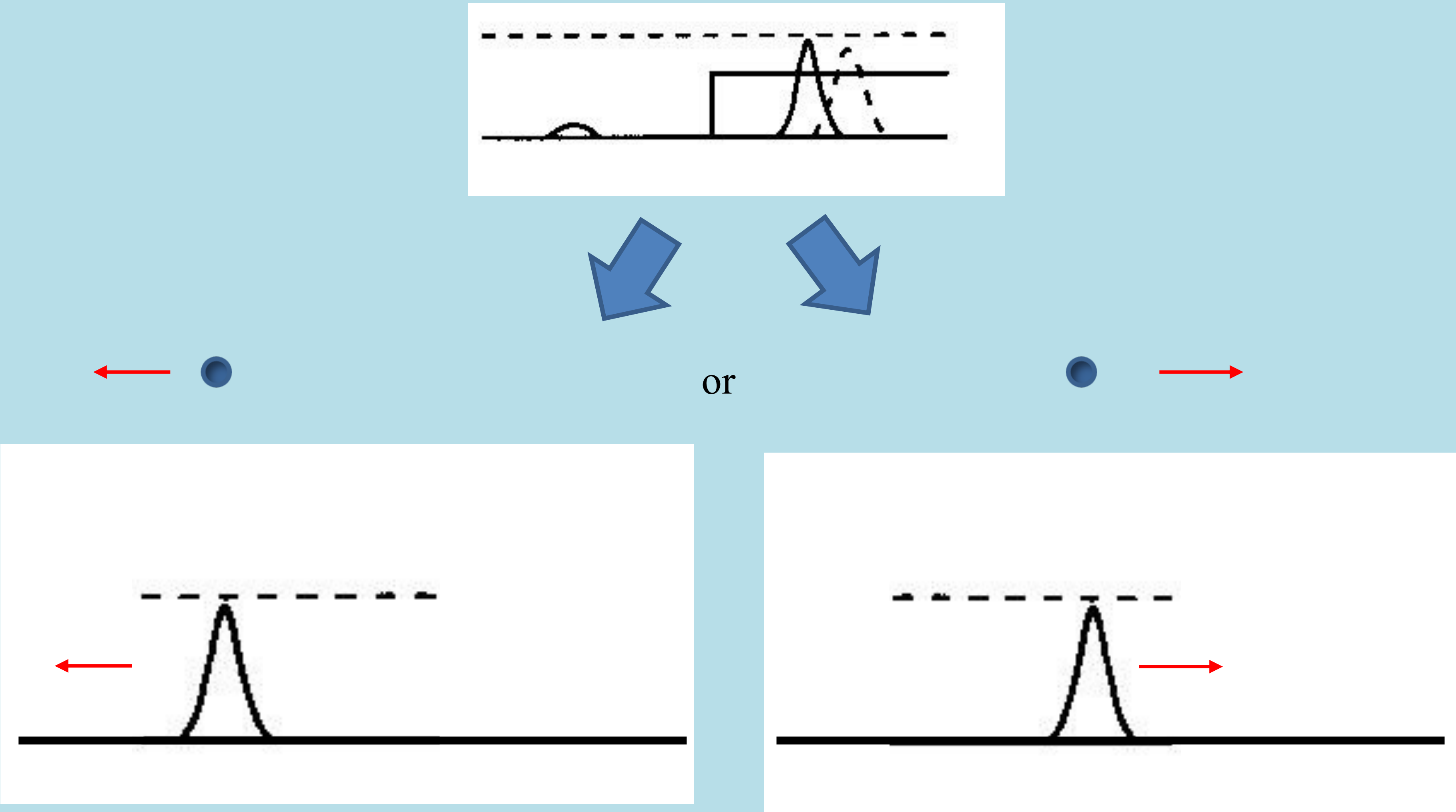




崩潰Collapse



在屏幕處對位置的觀測改變了電子的狀態！！



對位置的測量，強迫電子由包含兩個反向移動波包的波，
崩潰為有特定位置的波包，也就是粒子狀的態。

畢竟測量得有個測量值！如果立刻重測應該沒有不確定性。

測量本身強迫粒子狀態崩潰Collapse到此測量有特定值的狀態。

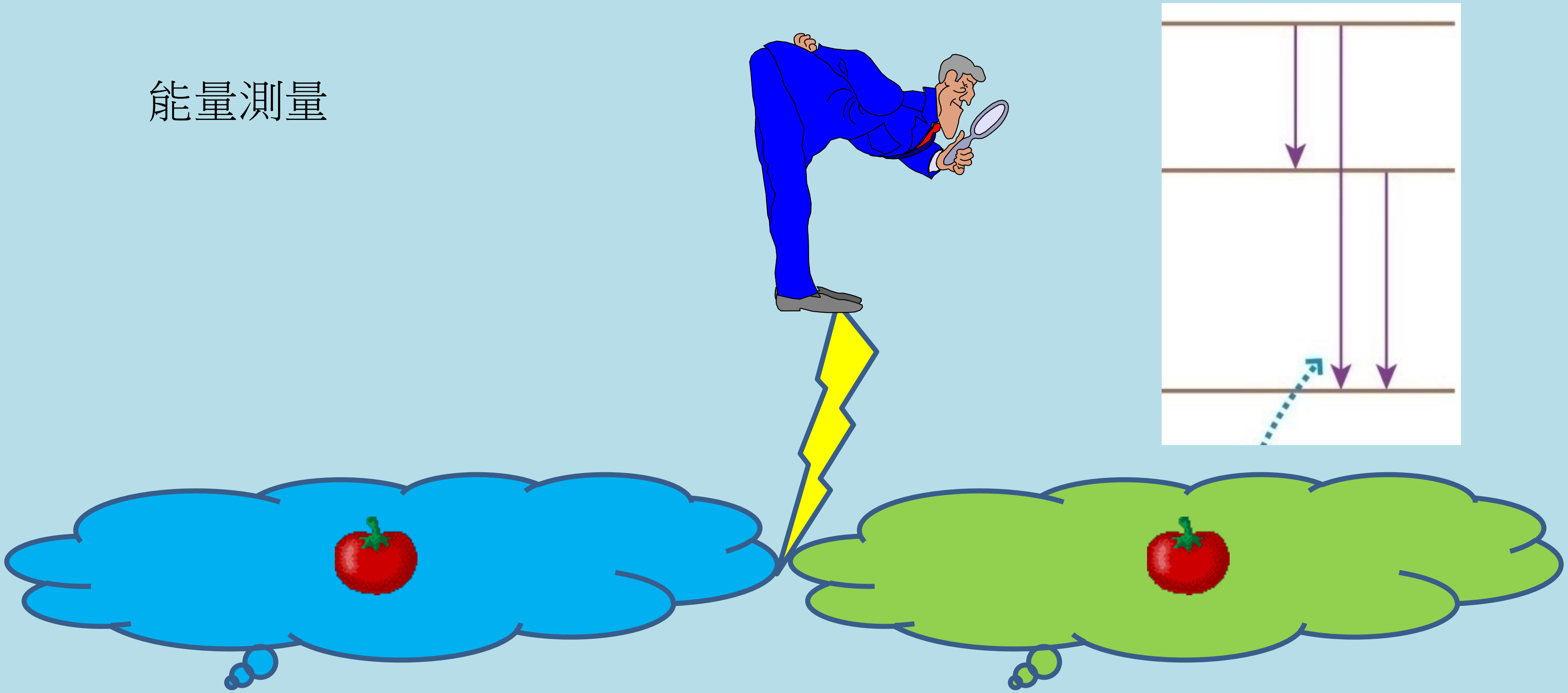
不同的測量會使粒子狀態崩潰到不同類的狀態！

測量動量就得崩潰動量有定值的狀態！ $\Delta p = 0$ 稱動量的本徵態，波狀的態。

測量位置就得崩潰位置有定值的狀態！ $\Delta x = 0$ 稱位置的本徵態， 粒子狀的態。

削足適履

能量測量



或者之前獨立演化的微觀系統。

在巨觀儀器干擾後，躍遷至另一狀態。

例如：電磁場可以引發一顆光子的放射吸收，

會使原本穩定的定態，可以躍遷到其他的定態。

在躍遷之前之後，獨立的微觀系統維持處於一定態！

量子世界特性三：所有有效的測量本質上必然擾動被觀察的系統！

實驗者即使再如何努力小心，都不可能是完全的客觀旁觀者，

他的觀察本質上就影響了粒子的表現。

量子世界特性一：一個粒子處於完全相同的狀態下，某些物理測量卻不是每次得到的結果都相同。

在確定狀態下，測量結果卻並不確定。

不確定結果的機率分布是確定而可以預測的。

量子世界特性二：電子的位置與動量不能同時精確測量，位置精確測定的態與動量精確測定的態是不相容的，因此電子的狀態是多面向的！

量子世界特性三：所有有效的測量本質上必然擾動被觀察的系統！

微觀物理有內在無法克服的不確定性！

以上這些性質也適用於一般算子$\hat{A}$的本徵函數！

正交定理

$\hat{A}$ 的所有本徵函數 $\psi_a(x)$彼此正交。本徵值a即足標。

$$\int_{-\infty}^{\infty} dx \cdot \psi_a(x)^* \cdot \psi_b(x) \ = \delta_{ba}$$

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

$$= \int_{-\infty}^{\infty} dx \cdot \left[\hat{A}\psi_a(x)\right]^* \cdot \psi_b(x) \ = a \int_{-\infty}^{\infty} dx \cdot \psi_a(x)^* \cdot \psi_b(x)$$

$$a \neq b \quad \int_{-\infty}^{\infty} dx \cdot \psi_a(x)^* \cdot \psi_b(x) = 0$$

$$\langle \psi_a, \psi_b \rangle = \delta_{ab}$$

以上證明用到算子$\hat{A}$的這個性質：

$$\int_{-\infty}^{\infty} dx \cdot \phi^*(x) \cdot \hat{A}\psi(x) = \int_{-\infty}^{\infty} dx \cdot \left[\hat{A}\phi(x)\right]^* \cdot \psi(x)$$

很多時候算子也可以看成作用在左邊的狀態函數上，例如$\hat{x}$算子：

$$\int_{-\infty}^{\infty} dx \cdot \phi(x)^*[x\psi(x)] = \int_{-\infty}^{\infty} dx \cdot [x\phi]^*\psi$$

$\hat{p}$算子也是：

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

具有這樣性質的算子稱為Hermitian：

$$\int_{-\infty}^{\infty} dx \cdot \phi(x)^*\left[\hat{A}\psi(x)\right] = \int_{-\infty}^{\infty} dx \cdot \left[\hat{A}\phi\right]^*\psi$$

Hermitian算子的期望值永遠是實數!

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

可測量的物理量由 Hermitian算子代表！

本徵值就是本徵態的期望值，Hermitian算子的期望值是實數！

因此Hermitian算子的本徵值必是實數。

展開定理：

任一狀態向量ψ可以此 $\hat{A}$ 本徵函數組成的基底作分量展開。

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

狀態向量在此基底的分量c_a可以寫成波函數與本徵函數的空間積分:

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

$$c_a = \langle \psi_a, \psi \rangle$$

$$\int_{-\infty}^{\infty} dx \cdot \psi_a(x)^* \cdot \psi(x) = \int_{-\infty}^{\infty} dx \cdot \psi_a(x)^* \cdot \sum_b [c_b \cdot \psi_b(x)]$$
$$= \sum_b \left[c_b \cdot \int_{-\infty}^{\infty} dx \cdot \psi_a(x)^* \cdot \psi_b(x) \right] = \sum_b [c_b \cdot \delta_{ba}] = c_a$$

一算子的本徵函數形成一組完整的基底，其線性疊加組成一向量空間。

一波函數以此基底作展開，疊加係數就如同一向量對一組基底的分量。

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！

狀態向量ψ（在此 $\hat{A}$ 本徵函數組成的基底）沿 $\psi_a(x)$ 的分量 c_a

= 對應於 $\hat{A}$ 測量得到結果是 a 的振幅 。

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

Measurement Theorem Generalized 推廣

$\hat{A}$測量得到結果是a的振幅，等於狀態向量ψ沿ψ_a的分量c_a，計算如下：

$$c_a = \vec{\psi} \cdot \vec{\psi}_a \rightarrow \int_{-\infty}^{\infty} dx \cdot \psi_a(x)^* \cdot \psi(x)$$

在線性空間中，分量就以ψ與ψ_a的內積來計算，所以以上的積分可以看成內積！

$$c_a = \int_{-\infty}^{\infty} dx \cdot \psi_a(x)^* \cdot \psi(x) \rightarrow \vec{\psi} \cdot \vec{\psi}_a \equiv \langle \psi_a | \psi \rangle$$

注意$\hat{A}$測量得到結果是a，就是發現狀態向量ψ處於本徵函數ψ_a，ψ崩潰為ψ_a。

以上結果可推廣為：

電子位於ψ狀態時，用另一套測量發現它處於狀態ϕ的振幅，等於ψ與ϕ的內積。

例如先測動量，確定處於ψ狀態時，可以再測位置，發現它處於狀態ϕ！

$$\int_{-\infty}^{\infty} dx \cdot \phi(x)^* \cdot \psi(x) \rightarrow \vec{\psi} \cdot \vec{\phi} \equiv \langle \phi | \psi \rangle$$

以動量算子的本徵函數為例：

$$u_p = \frac{1}{\sqrt{2\pi\hbar}} e^{i\frac{p}{\hbar}x}$$

u_p同時也是自由空間的定態、$\hat{H}$的本徵函數。

無限大位能井定態所滿足的上述正交、展開、測量定理在此都對！

不同本徵值的本徵函數解彼此正交！正交定理。Orthogonality

$$\int_{-\infty}^{\infty} dx \cdot u_{p'}(x) \cdot u_p(x) = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dx \cdot e^{i\frac{px}{\hbar}} e^{-i\frac{p'x}{\hbar}} = \delta(p - p')$$

$\psi(x)$可以$u_p(x)$展開：

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

Expansion Theorem 展開定理

分量就是動量空間波函數$\phi(p)$，就是波函數$\psi(x)$的Fourier Transform：

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

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

$\phi(p)$是疊加時，動量為p的本徵函數的配重，

電子在狀態$\psi(x)$時測量動量，得到值為p的機率，

即是$\phi(p)$的絕對值平方：$|\phi(p)|^2$。

Measurement Theorem

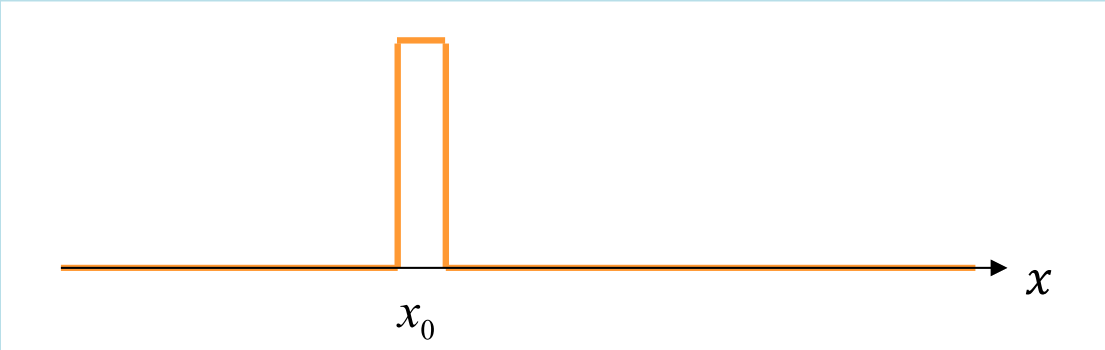
$$\psi(x) = \sum_a c_a \, \psi_a(x)$$

$|c_a|^2$是測量$\hat{A}$時得到結果是a的機率！

最後我們試試位置算子！

位置算子的本徵函數有確定位置！

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



正交定理

$$\int_{-\infty}^{\infty} dx'\, \delta(x' - x_1) \cdot \delta(x' - x_2) = \delta(x_2 - x_1)$$

收集所有可能x_0值所對應的本徵函數$\delta(x-x_0)$，

展開定理：$\psi(x)$可以所有的$\delta(x-x_0)$展開，展開的分量用標準公式計算。

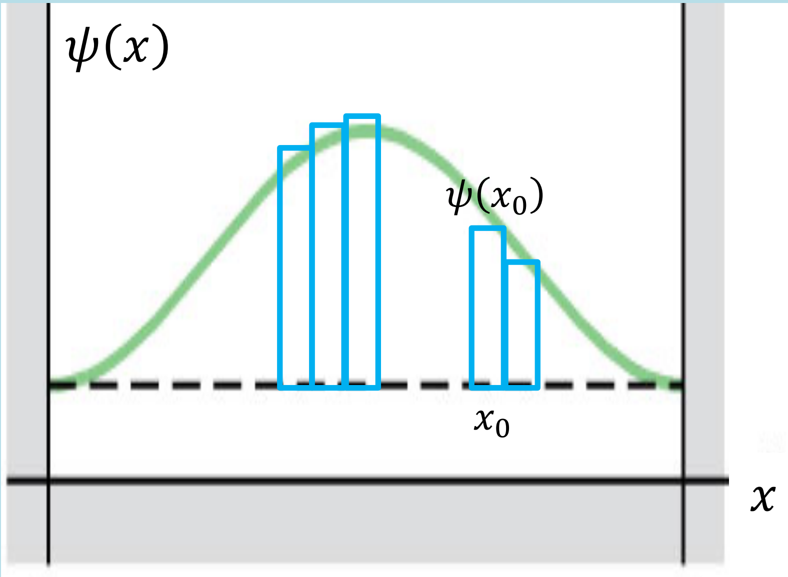
$$\int_{-\infty}^{\infty} dx'\,\delta(x'-x_0)\cdot\psi(x') = \psi(x_0)$$

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

狀態函數的值$\psi(x_0)$其實就是它自己以位置本徵函數$\delta(x-x_0)$展開時的分量。

波函數本質上原來是分量！

在圖上，很明顯一個函數可以寫成如一個一個$\delta(x-x_0)$疊加！分量即函數的值。



$$\psi(x) = \int_{-\infty}^{\infty} dx_0\,\psi(x_0)\,\delta(x-x_0)$$

分量　　本徵函數

Measurement Theorem 測量得到位置的值為x_0就是分量的絕對值平方$|\psi(x_0)|^2$ 。

量子力學的原則完整版

某瞬間時刻的狀態 ⟶ 狀態函數 $\psi(x)$ 可疊加，滿足歸一化條件。組成一無限維向量空間！

可測量的物理量 ⟶ 運算子 $\hat{A}$

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

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。

瞬間狀態$\psi(x)$隨時間t演化 ⟶ 波函數 $\Psi(x,t)$

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

狀態函數隨時間的演化由漢米爾頓量來負責！

4 Basic Assumptions of QM

A1. The wave function is the complete description of a quantum system.

A2. Hermitian operators are observables.

A3. The measurement axiom.

A4. Time evolution via the Schrödinger equation.

Measurement axiom. *If we measure the Hermitian operator $\hat{Q}$ on the (normalized) state Ψ, the possible outcomes for the measured values are the eigenvalues q_1, q_2, … of $\hat{Q}$ associated with the orthonormal eigenvectors ψ_1, ψ_2, …. With the state written as $\Psi = \sum_i \alpha_i \psi_i$, the probability p_i of measuring q_i is given by*

$$p_i = |\alpha_i|^2. \tag{5.3.26}$$

After the outcome q_i, the state of the system becomes

$$\Psi = \psi_i. \tag{5.3.27}$$

This is called the collapse of the wave function. If the spectrum of $\hat{Q}$ is degenerate after measuring a degenerate eigenvalue, the wave function collapses in the associated degenerate subspace (see remark 4 below).

摘要

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：

固定能量解ψ_E滿足與時間無關的薛丁格方程式可以寫成：

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

也就是：

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

Many important problems in physics can be cast as equations of the generic form

$$A\psi=\lambda\psi, \tag{6.1}$$

where A is a linear operator whose domain and range is a Hilbert space, ψ is a function in the space, and λ is a constant. The operator A is known, but both ψ and λ are unknown,

數學上這個關係稱為運算子$\hat{H}$的本徵函數問題！

原來，與時間無關的薛丁格方程式並不是波方程式，而是$\hat{H}$的本徵函數方程式！

定態的ψ_E是$\hat{H}$的本徵函數 Eigenfunction！對應的本徵值Eigenvalue為E。

摘要

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

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

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

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！

處於定態ψ_E的電子，能量的測量值為E，完全沒有不確定性！ $\Delta H = 0$

可以說定態ψ_E是具有特定確定能量的測量值為E的狀態。這是定態第三個意義。

一系列能量的本徵函數u_n滿足：

摘要

展開定理：任一狀態ψ可以u_n作展開。展開讓我們聯想到向量以基底展開：

$$\psi(x) = \sum_n [c_n \cdot u_n(x)] \quad \Rightarrow \quad \vec{a} = \sum_{m=1}^{l} a_m \hat{\imath}_m$$

正交定理：本徵函數彼此正交。這很像一組彼此正交的基底！

$$\int_{-\infty}^{\infty} dx \cdot u_m(x)^* \cdot u_n(x) = \delta_{mn} \quad \Rightarrow \quad \hat{\imath}_m \cdot \hat{\imath}_n = \delta_{mn}$$

分量c_a可以寫成態函數與本徵函數的空間積分:

$$c_n = \int_{-\infty}^{\infty} dx \cdot u_n(x)^* \cdot \psi(x) \quad \Rightarrow \quad a_m = \vec{a} \cdot \hat{\imath}_m$$

把狀態視為向量，展開與正交定理，就如同向量空間的向量分析一模一樣！

能量的本徵函數u_n形成一組完整的基底。

任一狀態函數可以此基底作展開，疊加係數c_n就如同向量對一組基底的分量。

摘要

這一展開式提供對無限大位能井位能下薛丁格波方程式的普遍解法：

將$t = 0$時的波函數，即起始條件，對定態解u_n展開如下：

$$\Psi(x,0) = \sum_{n=1}^{\infty} c_n u_n(x)$$

根據展開定理，這永遠可以做到！

$t = 0$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。

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n u_n(x) e^{-i\frac{E_n}{\hbar}t}$$

我們已經在自由薛丁格方程式用了這樣的策略！當時的正弦波就是定態。

很明顯，這個程序不只適用於無限大位能井，原則上適用於任何位能。

摘要

可見$|c_n|^2$就是測量能量時，得到結果是E_n的機率！

波函數沿本徵函數u_n的展開分量c_n，就是對$\hat{H}$測量得到結果是E_n的振幅。

Measurement Theorem 測量定理

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

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

沒有遺漏，可見對能量的測量結果只能是本徵值E_n其中之一，不能是其他的值。

如果還會測到其他值，總機率就要超過1了！

到此，無限大位能井內的電子，不一定是在定態，能量的量子化完全確立！

摘要

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，立刻再作一次能量的測量，結果一定確定還是E_n，

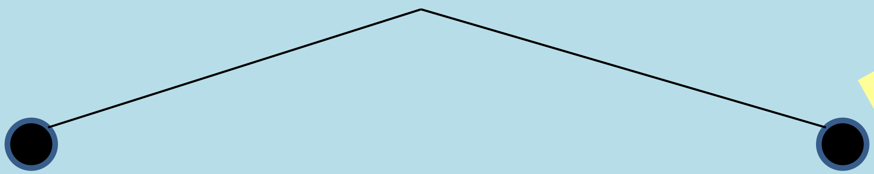
測量結果確定的狀態就是該物理量算子的本徵態。

可見第一次剛測完時，粒子狀態應該就是本徵函數$u_n(x)$。

所以第一次的測量使粒子的狀態由$\psi(x)$瞬間崩潰變成了$u_n(x)$。

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

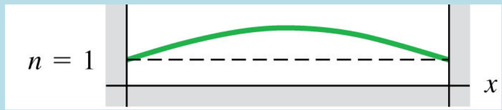
當然每一次測量結果不會是確定的！崩潰變成的狀態也就不確定。



$$\Psi(x,0) = \sin\frac{\pi}{a}x - \frac{1}{9}\sin\frac{3\pi}{a}x + \cdots$$

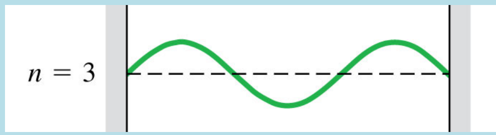
$E = E_1 = \left(\frac{\hbar^2}{2m}\right)\frac{\pi^2}{a^2}$

$P_1 \sim 1$



$E = E_3$

$P_3 \sim \frac{1}{81}$



$\cdots$

但不會測到E_{2m}。