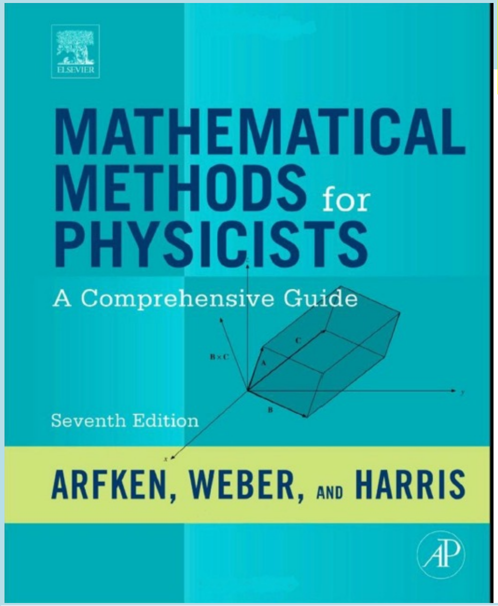
與時間無關的薛丁格方程式並不是波方程式，而是$\hat{H}$的本徵函數方程式！

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



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。

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

Chapter 8

Sturm-Liouville Theory

Characterization of the general features of eigenproblems arising from second-order differential equations is known as **Sturm-Liouville theory**. It therefore deals with eigenvalue problems of the form

$$\mathcal{L}\psi(x) = \lambda\psi(x), \tag{8.7}$$

where $\mathcal{L}$ is a linear second-order differential operator, of the general form

$$\mathcal{L}(x) = p_0(x)\frac{d^2}{dx^2} + p_1(x)\frac{d}{dx} + p_2(x). \tag{8.8}$$

The key matter at issue here is to identify the conditions under which $\mathcal{L}$ is a Hermitian operator.

動量算子$\hat{p}$定義為空間微分運算，那有位能時的能量算子可以寫成：

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

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

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

漢米爾或稱能量算子就定義為動量算子的平方加上位能算子。

薛丁格方程式就可以寫為：

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

⬇

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

這就是量子力學完整的薛丁格方程式。

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：

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。

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

定態的波函數是$\hat{H}$的本徵函數 Eigenfunction！

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

控制波函數時間演化的的薛丁格方程式。

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

因此：定態波函數的時間演化滿足：

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

此時間微分方程式很容易解出：

$$\Psi(x,t) = \Psi(x,0)e^{-i\frac{E}{\hbar}t} = \psi_E(x)e^{-i\frac{E}{\hbar}t}$$

$\hat{H}$的本徵函數一定是可分離的！

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。

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

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

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

$$\Delta H = 0$$

處於定態ψ_E的電子，能量的測量值為E，完全沒有不確定性！

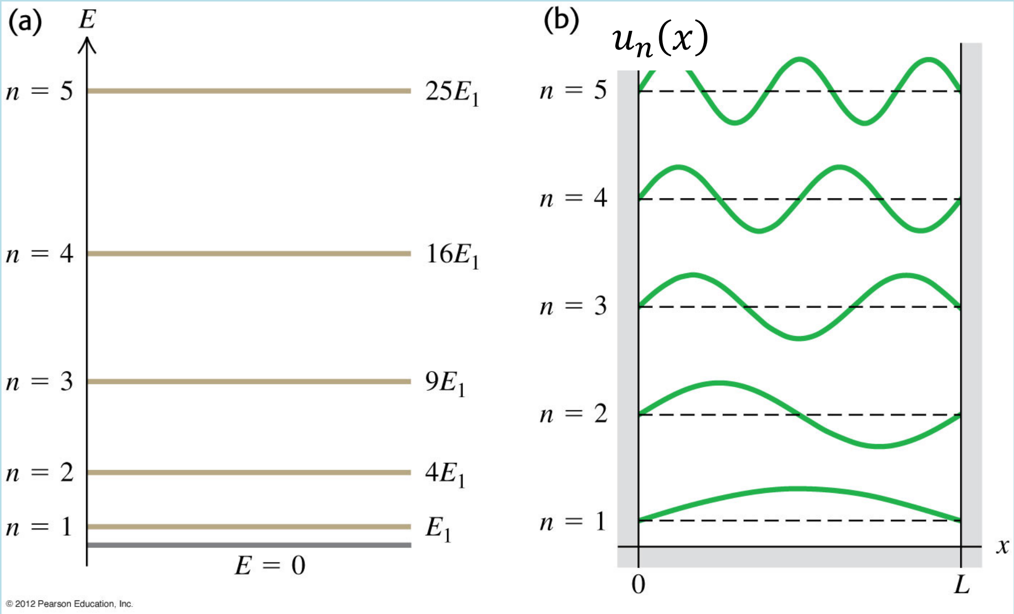
可以說定態ψ_E是具有特定確定能量的測量值為E的狀態。

無限大位能井$\hat{H}$的本徵函數滿足：

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

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

$(\Delta H)^2 = 0$



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！ $\Delta H = 0$

這樣的態有什麼用？

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，結果一定確定還是同樣的值，無不確定性。

因此$\Delta H = 0$，此時一定存在於某一個本徵態！

那麼、剛剛測得的能量結果一定只能是某一本徵值E_n！

驚人的：在此位能中任意一次能量測量結果只能是某本徵值E_n，不會測到其他值。

到此，無限大位能井內，電子能量的量子化完全確立！不一定是在定態。

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。

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，

測量完畢後，狀態已經不會再是結果不確定的狀態$\psi(x)$，

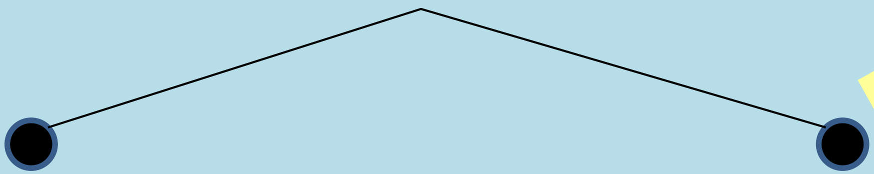
而是結果完全確定的本徵函數$u_n(x)$。

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

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

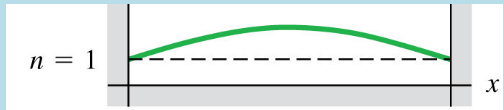
在非本徵狀態$\psi(x)$，測量結果不會是確定的！

崩潰變成的態也就不確定。

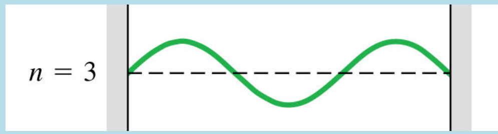


$$\Psi(x,0) = \sin\frac{\pi}{a}x - \frac{1}{9}\sin\frac{3\pi}{a}x + \cdots$$

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



$$E = E_3$$



但不會測到其他值。

解能量量算子的本徵函數、是在決定你測量能量後崩潰到什麼狀態。

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 $\hat{A} \rightarrow a$

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，

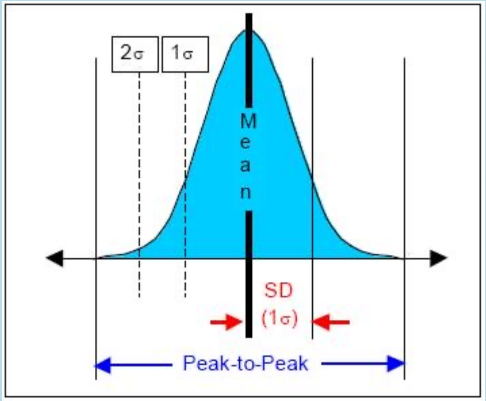
隱含：物理量$\hat{A}$測量時如古典量，也就是有確定的值。

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：



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

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

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

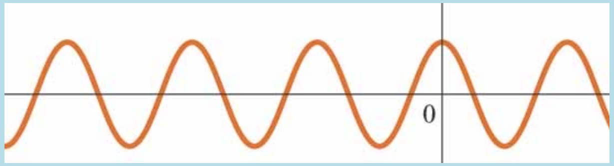
$$\Delta A = 0$$

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。

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！

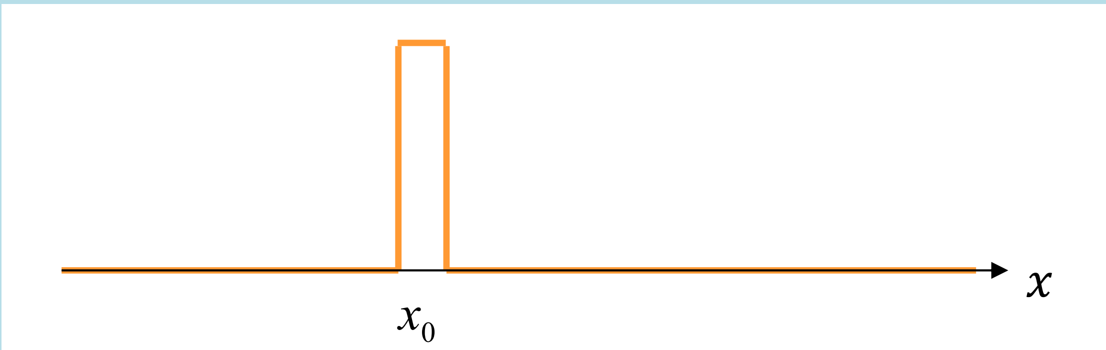
波函數是一個delta function！

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

這是位置算子$\hat{x}$的本徵函數：

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

$$\Delta x = 0$$



對任一狀態$\psi(x)$作某物理量的測量，若所得到的結果是某一a，
剛測量完時，立刻再作一次能量的測量，結果一定確定還是a，
所以測量第一次完畢後，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$\psi_a(x)$。

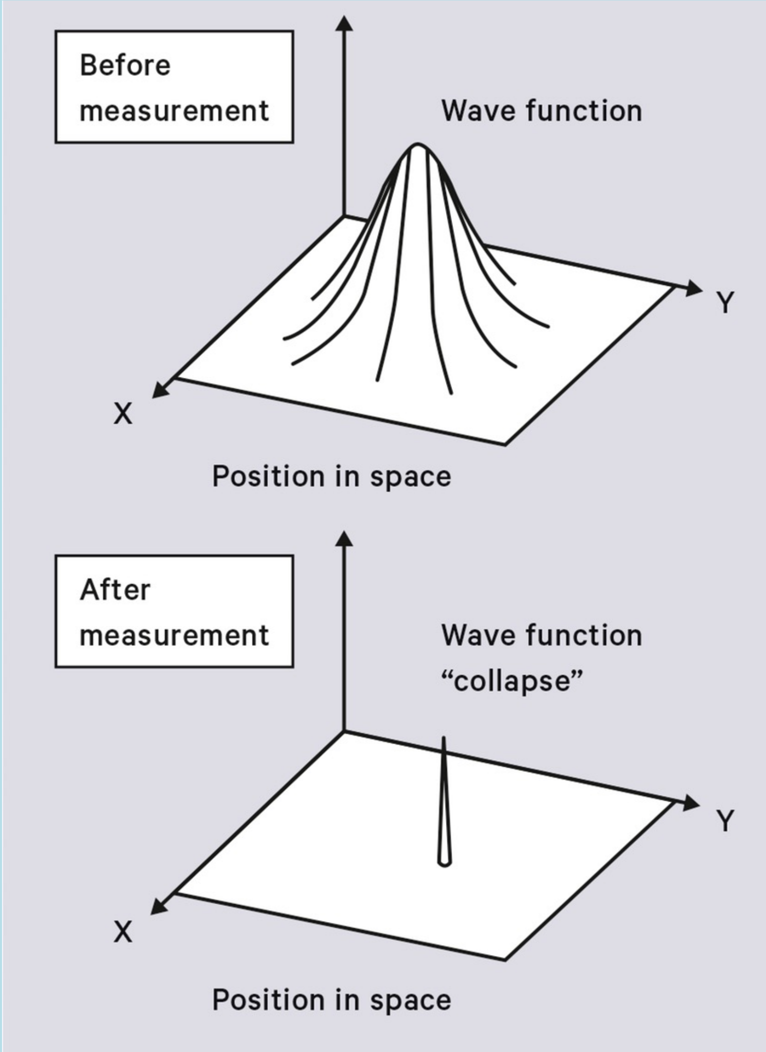
所以第一次的測量使粒子的狀態由$\psi(x)$瞬間崩潰變成了$\psi_a(x)$。

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

物理量$\hat{A}$的本徵函數，就是$\hat{A}$一測量完後的狀態！測到的值就是本徵值！

例如位置的測量會使狀態崩潰為位置本徵函數其中之一：

$$\psi(x) \xrightarrow[\hat{x}\to x_0]{} \delta(x-x_0)$$



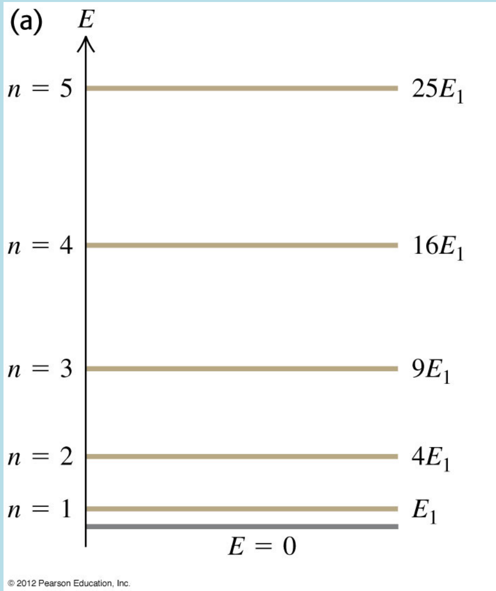
$\psi(x)$

$\hat{\mathcal{A}}$

那狀態對測量結果的影響為何呢？

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！

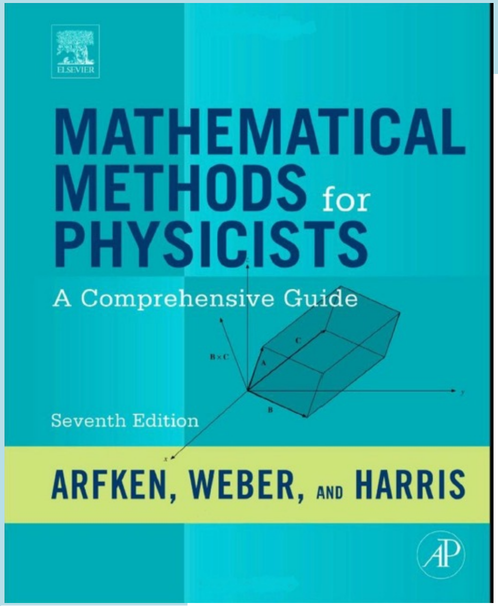


算子有它的堅持！

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。

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

本徵函數有許多共通的性質：



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**.

8.5 SUMMARY, EIGENVALUE PROBLEMS

Because any Hermitian operator on a Hilbert space can be expanded in a basis and is therefore mathematically equivalent to a matrix, all the properties derived for matrix eigenvalue problems automatically apply whether or not a basis-set expansion is actually carried out. It may be helpful to summarize some of those results, along with some that were developed in the present chapter.

1. A second-order differential operator is Hermitian if it is self-adjoint in the differential-equation sense and the functions on which it operates are required to satisfy appropriate boundary conditions. In that event, the scalar product consistent with Hermiticity is an unweighted integral over the range between its boundaries.
2. If a second-order differential operator is not self-adjoint in the differential-equation sense, it will nevertheless be Hermitian if it satisfies appropriate boundary conditions and if the differential equa

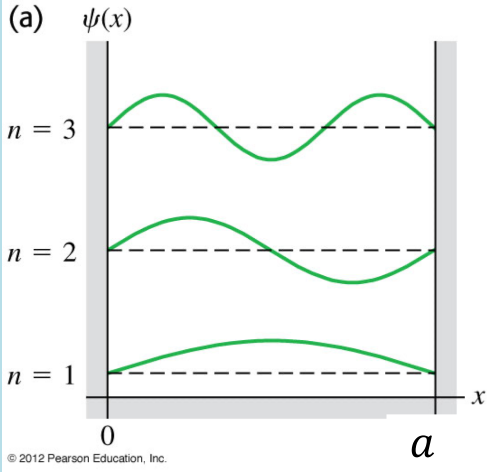
任何可行的狀態函數，都可以展開成本徵函數的疊加！

3. A Hermitian operator on a Hilbert space has a complete set of eigenfunctions. Thus, they span the space and can be used as basis for an expansion.
4. The eigenvalues of a Hermitian operator are real.
5. The eigenfunctions of a Hermitian operator corresponding to different eigenvalues are orthogonal, using the appropriate scalar product.

不同本徵值的本徵函數彼此正交

6. Degenerate eigenfunctions of a Hermitian operator Gram-Schmidt or any other orthogonalization process.
7. Two operators have a common set of eigenfunctions if and only if they commute.
8. An algebraic function of an operator has the same eigenfunctions as the original operator, and its eigenvalues are the corresponding function of the eigenvalues of the original operator.
9. Eigenvalue problems involving a differential operator may be solved either by expressing the problem in any basis and solving the resulting matrix problem or by using relevant properties of the differential equation.
10. The matrix representation of a Hermitian operator can be brought to diagonal form by a unitary transformation. In diagonal form, the diagonal elements are the eigenvalues, and the eigenvectors are the basis functions. The orthonormal eigenvectors are the columns of the unitary matrix U^{-1} when a Hermitian matrix H is transformed to the diagonal matrix $\mathsf{U}\mathsf{H}\mathsf{U}^{-1}$.

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。
大致分為兩部分：展開與測量！
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：

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

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

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

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

$= 0$ when $n \neq m$

$= 1$ 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components 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！

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*,

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

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

so that

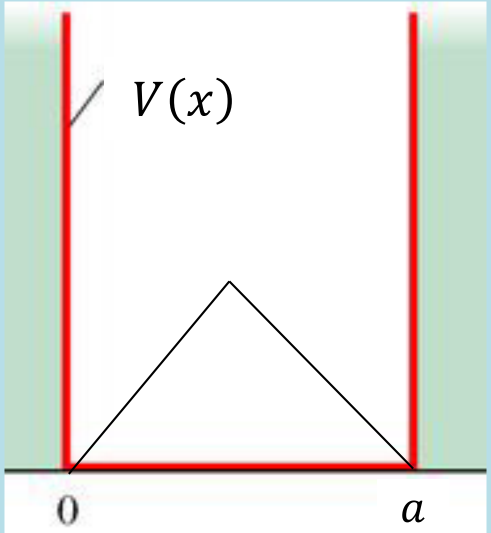
$$|A_n|^2 = \frac{96}{\pi^4 n^4} \qquad \text{for } n \text{ odd}$$
$$= 0 \qquad \text{for } n \text{ even}$$

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:

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



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。

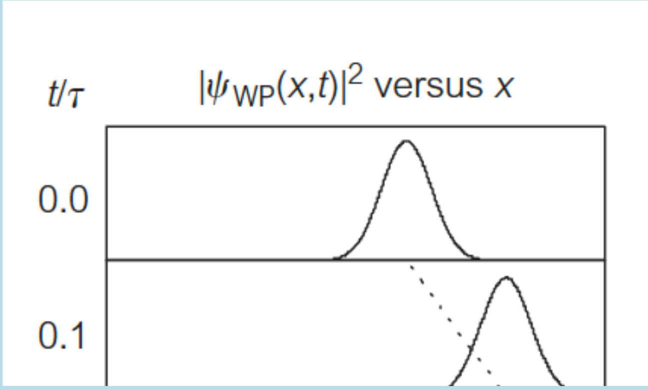
$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n u_n(x) e^{-i\frac{E_n}{\hbar}t}$$

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。

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。



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

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

(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

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

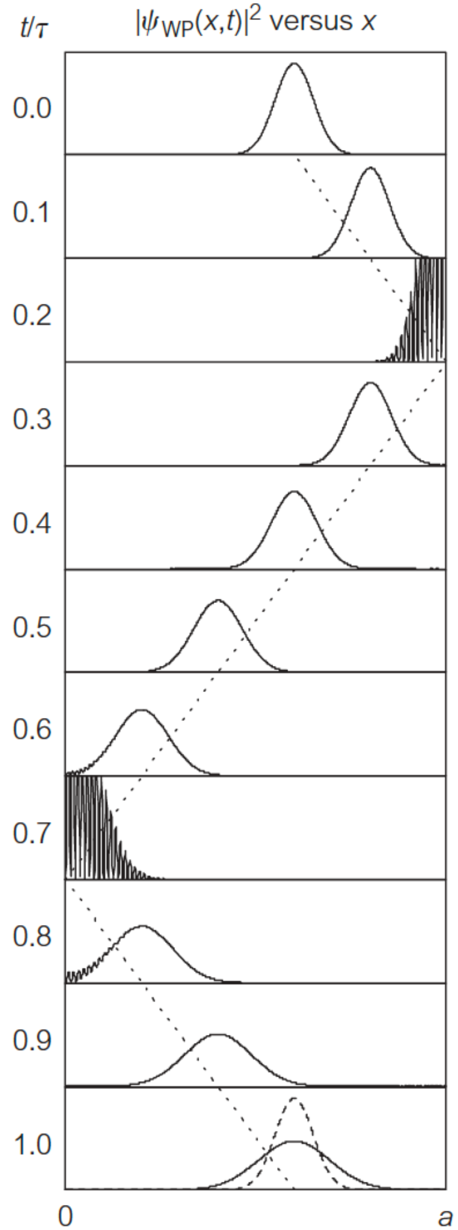


Figure 5.9. Time-development of $|\psi(x,t)|^2$ versus x for a Gaussian-like wave packet in the standard infinite well, over one classical period (left) and 10 classical periods (right); the classical periodicity and the spreading time (t_0) are chosen to be comparable. The classical trajectory is shown 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.

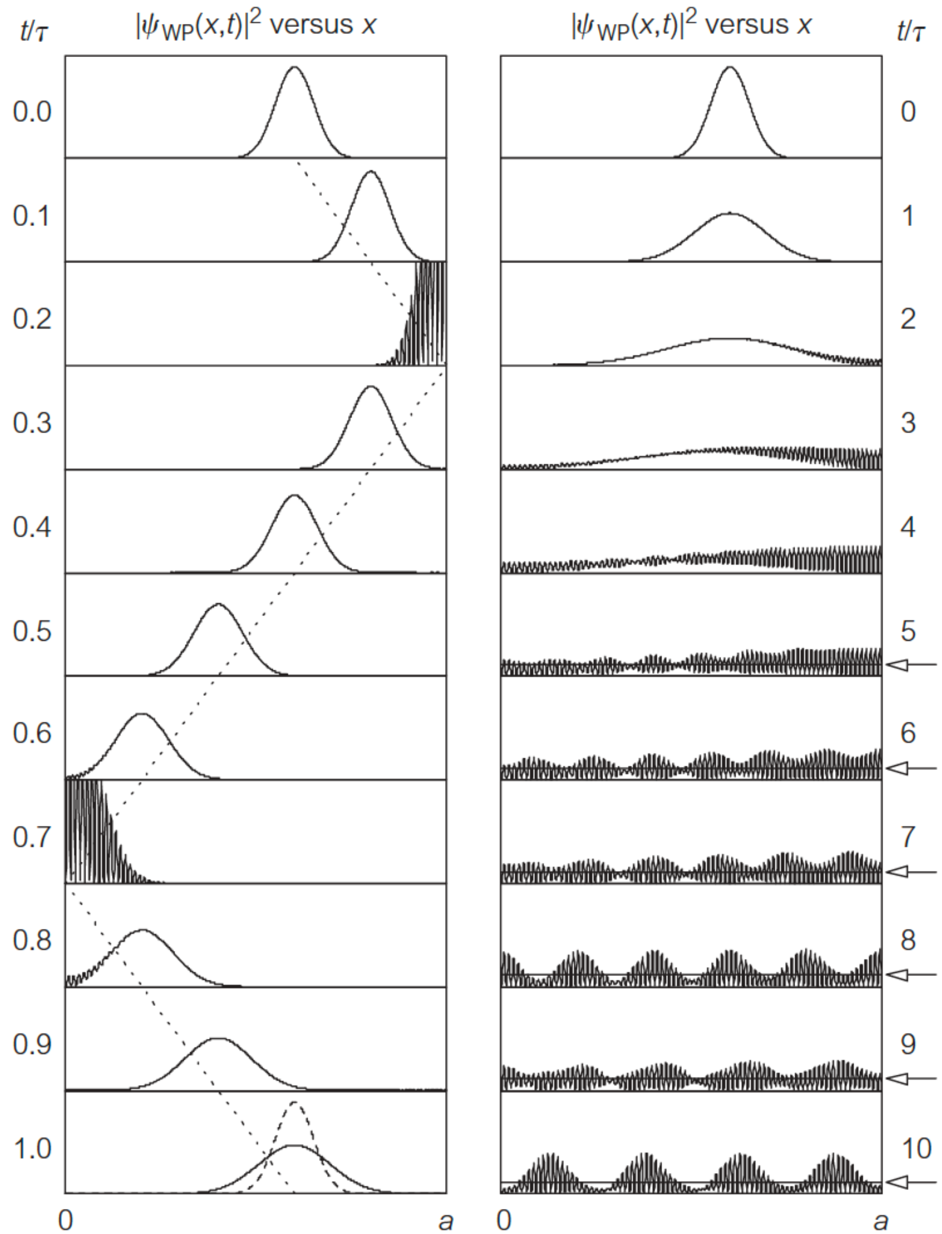


Figure 5.9. Time-development of $|\psi(x,t)|^2$ versus x for a Gaussian-like wave packet in the standard infinite well, over one classical period (left) and 10 classical periods (right); the classical periodicity and the spreading time (t_0) are chosen to be comparable. The classical trajectory is shown 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.

任意算子的本徵函數普遍具有的兩個重要性質。 展開與測量！

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：$|\phi(p)|^2$。

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

$\phi(p)$就是以動量的本徵函數：自由電子波，作展開的分量！

自然的猜測：對於以能量本徵函數u_n展開的瞬間狀態函數$\psi(x)$，

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

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

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！

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

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

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

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

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

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

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

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

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

測量能量時，得到結果只能是E_n其中之一！

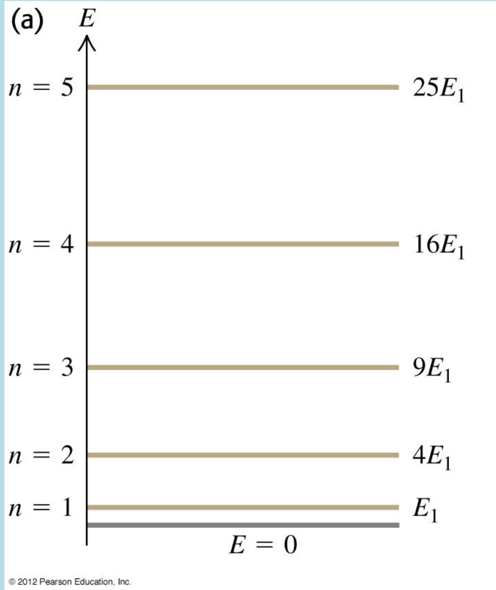
這很容易理解：對一狀態$\psi(x)$作能量的測量，若立刻重測，結果一定確定，此時一定在某一本徵態，因此測得結果只能是某一本徵值E_n， 不會測到其他值。

真是如此，那機率總和必須等於1！

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

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

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



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

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！

$\psi(x)$

$\hat{\mathcal{A}}$

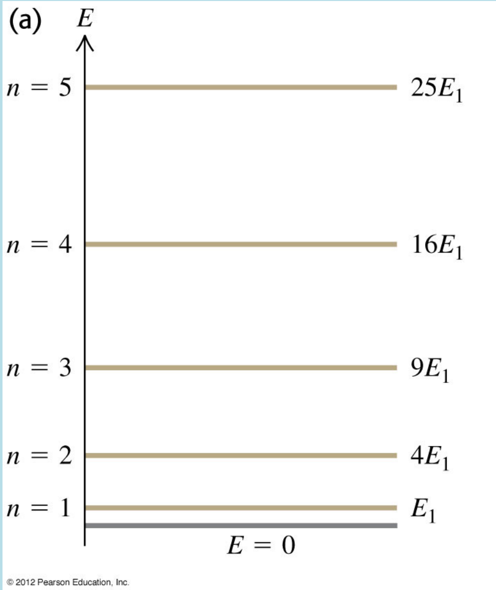
不同的狀態下，機率的分佈不同！

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

但可能的測量結果卻一樣！

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。

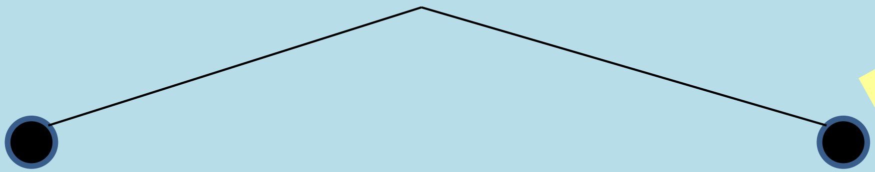
得到某eigenvalue時，粒子的狀態會崩潰為何種狀態(eigenfunction)。

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，

測量使粒子的狀態由$\psi(x)$瞬間崩潰變成了$u_n(x)$。

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

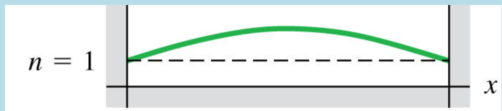
在非本徵狀態$\psi(x)$，測量結果不會是確定的！崩潰變成的態也就不確定。



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

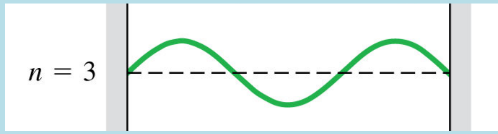
$E = E_1 = \left(\frac{\hbar^2}{2m}\right)\frac{\pi^2}{a^2}$

$P_1 \sim 1$



$E = E_3$

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



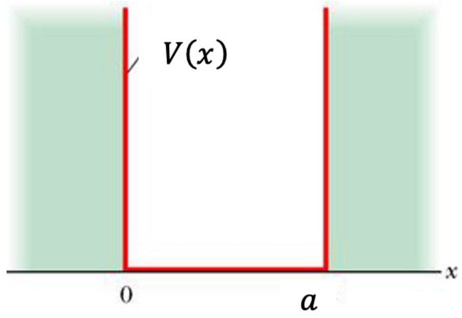
$\cdots$

但不會測到E_{2m}。

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。

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:

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

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

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:

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

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 $\frac{1}{5}$ 。

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。

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

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

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

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

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

以上證明用到算子$\hat{A}$的這個性質：

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

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：

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

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

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

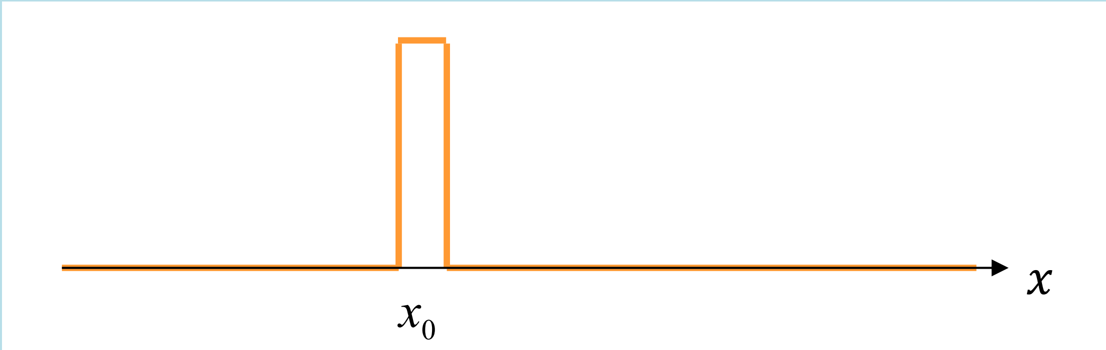
$$\psi(x) = \sum_a c_a \, \psi_a(x)$$

$|c_a|^2$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。

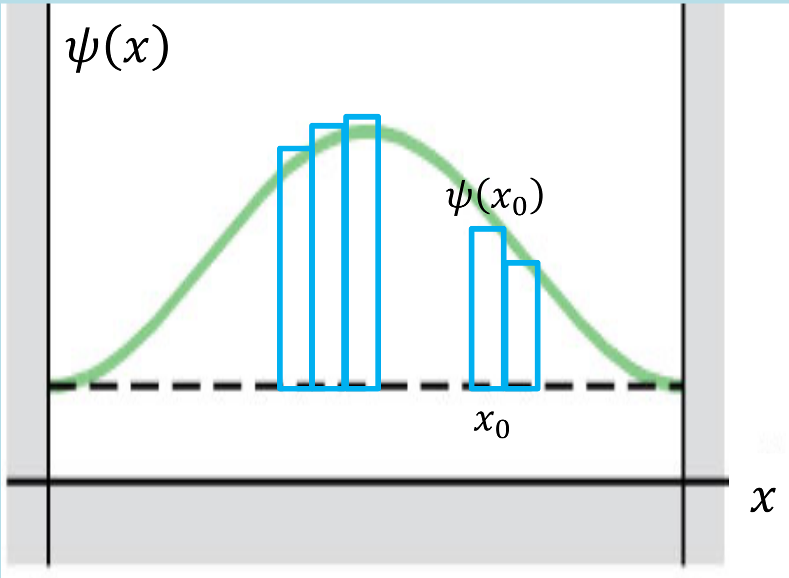
$$\int_{-\infty}^{\infty} dx'\,\delta(x'-x_0)\cdot\psi(x') = \psi(x_0)$$

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

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。

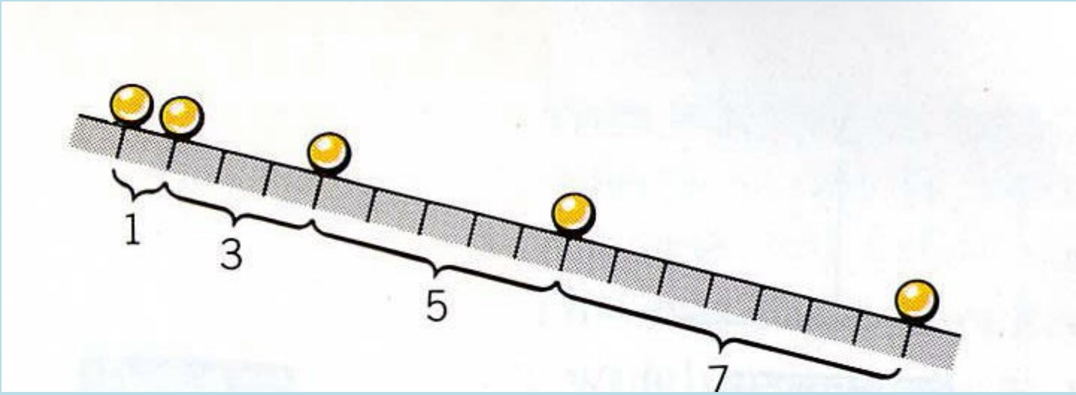


$$\psi(x) = \int_{-\infty}^{\infty} dx_0\,\psi(x_0)\,\delta(x-x_0)$$

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$|\psi(x_0)|^2$ 。

古典力學的原則



一個粒子一直都有一個特定的位置：$x(t)$！

此位置函數$x(t)$滿足運動方程式：

$$m\frac{d^2x}{dt^2} = -\frac{\partial V}{\partial x}$$

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：

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

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！

以上的結果與一般向量分析中，求向量的分量的方法神似：

狀態函數ψ可以疊加 ➡ 向量$\vec{a}$可以相加

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：

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

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:

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

把狀態類比於向量，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類比於一組完整的基底。

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。

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：

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

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:

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

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：

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

兩個函數乘積的積分滿足線性代數中兩向量的內積的所有性質！

大膽引進一符號$\langle\psi,\phi\rangle$來表達兩個狀態函數ψ,ϕ的內積：

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

這個內積在前換互換後，會變為複數共軛。

$$\langle\psi,\phi\rangle^* = \left(\int_{-\infty}^{\infty} dx \cdot \psi^* \cdot \phi\right)^* \equiv \int_{-\infty}^{\infty} dx \cdot \phi^* \cdot \psi = \langle\phi,\psi\rangle$$

可見一個狀態函數ψ與自己的內積一定是實數，

$$\langle\psi,\psi\rangle^* = \langle\psi,\psi\rangle$$

對應向量的長度平方。

這個內積可以用來書寫一個狀態函數ψ的歸一化條件：

$$\int_{-\infty}^{\infty} dx \cdot \psi(x)^* \cdot \psi(x) \equiv \langle\psi,\psi\rangle = 1$$

ψ只能是單位向量！

用這一內積符號：$\displaystyle\int_{-\infty}^{\infty} dx \cdot \psi(x)^* \cdot \phi(x) \equiv \langle \psi, \phi \rangle$

如此u_n的正交定理可以簡化寫成：

$$\int_0^a dx \cdot u_n^*(x) u_m(x) = \delta_{mn} \quad \rightarrow \quad \langle u_n, u_m \rangle = \delta_{mn}$$

函數展開的分量可以寫成 ：

$$c_n = \int_0^a dx \cdot u_n^*(x) \psi(x) \quad \rightarrow \quad c_n = \langle u_n, \psi \rangle$$

u_n就是正交基底。

這是驚人的簡化，省去書寫積分的麻煩。

更重要、它揭露了量子狀態、即狀態函數的數學結構：有內積的向量空間。