量子力學的原則完整版

可疊加，組成一無限維向量空間！

某瞬間時刻的狀態 ⟶ 複數狀態函數 $\psi(x)$ 滿足歸一化條件。

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。

2. A particle's wavefunction at $t = 0$ is:

$$\Psi(x,0) = \sqrt{\frac{30}{a^5}}\,x(a-x) \quad 0 < x < a,$$

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

Calculate the expectation values: $\langle x^2\rangle, \langle p^2\rangle$. (25) 提示：$p = -i\hbar\frac{\partial}{\partial x}$

解答：

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

$$= \frac{30}{a^5}\int_0^a dx \cdot x^2(a^2x^2 - 2ax^3 + x^4) = \frac{30}{a^5}\int_0^a dx \cdot (a^2x^4 - 2ax^5 + x^6)$$

$$\frac{30}{a^5}\left(\frac{1}{5}a^7 - \frac{1}{3}a^7 + \frac{1}{7}a^7\right) = \frac{30}{a^5}\frac{1}{105}a^7 = \frac{2}{7}a^2$$

$$\langle p^2\rangle = \int_{-\infty}^{\infty} dx \cdot \Psi^*(x) \cdot \frac{1}{2m}\left(-i\hbar\frac{\partial}{\partial x}\right)^2 \Psi(x) = -\frac{30}{a^5}\hbar^2\int_0^a dx \cdot x(a-x)\frac{\partial^2 x(a-x)}{\partial x^2}$$

$$= \frac{30}{a^5}\hbar^2\int_0^a dx \cdot x(a-x)\cdot 2 = \frac{60}{a^5}\hbar^2\left(\frac{a^3}{2} - \frac{a^3}{3}\right) = \frac{10}{a^2}\hbar^2$$

In $\langle p^2\rangle$, you must keep the two derivatives in the middle to get the right answer. To see why, check out my careful discussion in the PowerPoint file. You cannot move derivative operators around in your formula. That is a key difference between classical and quantum physics!

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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！

薛丁格方程式

運用以上的原則：

薛丁格方程式的可分離separable解，滿足與時間無關的薛丁格方程式：

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

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

這些是描述Stationary State定態的解ψ_E。定態解的所有測量期望值與時間無關。

定態的波函數的時間演化就是函數$\psi_E(x)$乘上一個Phase factor：$e^{-i\frac{E}{\hbar}t}$。

左邊就是量子力學中對應的Hamiltan運算子，此式可以寫成：

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

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。

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

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！ $\Delta H = 0$

這樣的能量的本徵函數通常有一系列：$u_n, n = 1,2,\cdots$！

我們發現任一狀態函數ψ可以以一系列能量的本徵函數u_n展開！

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

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

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

能量的期望值等於：

$$\langle H\rangle = \int_{-\infty}^{\infty} dx \cdot \psi^*(x) \cdot \hat{H}\psi(x) = \sum_n \underbrace{E_n}_{\text{測量結果}} \cdot \underbrace{|c_n|^2}_{\text{機率}}$$

展開分量c_n的絕對值平方，就是對$\hat{H}$測量得到結果是E_n的機率。

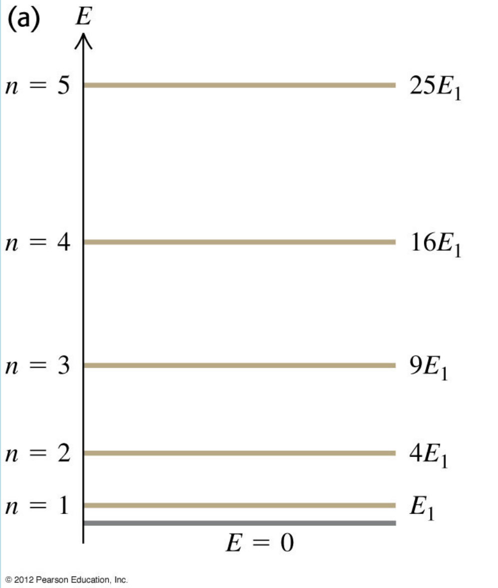
這強烈暗示測量能量時，得到結果只能是E_n其中之一！不會測到其他的值。

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 $\boxed{\text{measurement of the energy must be one of the eigenvalues of the energy operator.}}$ Under

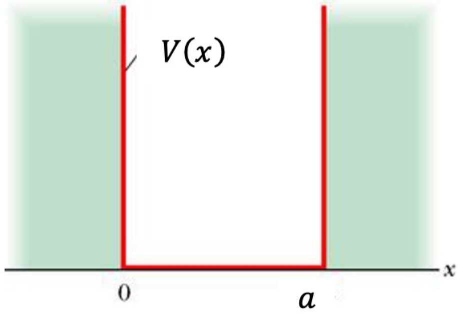
沒有遺漏，可見對能量的測量結果只能是本徵值E_n其中之一，不能是其他的值。

如果還會測到其他值，總機率就要超過1了！

Measurement Theorem 測量定理

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.

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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 $\frac{1}{5}$。

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

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

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

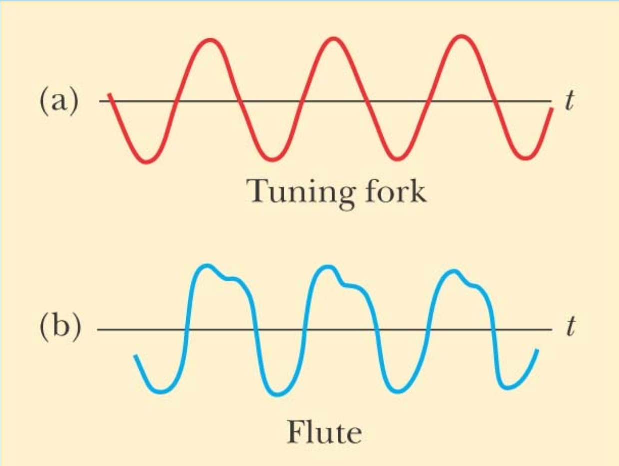
$$= \int_{-\infty}^{\infty} dx \cdot \psi^*(x) \cdot \hat{H} \cdot \left[\sqrt{\frac{4}{5}}u_1(x) + \sqrt{\frac{1}{5}}u_2(x)\right]$$

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

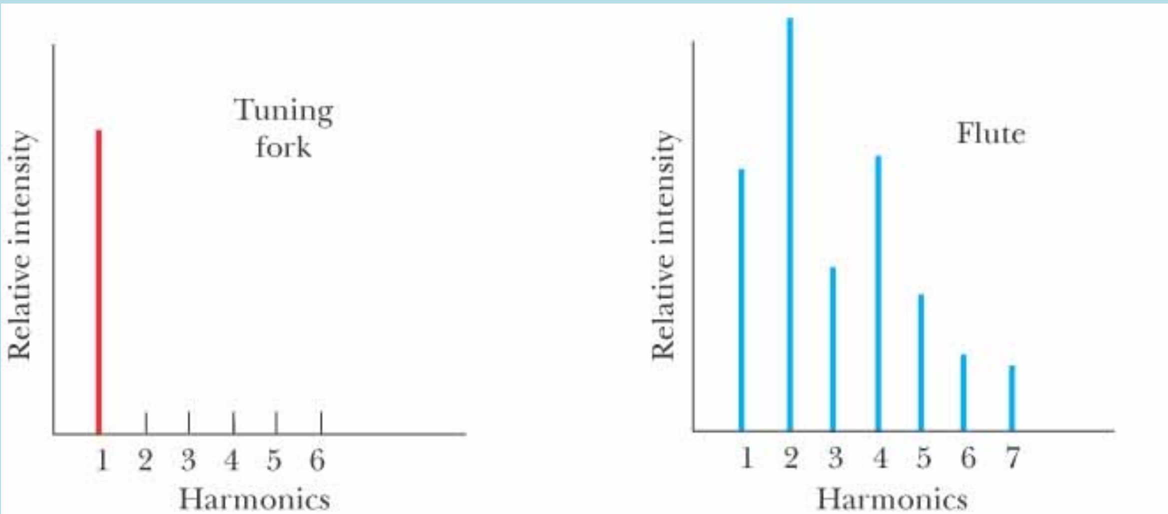
$$= \frac{4}{5}E_1 + \frac{1}{5}E_2 = |c_1|^2E_1 + |c_2|^2E_2$$

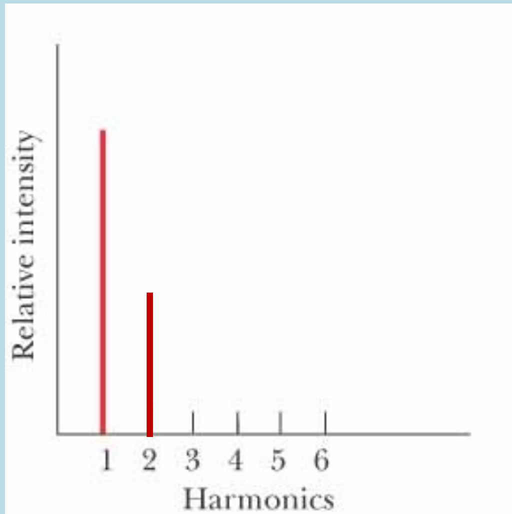
$$\frac{4}{5} + \frac{1}{5} = 1$$

測量結果 機率

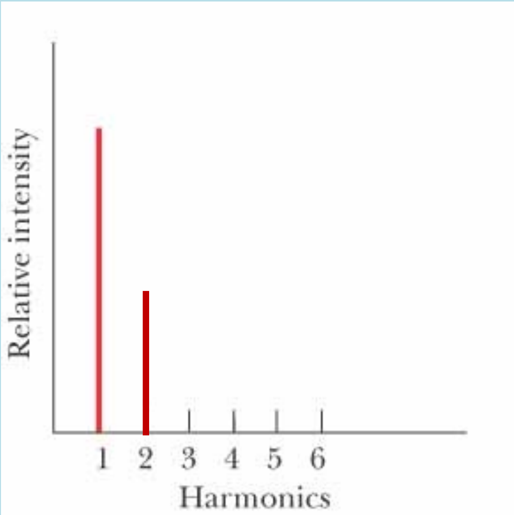


$$\Psi(x,0) = \sqrt{\frac{4}{5}}\left(\sqrt{\frac{2}{a}}\sin\frac{\pi x}{a}\right) + \sqrt{\frac{1}{5}}\left(\sqrt{\frac{2}{a}}\sin\frac{2\pi x}{a}\right)$$

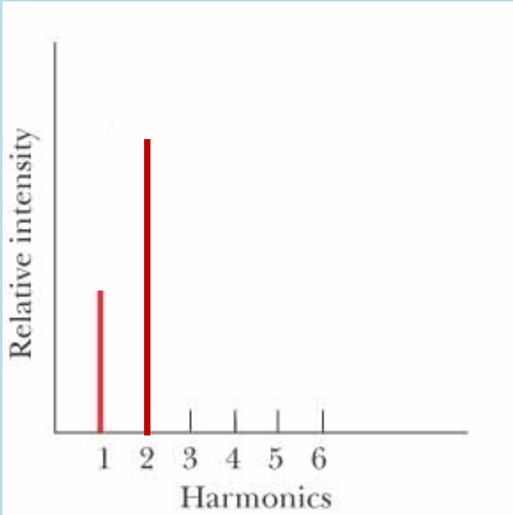




$$\sqrt{\frac{4}{5}}\left(\sqrt{\frac{2}{a}}\sin\frac{\pi x}{a}\right)+\sqrt{\frac{1}{5}}\left(\sqrt{\frac{2}{a}}\sin\frac{2\pi x}{a}\right)$$



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



這兩個不同的狀態，可以測到的能量值竟然完全一樣：E_1, E_2。

機率的分佈不同！$2:1$與$1:2$。

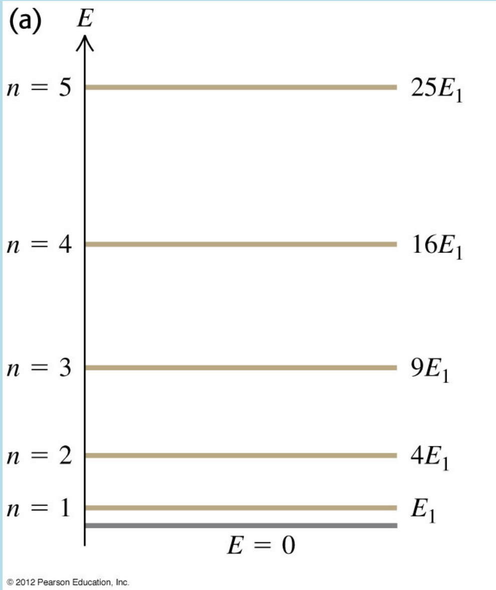
$\psi(x)$

$\hat{\mathcal{A}}$

不同的狀態下，機率的分佈不同！
但可能得到的測量結果卻一樣！

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

描述測量的算子是很有個性的！
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。

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$u_n(x)$。

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

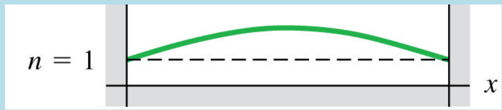
在特定狀態，每一個初次測量結果不會是確定的！

崩潰變成的態也就不確定。

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

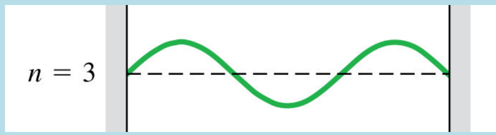
$E = E_1 = \left(\frac{\hbar^2}{2m}\right)\frac{\pi^2}{a^2}$

$P_1 \sim 1$



$E = E_3$

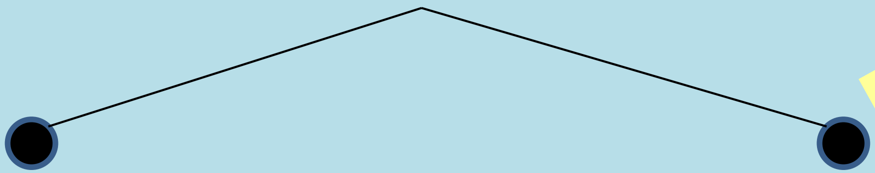
$P_3 \sim \frac{1}{81}$



$\cdots$

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。



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

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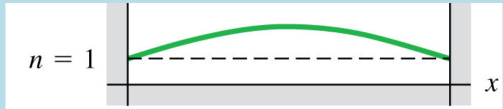

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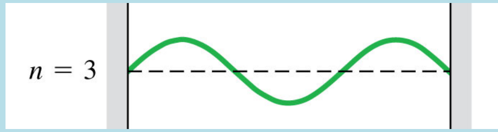
$P_3 \sim \frac{1}{81}$



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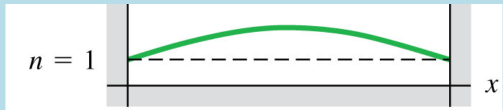
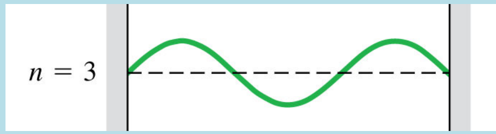


$E = E_3$

$P_3 \sim 1$



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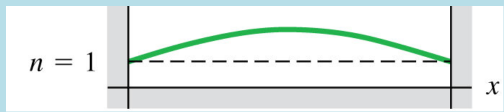
兩個不同的狀態，測到一的樣能量值，如E_1，就崩潰到同樣狀態。



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).

狀態以定態解展開還提供了對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。

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

B. For a later time $t = t_0$, write down the wave function $\psi(x, t_0)$. There is no need to simplify the answer. (15)

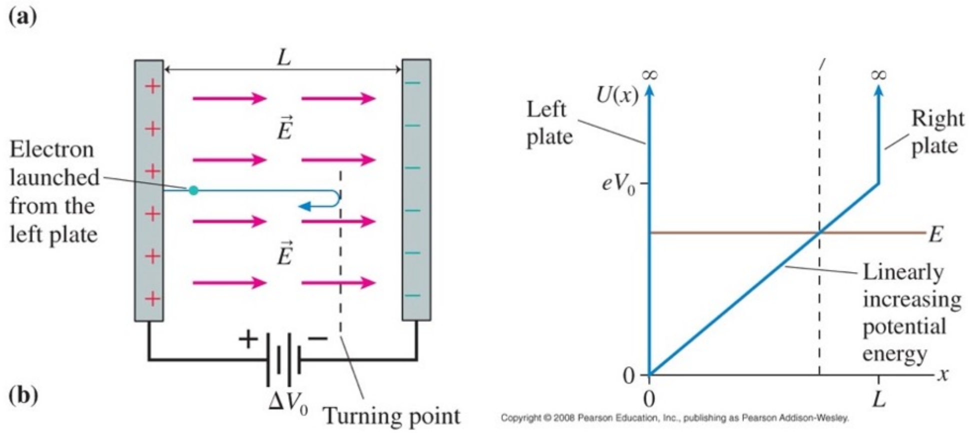
B. $t = 0$時此狀態可以視為定態$u_{1,2}$的如上疊加，接著定態隨時間個自演化，位能下薛丁格方程式要求u_n乘上$e^{-i\frac{E_n}{\hbar}t}$。乘完之後依同樣方式疊加，整個波函數也就滿足薛丁格波方程式。因此

$$\Psi(x,t) = \sqrt{\frac{4}{5}}\left(\sqrt{\frac{2}{a}}\sin\frac{\pi x}{a}\right)e^{-i\frac{E_1}{\hbar}t} + \sqrt{\frac{1}{5}}\left(\sqrt{\frac{2}{a}}\sin\frac{2\pi x}{a}\right)e^{-i\frac{E_2}{\hbar}t}。$$

注意兩個定態的能量E_1, E_2是不一樣的。。

與時間無關的薛丁格方程式：描述在一位能$V(x)$中Stationary State定態的解ψ_E：

1. An electron (charge e) is moving inside a parallel capacitor of constant electric field with separation L and fixed voltage difference V_0. Write down the time independent Schrodinger equation for the stationary states $\psi_E(x)$ of energy E in $0 < x < L$. Can you guess if its energy is quantized? Why? No need to solve it. (15)



解答：The potential energy of the electron is $V(x) = \frac{eV_0}{L}x$. Therefore the time independent Schrodinger equation is

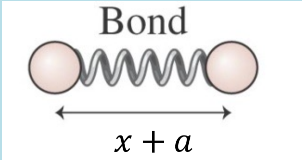
$$-\frac{\hbar^2}{2m}\frac{d^2\psi_E(x)}{dx^2} + V(x)\cdot\psi_E(x) = -\frac{\hbar^2}{2m}\frac{d^2\psi_E(x)}{dx^2} + \frac{eV_0}{L}x\cdot\psi_E(x) = E\cdot\psi_E(x)$$

This is a complicated differential equation. The solution we have for step potential: $\psi_E = Ae^{ikx} + Re^{-ikx}$ *totally* cannot apply here. Some of you still copy here the formula $k \equiv \sqrt{\frac{2m(E-V(x))}{\hbar^2}}$. But it does not make sense. The lefthand side is a constant but the righthand side is x- Screenshot

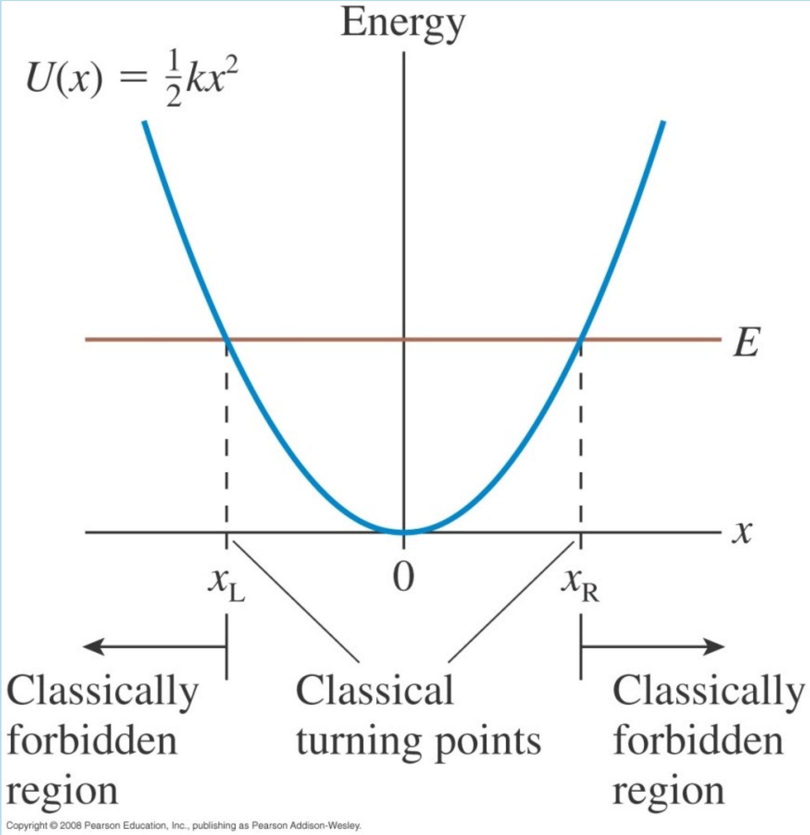
簡諧振盪器、量子彈簧、

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+\frac{1}{2}kx^2\right]\psi_E(x)=E\psi_E(x)$$

$$\frac{\hbar^2}{2m}\frac{d^2\psi_E}{dx^2}=\left(\frac{1}{2}kx^2-E\right)\psi_E$$



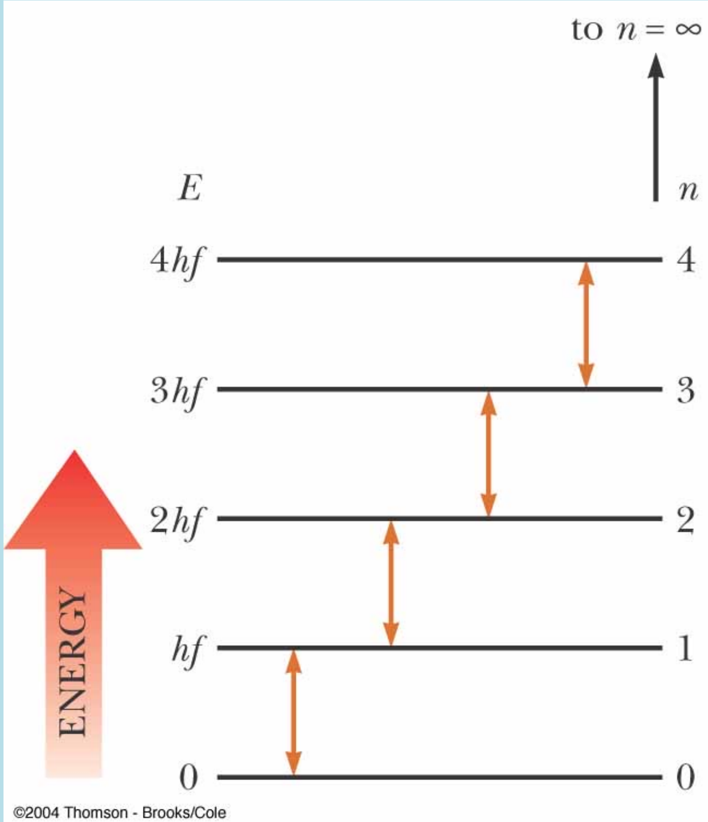
最簡單的量子彈簧就是雙原子分子！



黑體輻射以及空腔輻射也是一系列的量子彈簧。

如果要解釋黑體輻射，量子彈簧的能量變化必需是能階狀的！

Max Planck 在1900 開啟了量子革命的第一槍！



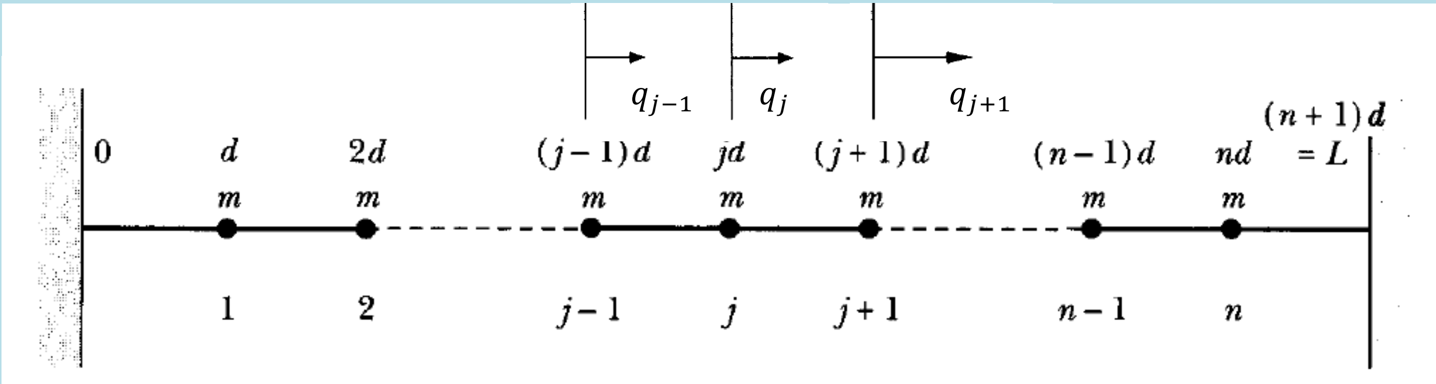
量子彈簧的能量不是連續的，而是固定量子的整數倍（離散型式）

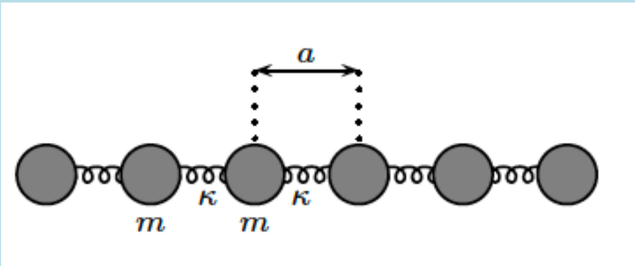
量子(Quantum)的大小與頻率成正比！

$E_n = n \cdot hf$ h: Planck Constant $h = 6.625 \times 10^{-34} \mathrm{J} \cdot s$

12.9 The Loaded String*

固體內原子晶格的振動也是一系列量子彈簧

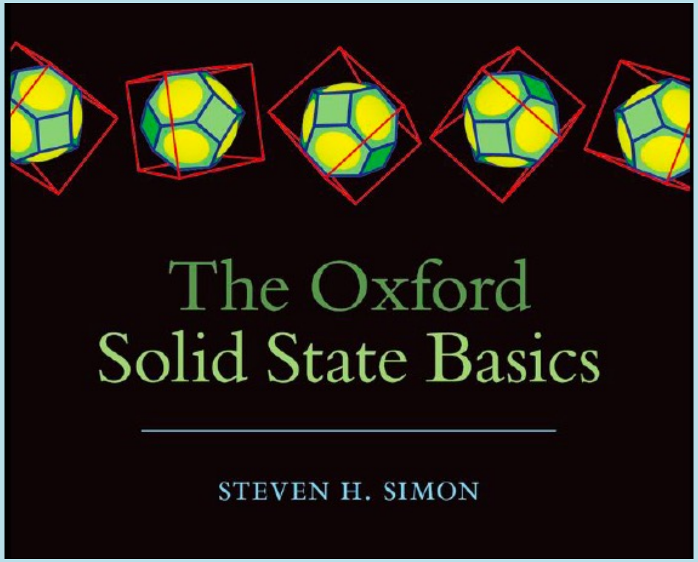




Vibrations of a One-Dimensional Monatomic Chain

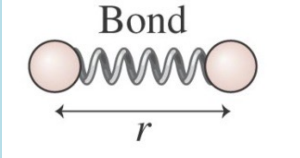
9

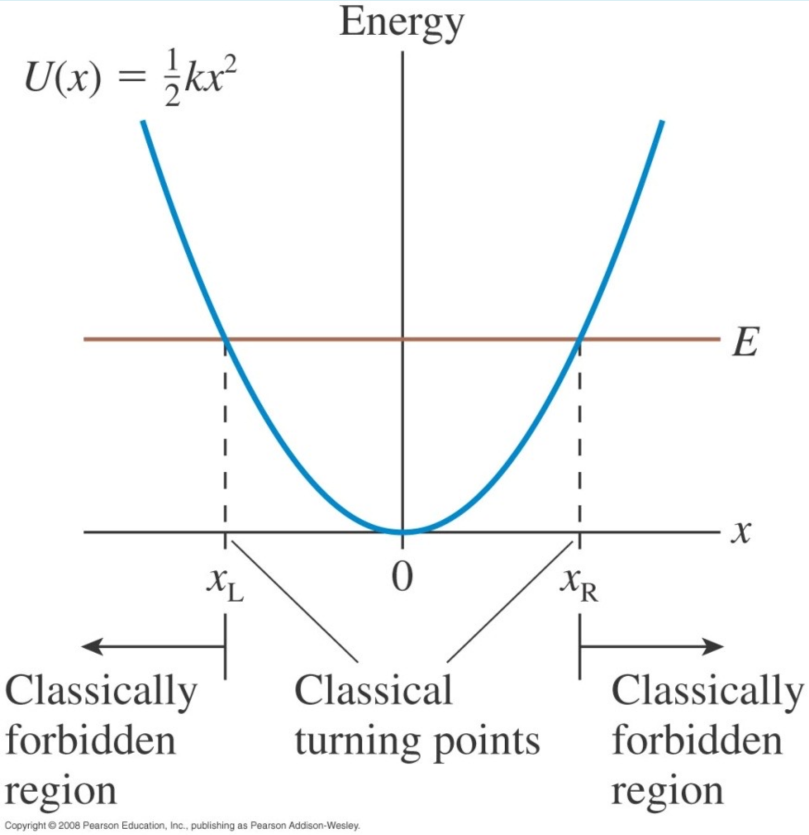
In Chapter 2 we considered the Boltzmann, Einstein, and Debye models of vibrations in solids. In this chapter we will consider a more detailed model of vibration in a solid, first classically, and then quantum-

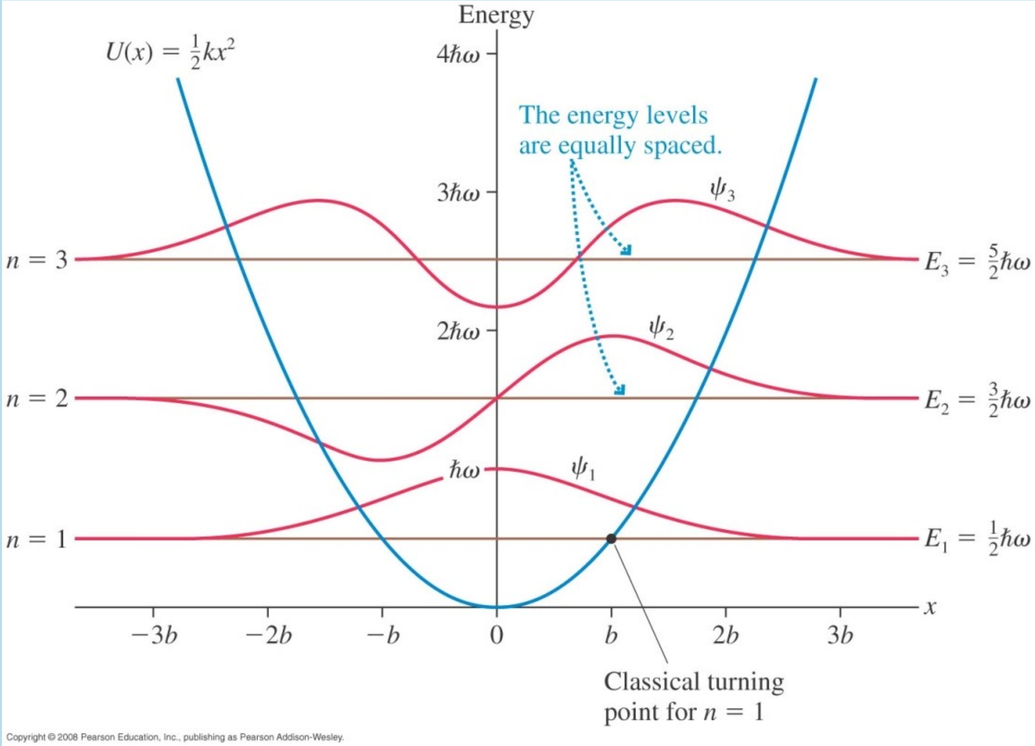


量子簡諧振盪器Simple Harmonic Oscillator SHO、量子彈簧

$$\frac{d^2\psi_E}{dx^2} = \frac{2m}{\hbar^2}\left(\frac{1}{2}kx^2 - E\right)\psi_E$$







$$E_n = \left(n - \frac{1}{1}\right)\hbar\omega$$

波函數會進入古典禁止區域

能量是量子化的！

Villa Herwig, Arosa Switzerland 1925

薛丁格從無到有 from scratch猜出一個波方程式：

Schrodinger Wave Equation

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

注意：波函數是複數！

1926. № 6.

ANNALEN DER PHYSIK.

VIERTE FOLGE. BAND 79.

1. *Quantisierung als Eigenwertproblem;*
von E. Schrödinger.

(Zweite Mitteilung.)[1]

Quantisation as an eigenvalue problem;
by E. Schrödinger*

1. Der Plancksche Oszillator. Die Entartungsfrage.

Wir behandeln zunächst den eindimensionalen Oszillator. Die Koordinate q sei die Elongation multipliziert mit der Quadratwurzel aus der Masse. Die beiden Formen der kinetischen Energie sind dann

$$\bar{T} = {}^1/_2\,\dot{q}^2\,, \qquad T = {}^1/_2\,p^2\,. \tag{20}$$

Die potentielle Energie sei

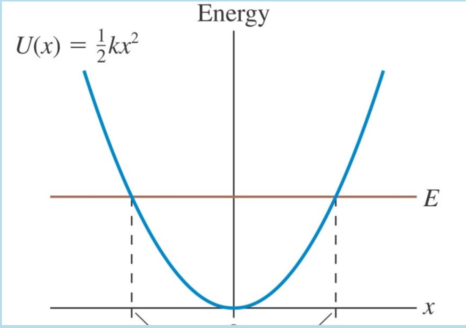
$$V(q) = 2\pi^2 \nu_0^2 q^2\,, \tag{21}$$

wo ν_0 die Eigenfrequenz im Sinne der Mechanik. Dann lautet Gleichung (18) für diesen Fall:

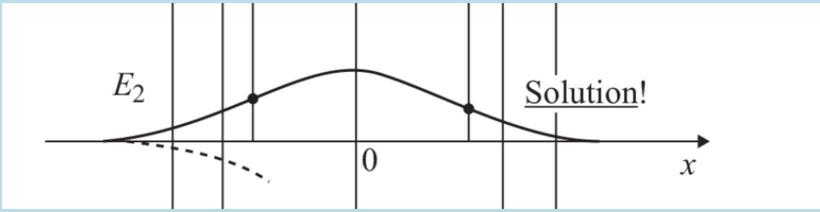
$$\frac{d^2\psi}{dq^2} + \frac{8\pi^2}{h^2}(E - 2\pi^2\nu_0^2 q^2)\,\psi = 0\,. \tag{22}$$

先讓我們定性的來猜一下它的解。

彈力位能是左右對稱的，對稱點在原點：$x = 0$。



物理結果應該左右對稱，所以，定態方程式的解或許也是對稱的？例如：

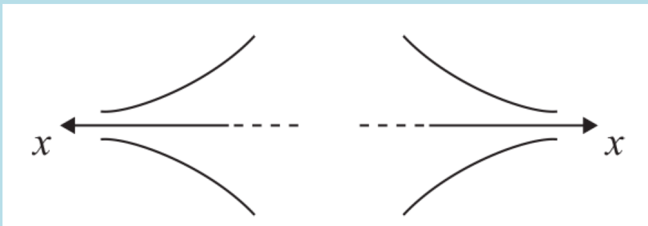


這樣的對稱的解稱為：偶函數。

偶函數在原點的斜率必須為零！斜率在原點才能連續。

可以猜想到，在無限限遠處，波函數解ψ及其斜率ψ'會漸漸趨近於零。

$x \to \infty, \psi, \psi' \to 0$，如下：



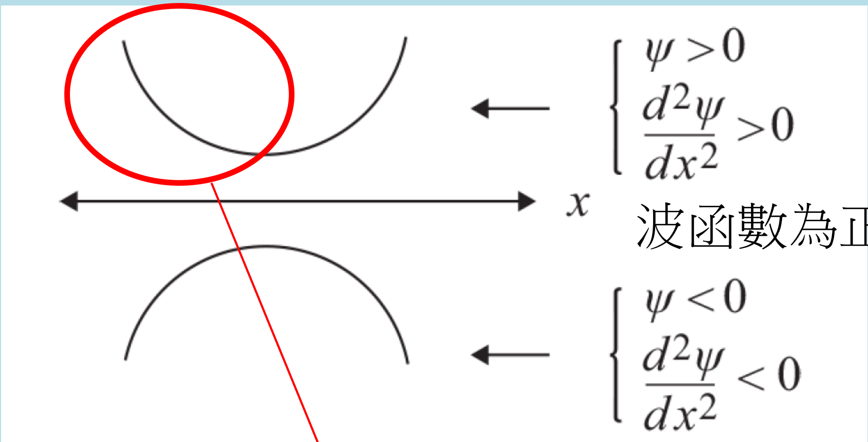
在$x \to -\infty$附近，會與$x \to \infty$對稱！

在$x \to \pm\infty$兩者之間，解的變化就由方程式決定，我們也有一些定性的了解：

$$\frac{d^2\psi_E}{dx^2} = \frac{2m}{\hbar^2}(V(x) - E)\psi_E \qquad \frac{\psi''}{\psi} = \frac{2m}{\hbar^2}[V(x) - E]$$

$V(x) - E$的正負號會決定$\frac{\psi''}{\psi}$的正負號！而ψ''是斜率的變化！

若$V(x) > E$，這是古典不容許的區域！

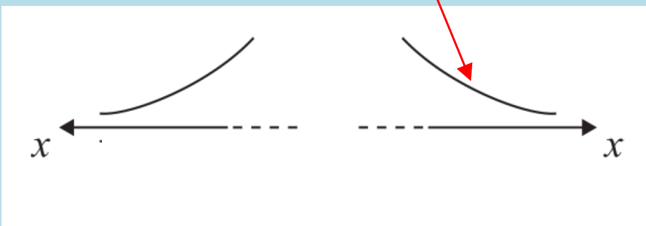


波函數為正，ψ''為正，x增加時，斜率增加！

波函數為負，ψ''為負，x增加時，斜率減小！

通常就說：x增加時，波函數會趨離x軸而彎曲。

$+\infty$處就是這樣的例子：x增加時，負的斜率增加，傾斜度減小到零，

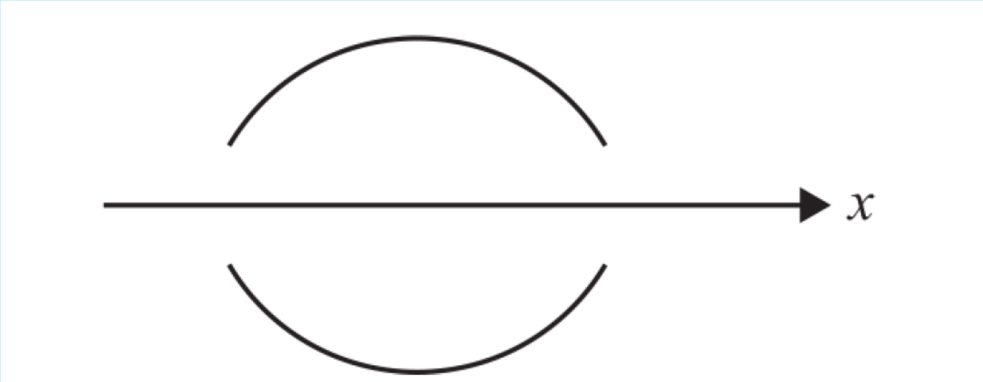


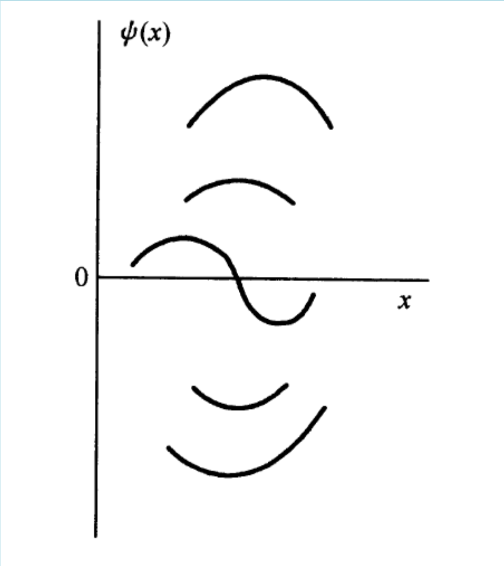
定性上類似指數遞減。

$$\frac{\psi''}{\psi} = \frac{2m}{\hbar^2}[V(x) - E]$$

$V(x) < E$的區域是古典容許的！

波函數ψ為正時，ψ''為負，x增加時，斜率減小！





波函數ψ為負時，ψ''為正，x增加時，斜率增加！

x增加時，波函數會趨向x軸而彎曲，。

穿過x軸後又會趨向x軸彎曲，再一次又穿過x軸，典型的情況會來回穿過x軸。

結論：在古典不容許的區域，定性上類似指數遞減！

在古典容許的區域，定性上類似來回振盪！

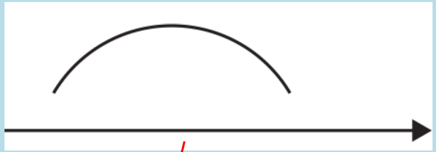
策略：考慮一系列的能量值，大小不同，因此折返點不同。

已知當$x \to \infty$， 波函數解ψ及其斜率ψ'會趨近於零。

從$x \to \infty$出發向內朝原點前進，以斜率變化ψ''的正負，定性得到函數的行為。

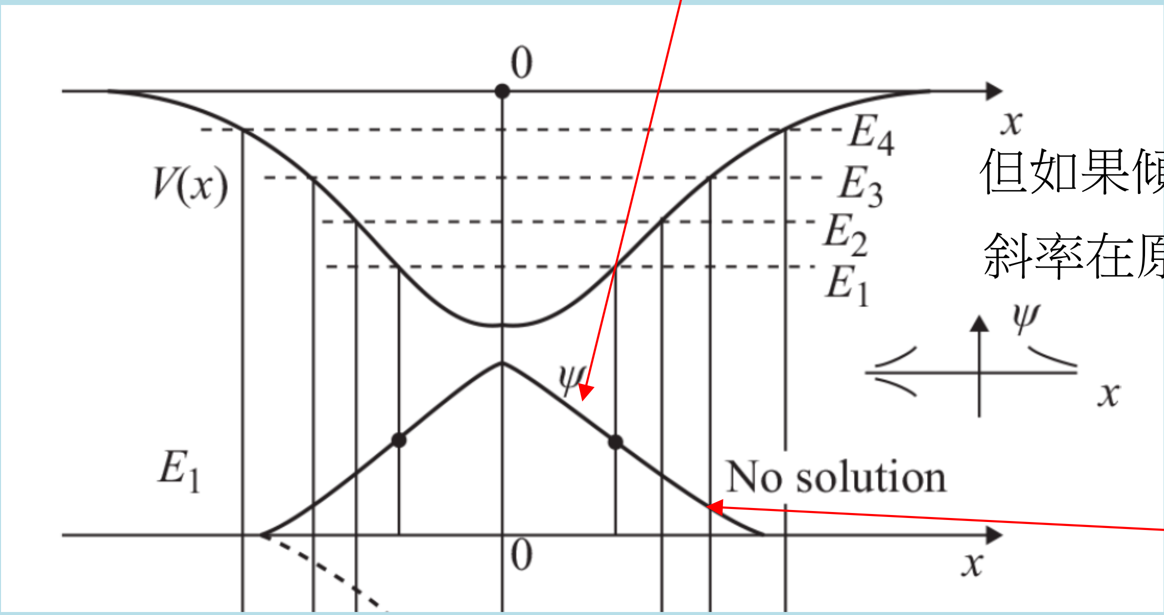
而當地$V(x) - E$的正負號，也就是是否為古典容許區域，會決定$\frac{\psi''}{\psi}$的正負號！

對於E_1：



在折返點內，曲線趨向x軸彎曲。

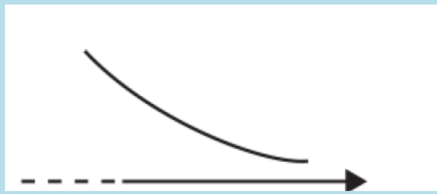
向原點靠近時，傾斜度又開始漸漸下降！



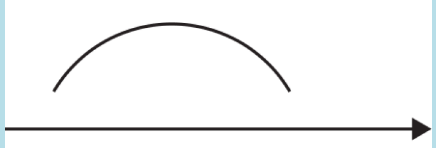
但如果傾斜度到達原點，來不及降為零！

斜率在原點就無法連續，此解不成立！

對於E_1，沒有解！



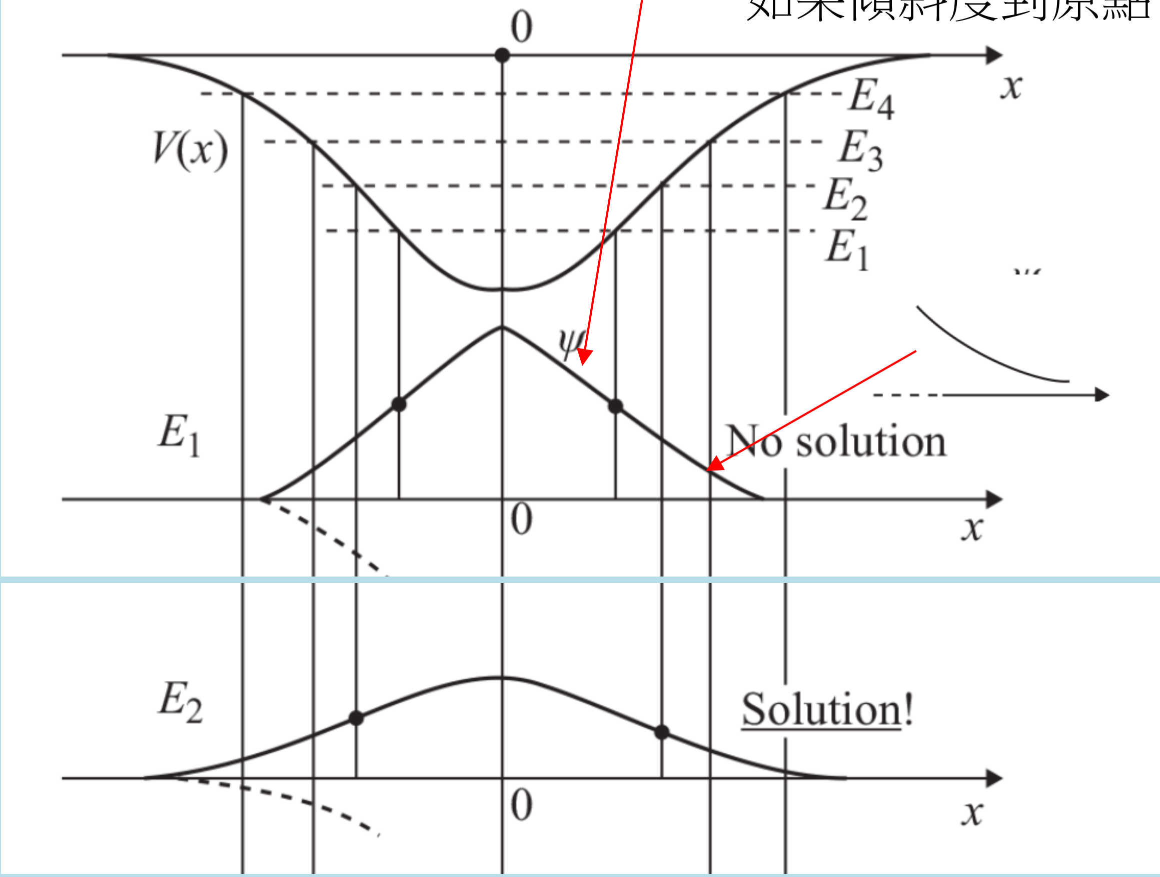
折返點外，$x \to \infty$，傾斜度漸漸趨近零！向內走，傾斜度漸漸增加。



由遠處向原點靠近，傾斜度漸漸增加！

到折返點後，傾斜度又漸漸減小。

如果傾斜度到原點，來不及降為零，解不成立。



對於E_2，折返點右移！

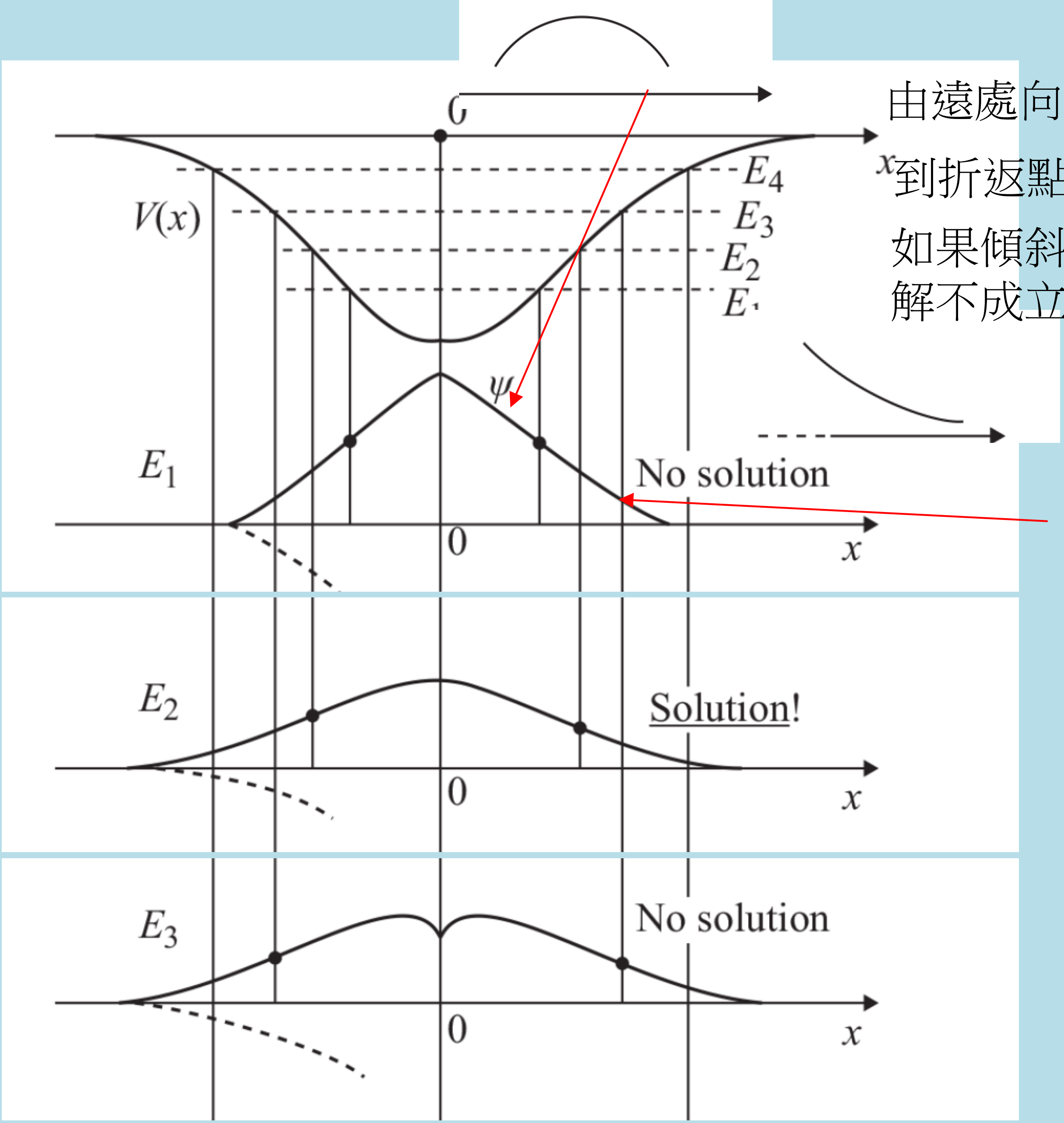
傾斜度有較大間隔下降！

傾斜度在原點恰好降為零！

$E = E_2$，定態方程式有解！

所以條件必須剛好成立，定態方程式才會有解！

能量必須恰好使得傾斜度在∞由零加大，在折返點開始減小，到原點恰好減到零！



由遠處向原點靠近，傾斜度漸漸增加！

到折返點後，傾斜度又漸漸減小。

如果傾斜度到原點，來不及降為零，解不成立。

對於E_2，折返點右移！

傾斜度有較大間隔下降！

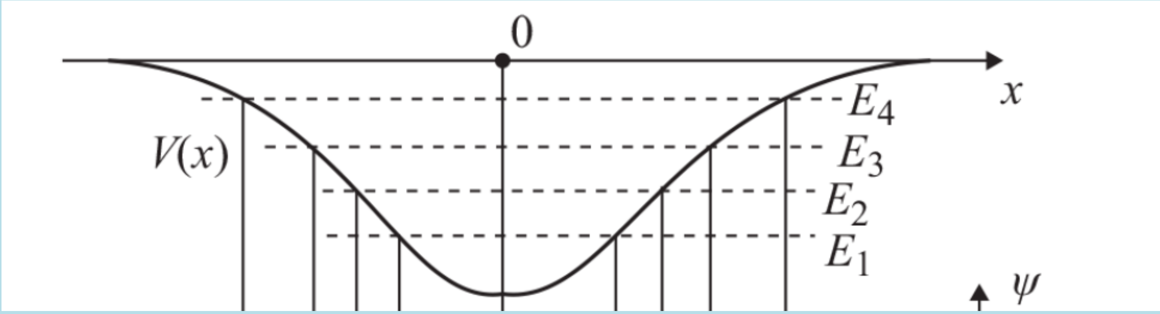
傾斜度在原點恰好降為零！

$E = E_2$，定態方程式有解！

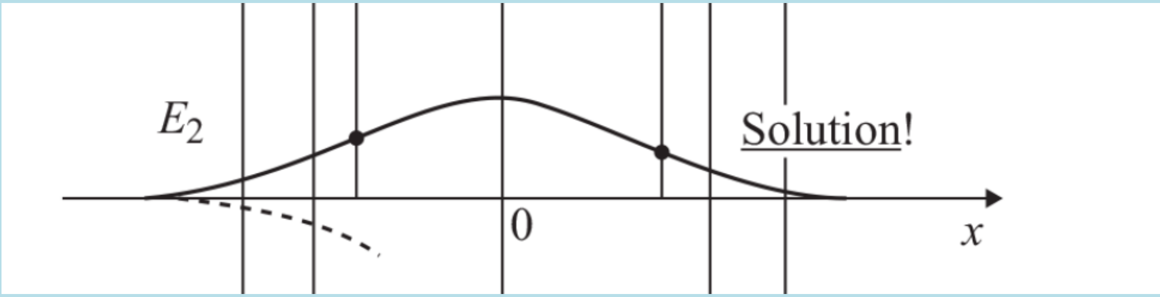
對於大於E_2的E_3，斜率在原點前變號！但函數不為零，解又不成立了。

在以上的範圍，能量只能是E_2，大一點小一點都不行，能量是量子化的。

位能左右對稱，



定態方程式的解是對稱的：偶函數。



見課本3-6

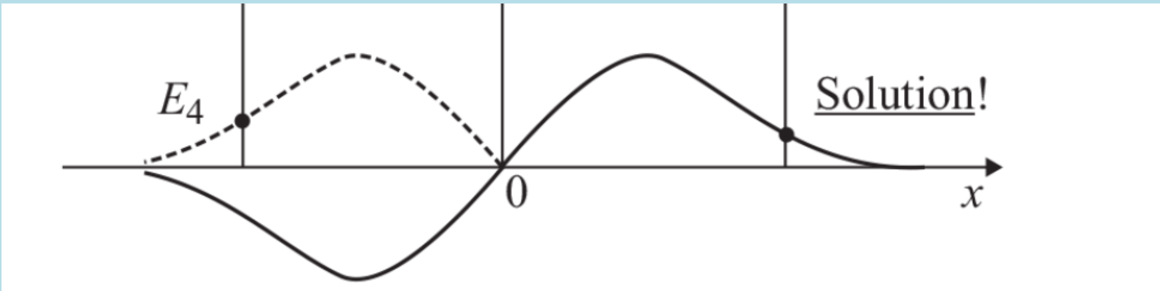
有較細緻的討論。

偶函數在原點的斜率必須為零！

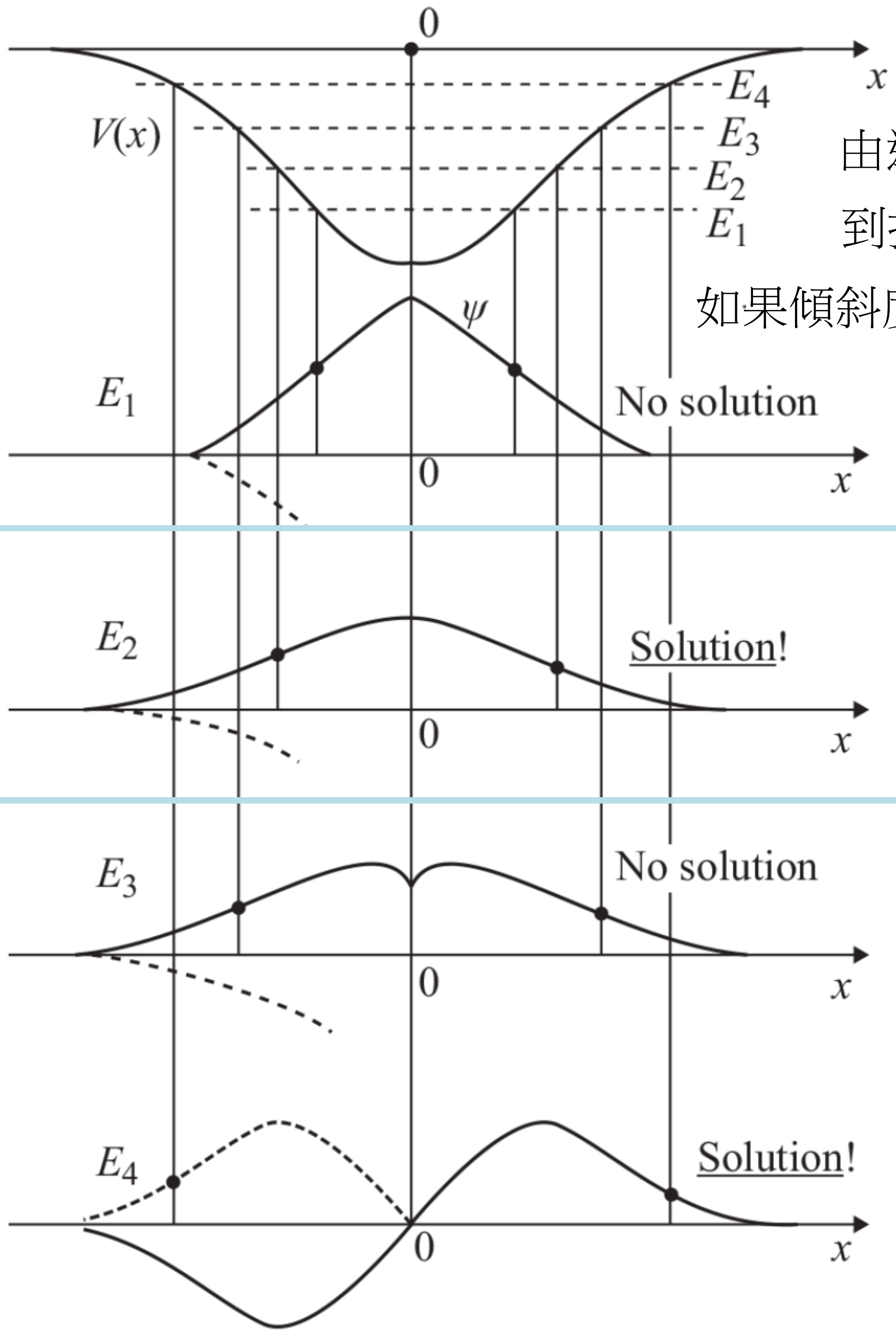
物理應該對稱，但物理是由狀態函數的平方決定，

狀態波函數也可以是反對稱，意思是右邊函數式左邊函數乘-1。

定態方程式的解也可以反對稱的：稱為奇函數，例如：



但注意！如此奇函數在原點的函數值必須為零！



由遠處向原點靠近，傾斜度漸漸增加！

到折返點後，傾斜度又漸漸減小。

如果傾斜度到原點，來不及降為零，解不成立。

對於E_2，折返點右移！

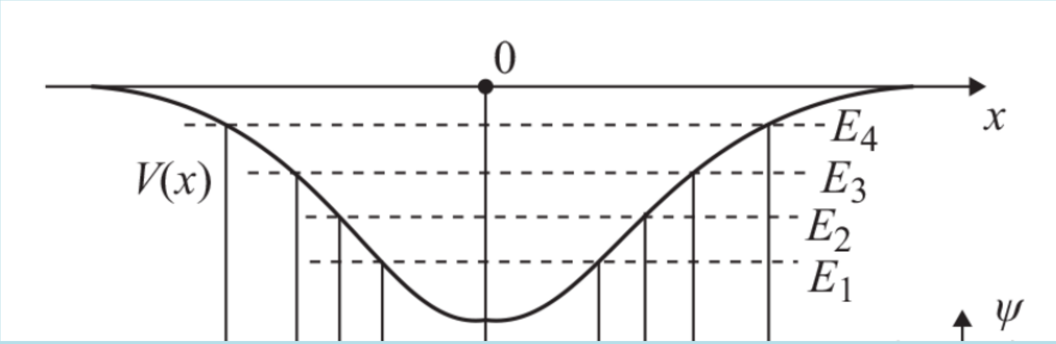
傾斜度有較大間隔下降！

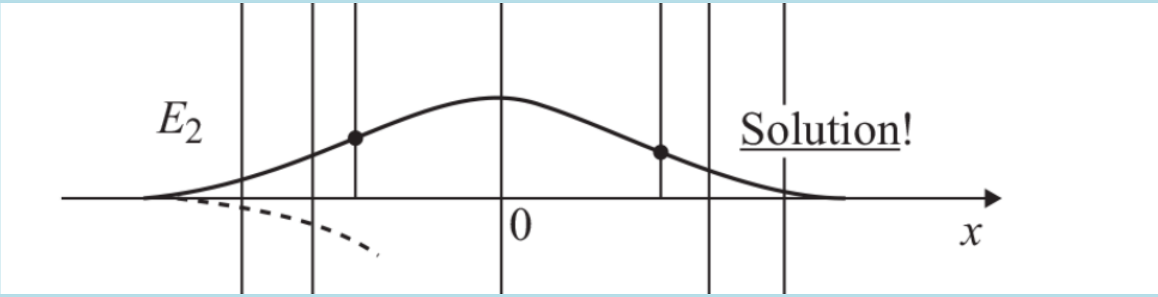
傾斜度在原點恰好降為零！

$E = E_2$，定態方程式有解！

對於大於E_2的E_3，斜率在原點前變號，但函數不為零！解不成立。

但直到某更大的E_4，原點函數值降為零，此解成立。是一奇函數解！

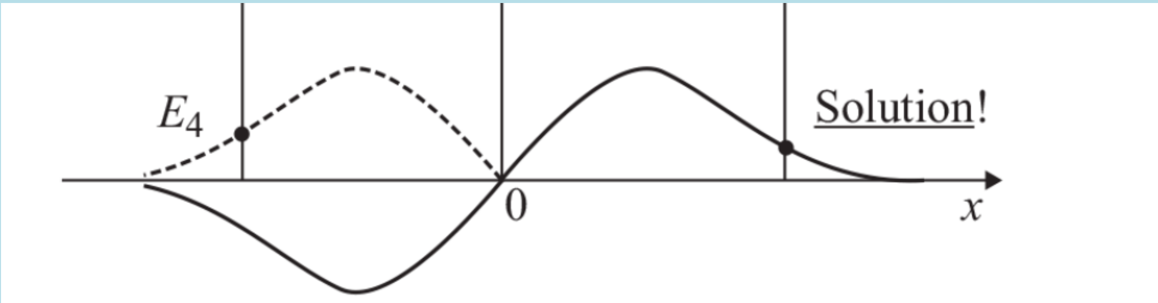




這是偶函數。

所以條件必須剛好成立，定態方程式才會有解！

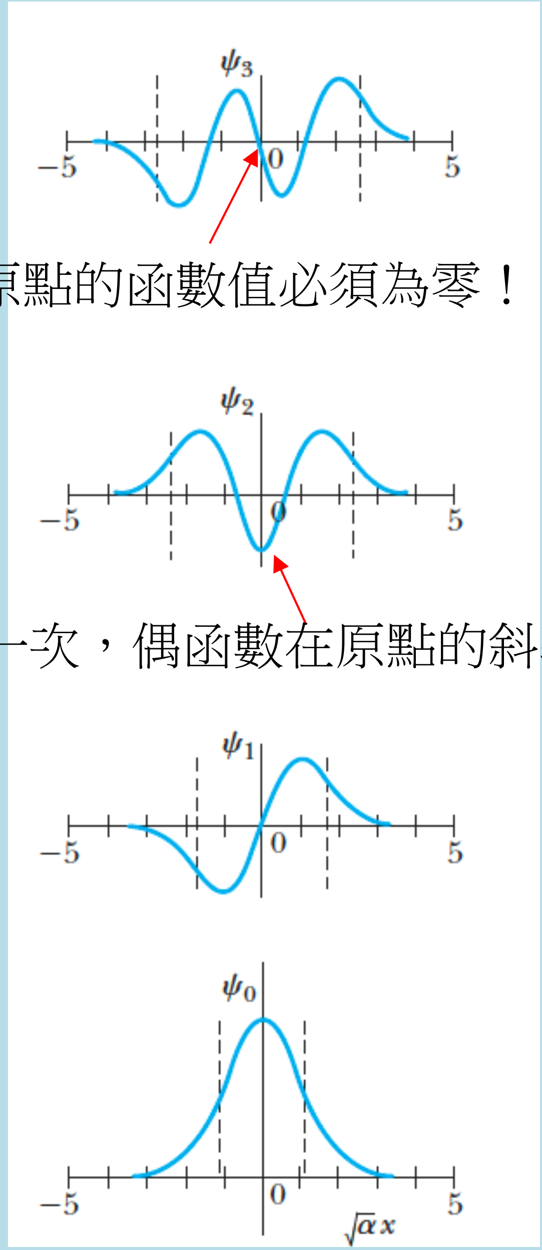
能量必須恰好使得傾斜度在∞由零加大，在折返點開始減小，到原點恰好減到零！



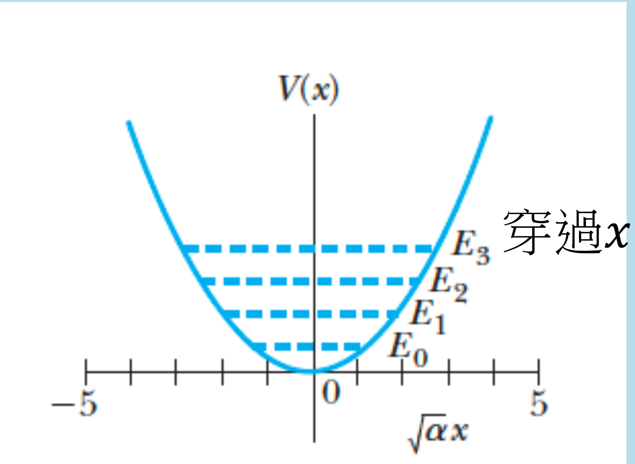
這是奇函數。

能量必須使得傾斜度在∞由零加大，在折返點開始減小直到變號，

函數值開始減小，同時使函數值在原點洽降到零！

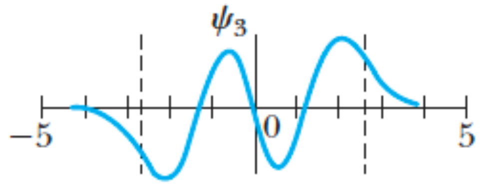


穿過x軸一次，奇函數在原點的函數值必須為零！

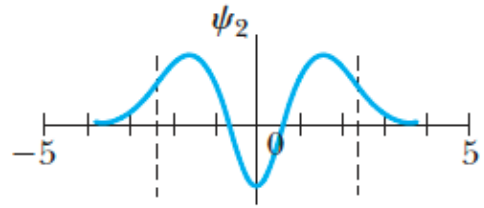


穿過x軸一次，偶函數在原點的斜率必須為零！

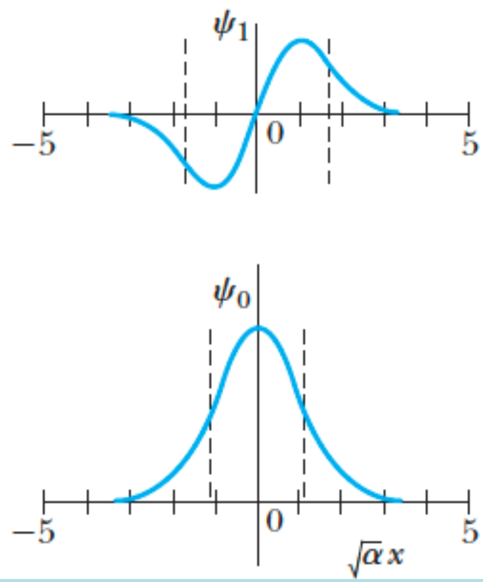
能量再增加，折返點距原點越遠，函數曲線可以來回穿過x軸數次，
但必須滿足以上條件才是解。



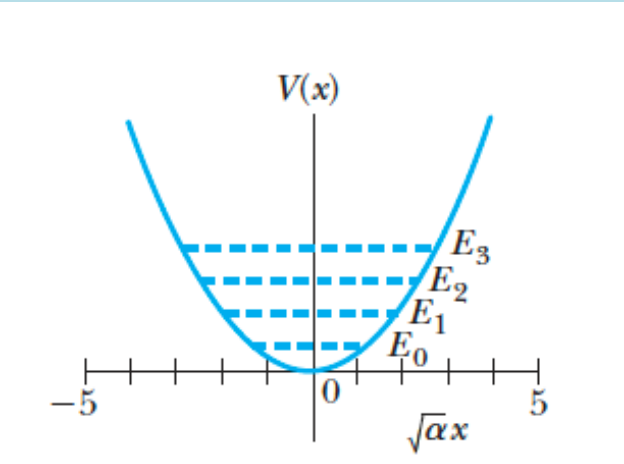
穿過x軸一次後使奇函數在原點的函數值為零！ 此能量給出一個解，共穿過x軸三次。

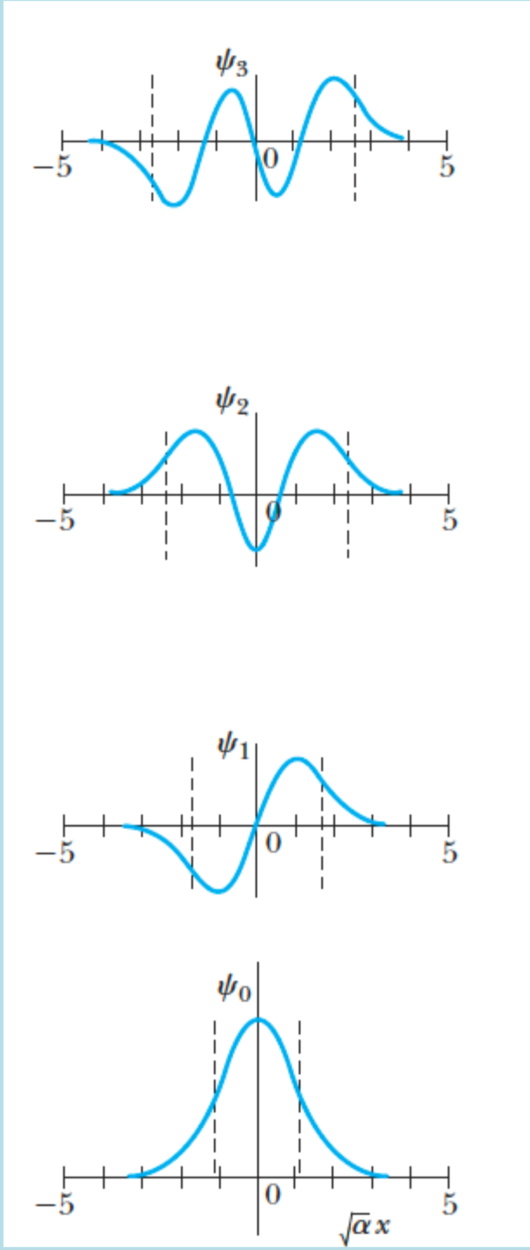


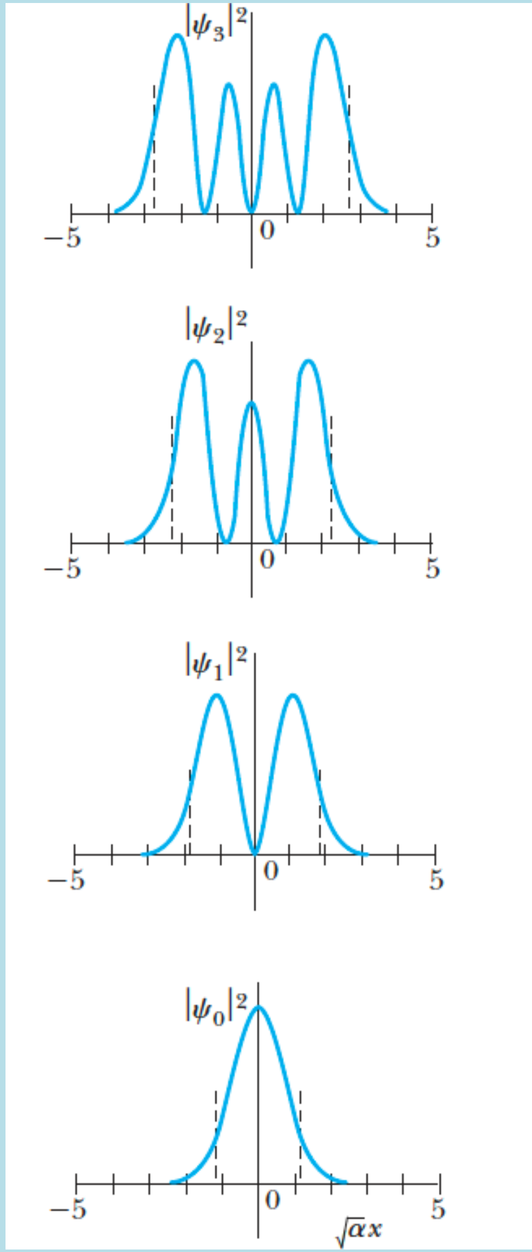
穿過x軸一次後使偶函數在原點的斜率為零！此能量給出一個解，共穿過x軸二次。



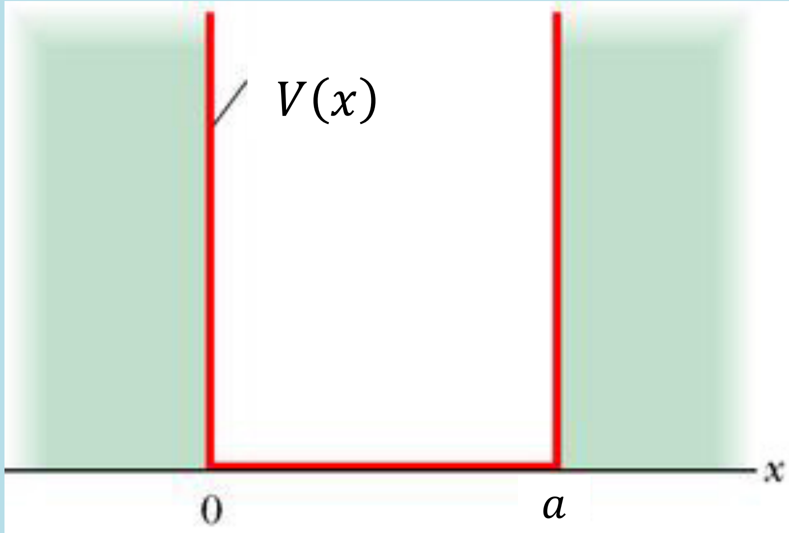
第n個能階定態解會有個$n-1$個Node節點。

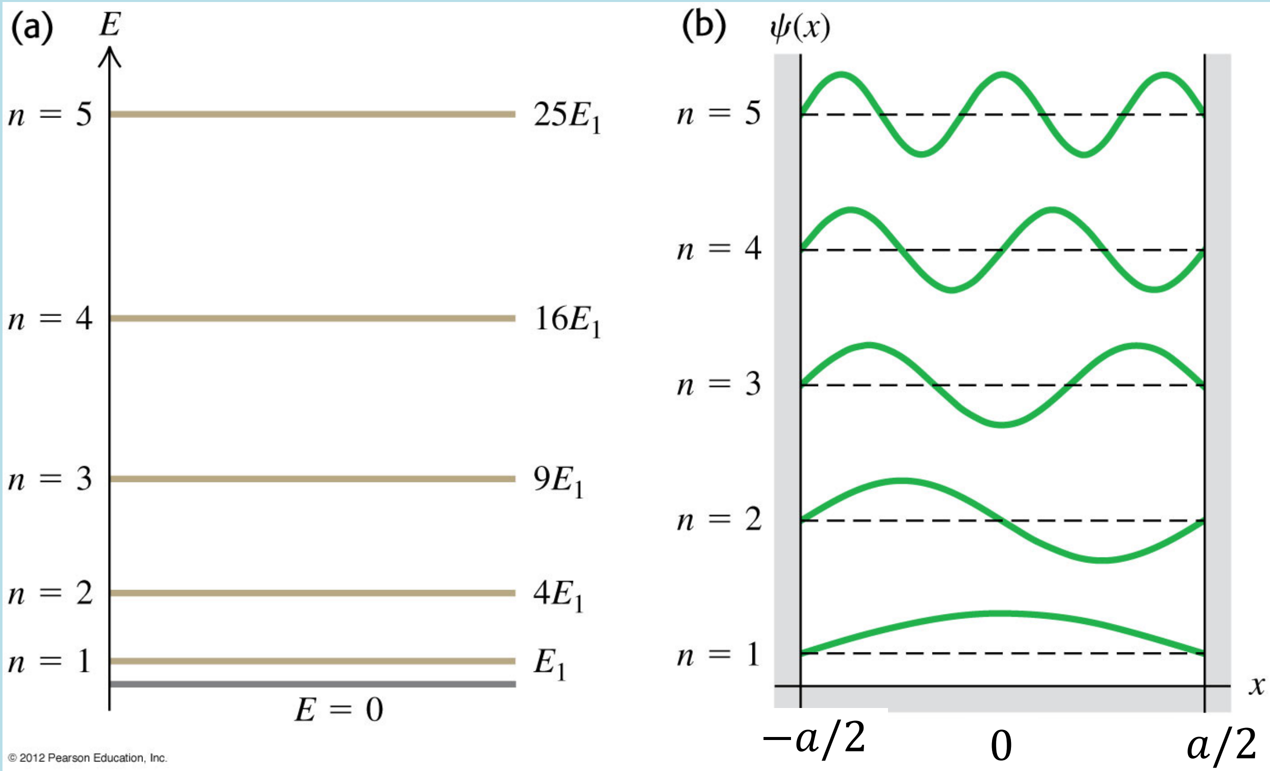






偶函數、奇函數隨能量增加間隔出現！

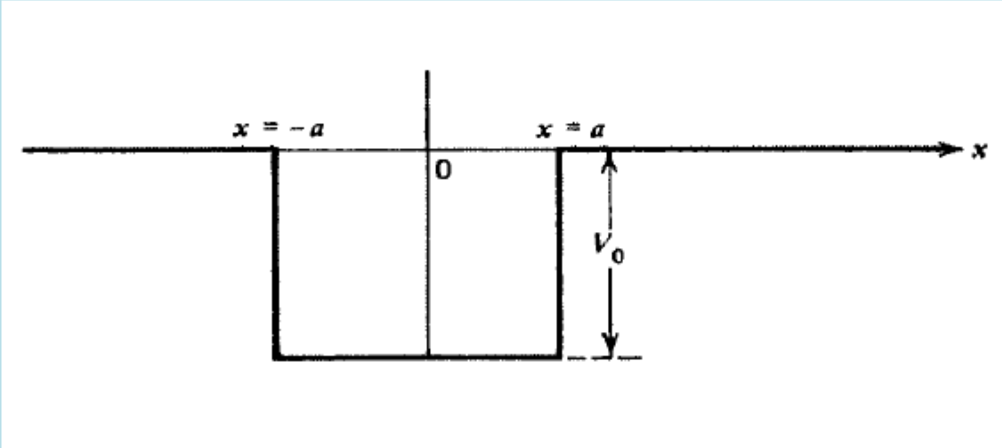




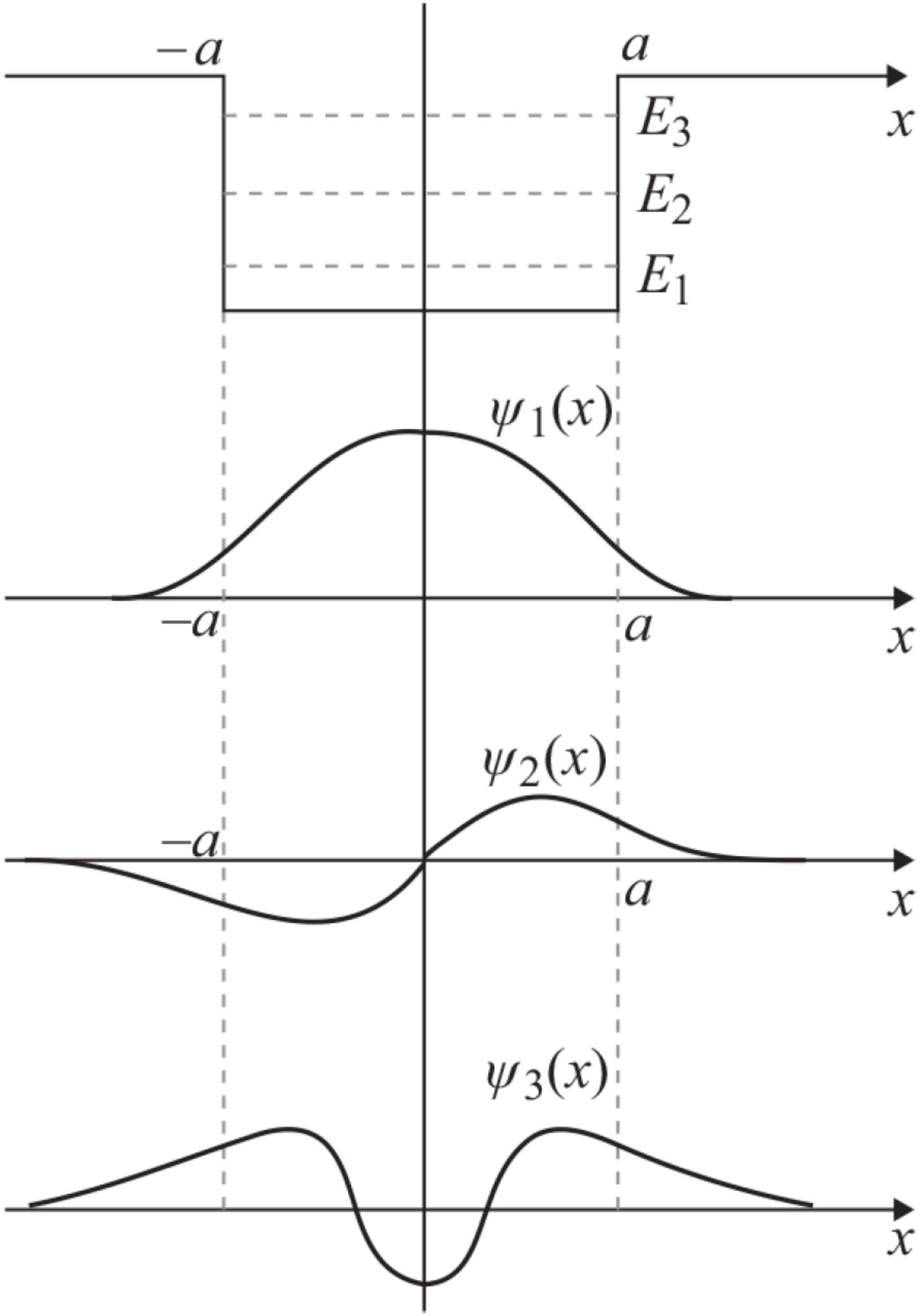
能量只有在這些值，定態方程式才有滿足邊界條件的解！

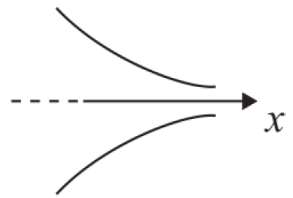
偶函數、奇函數也是間隔分佈！　　第n個能階定態解會有個$n-1$個Node節點。

有限位能井 Finite Potential Well



$$
\begin{aligned}
V(x) &= 0 && x < -a \\
&= -V_0 && -a < x < a \\
&= 0 && a < x
\end{aligned}
$$





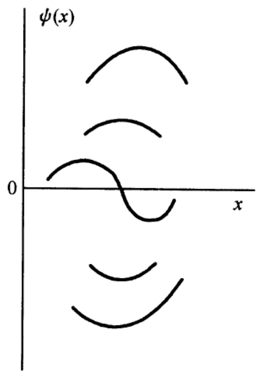
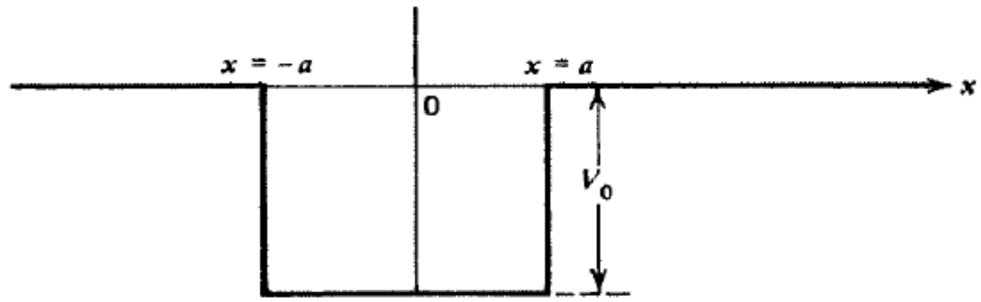


Figure 6.7

Sketching eigenstates of a finite square well potential. The energies are $E_1 < E_2 < E_3$, and the corresponding eigenstates are ψ_1, ψ_2, and ψ_3, with ψ_1 the ground state.

有限位能井 Finite Potential Well



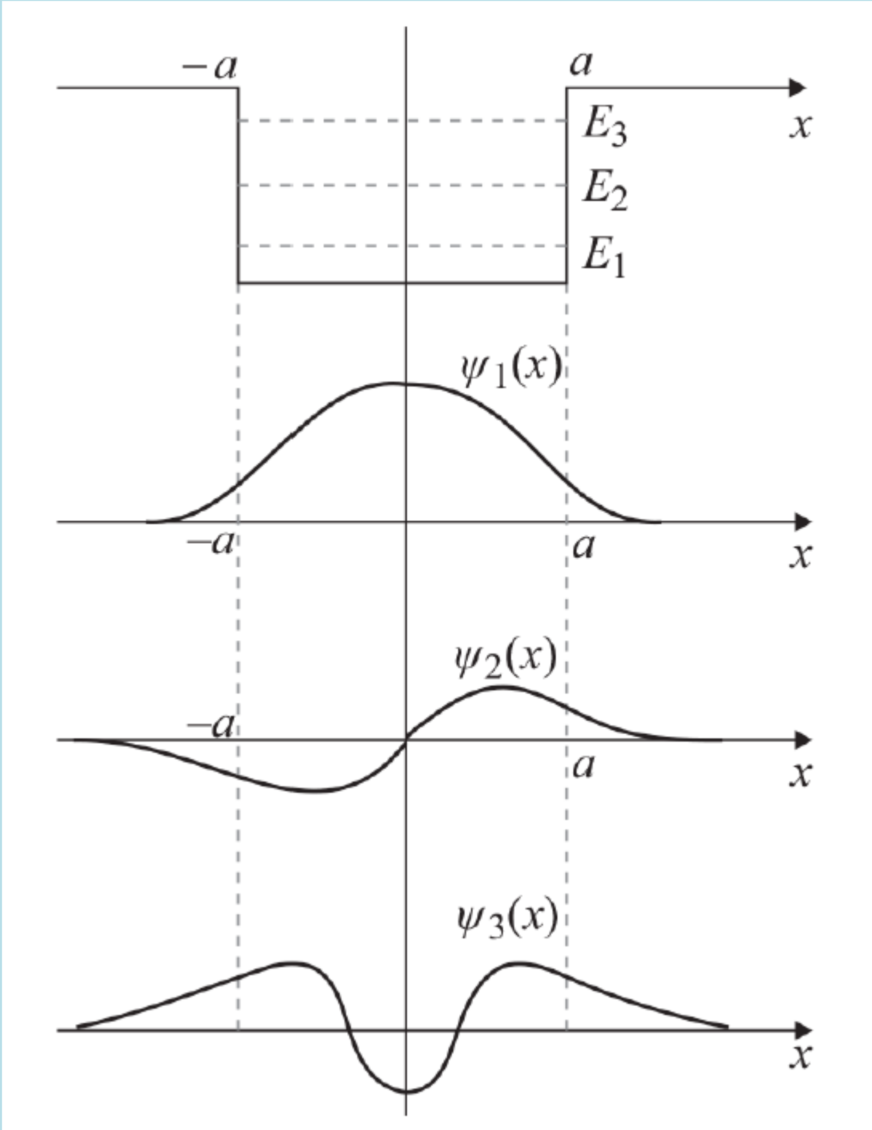
$$
\begin{aligned}
V(x) &= 0 & x &< -a \\
&= -V_0 & -a < x &< a \\
&= 0 & a &< x
\end{aligned}
$$

functions. To solve the Schrödinger equation, we have to examine how the equation looks in the various regions where the potential is constant and then use boundary conditions to match the solutions across the points where the potential is discontinuous. We have the equation

一維位能的問題有時可以分解為一段段常數位能的區域，可以分開求解。

然後在邊界處，以連續條件將得到的各個解聯(match)起來。

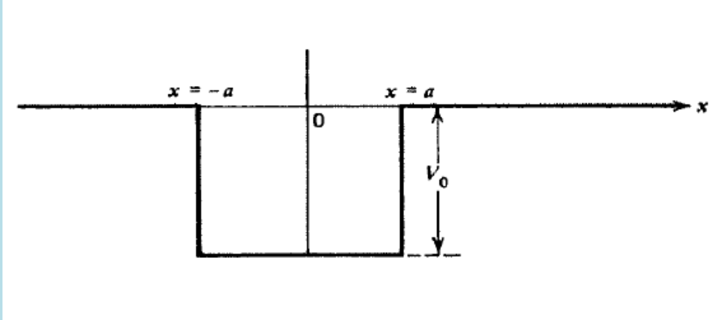
首先考慮$E < 0$，能量可能為離散的定態



在位能井內，電子如同自由粒子！

$-a < x < a$　　$0 > E > V = -V_0$

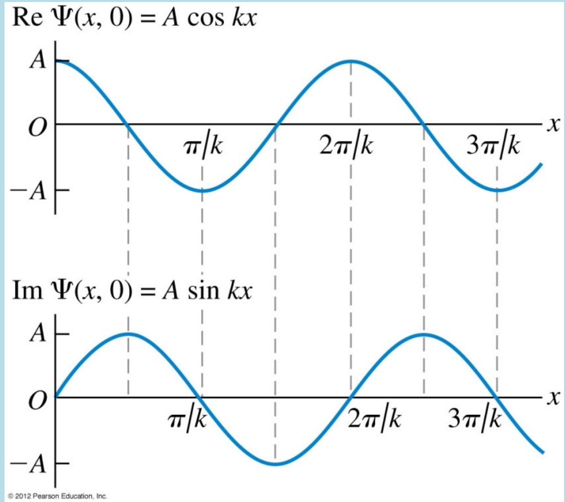
在此區域古典的粒子可以存在。



$$\frac{d^2\psi_E}{dx^2} = \frac{2m}{\hbar^2}[V - E]\psi_E = -\frac{2m}{\hbar^2}[V_0 - |E|]\psi_E$$

$$\frac{d^2\psi_E}{dx^2} = -q^2\psi_E \qquad q \equiv \sqrt{\frac{2m}{\hbar^2}(V_0 - |E|)}$$

解也如同自由粒子波！



$$\psi_E = C_1 e^{iqx} + C_2 e^{-iqx}$$

$$= A\cos qx + B\sin qx$$

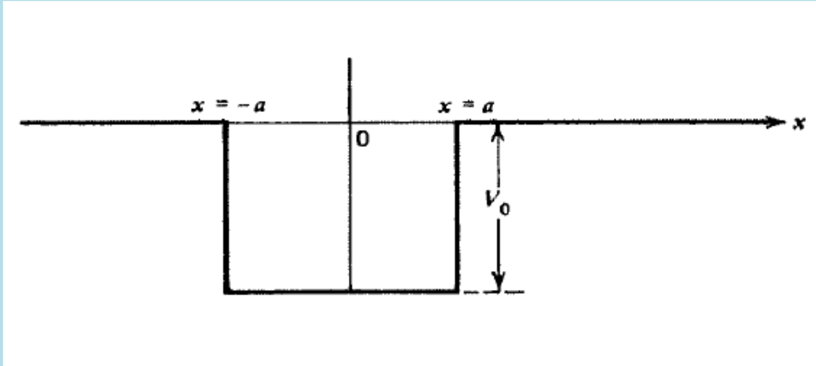
這兩個解分別是偶函數與奇函數。

可以分開考慮！

從偶函數開始：$\psi_E = A\cos qx$

在位能井外：

$x < -a$, 及 $x > a$　　$E < V = 0$



古典的粒子不能存在這樣的區域，

方程式差一個負號！

$$\frac{d^2\psi_E}{dx^2} = \alpha^2\psi_E \quad E)\psi_E \equiv \alpha^2\psi_E$$

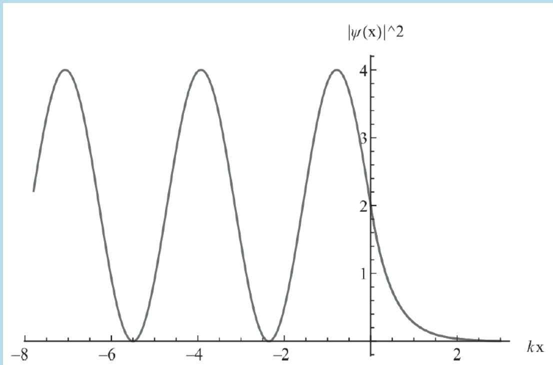
$$\alpha \equiv \sqrt{\frac{2m}{\hbar^2}|E|}$$

$$\psi_E(x) = C_1 e^{\alpha x} + C_2 e^{-\alpha x}$$

為使無限遠處，波函數不發散：

$x > a$　　$\psi_E(x) = C_2 e^{-\alpha x}$

$x < -a$　　$\psi_E(x) = C_1 e^{\alpha x}$



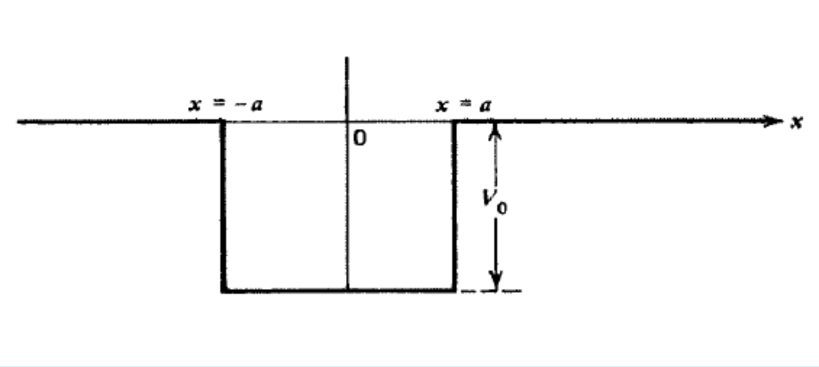
古典粒子不能存在，就表現在波函數指數遞減之上！

在量子力學中，此區域波函數還是有解，只是不再是正弦波，而是指數函數。

在位能井邊界上：

$x = -a$, 及 $x = a$

$\psi(x)$必須連續！



否則微分會是無限大，微分決定流量，不能是無限大。

先從偶函數開始討論：Even Function。

$x = a$

$\psi_E(x) = A\cos qx$ $\qquad$ $\psi_E(x) = C_2 e^{-\alpha x}$

$$A\cos qa = C_2 e^{-\alpha a}$$

$x = -a$

$\psi_E(x) = A\cos qx$ $\qquad$ $\psi_E(x) = C_1 e^{\alpha x}$

$$A\cos qa = C_1 e^{-\alpha a}$$

兩邊對稱，解是一樣的！只要考慮一邊即可。

$x = a$ $\psi(x)$與其微分都必須連續！

$\psi'_E(x) = -Aq\sin qx$ $\psi'_E(x) = -\alpha C_2 e^{-\alpha x}$

$Aq\sin qa = \alpha C_2 e^{-\alpha a}$

$\psi(x)$連續的條件：

$A\cos qa = C_2 e^{-\alpha a}$

兩式相除，即消去常數：

$q\tan qa = \alpha$

$$\alpha \equiv \sqrt{\frac{2m}{\hbar^2}|E|}$$

$$q \equiv \sqrt{\frac{2m}{\hbar^2}(V_0 - |E|)}$$

注意角波數q與α都是隨能量E變化的變數，而E是我們要由上式求解的對象。

角波數q，可轉為無單位的數值變數 y ：定義 $qa \equiv y$

$y\tan y = \alpha a$

另一個變數α可以用y表示出來，因為：

$$\alpha^2 + q^2 = \frac{2mV_0}{\hbar^2}$$

λ是常數！

$$\alpha a = \sqrt{\frac{2mV_0a^2}{\hbar^2} - y^2} \equiv \sqrt{\lambda - y^2}$$

$$y\tan y = \sqrt{\lambda - y^2}$$

$$y \tan y = \sqrt{\lambda - y^2}$$

$$\tan y = \frac{\sqrt{\lambda - y^2}}{y}$$

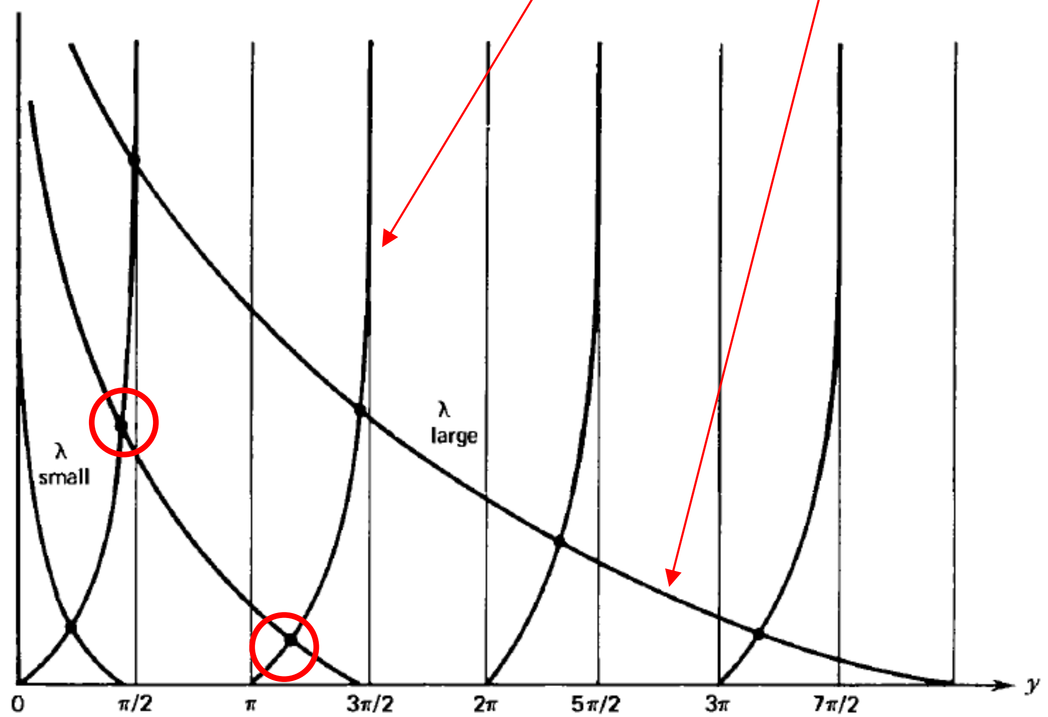


Figure 4-7 Location of discrete eigenvalues for even solutions in a square well. The rising curves represent tan y; the falling curves are $\sqrt{\lambda - y^2}/y$ for different values of λ.

$qa \equiv y$ 由y的解即得到q，也就得到E。

$x = a$ Odd Function

$$\psi_E(x) = A \sin qx$$

$$\psi'_E(x) = Aq \cos qx$$

$$\psi_E(x) = C_2 e^{-\alpha x}$$

$$\psi'_E(x) = -\alpha C_2 e^{-\alpha x}$$

$$\alpha \equiv \sqrt{\frac{2m}{\hbar^2}|E|}$$

$$q \equiv \sqrt{\frac{2m}{\hbar^2}(V_0 - |E|)}$$

$$A \sin qa = C_2 e^{-\alpha a}$$

$$Aq \cos qa = -\alpha C_2 e^{-\alpha a}$$

兩式相除，即消去常數：

$$q \cot qa = -\alpha$$

角波數q，可轉為無單位的數值變數 y ：定義 $qa \equiv y$

$$y \cot y = -\alpha a$$

另一個參數α可以用 y 表示出來，因為：

$$\alpha^2 + q^2 = \frac{2mV_0}{\hbar^2}$$

λ是常數！

$$\alpha a = \sqrt{\frac{2mV_0 a^2}{\hbar^2} - y^2} \equiv \sqrt{\lambda - y^2}$$

$$y \cot y = \sqrt{\lambda - y^2}$$

$$y\cot y = -\sqrt{\lambda - y^2} \quad \Rightarrow \quad -\cot y = \frac{\sqrt{\lambda - y^2}}{y}$$

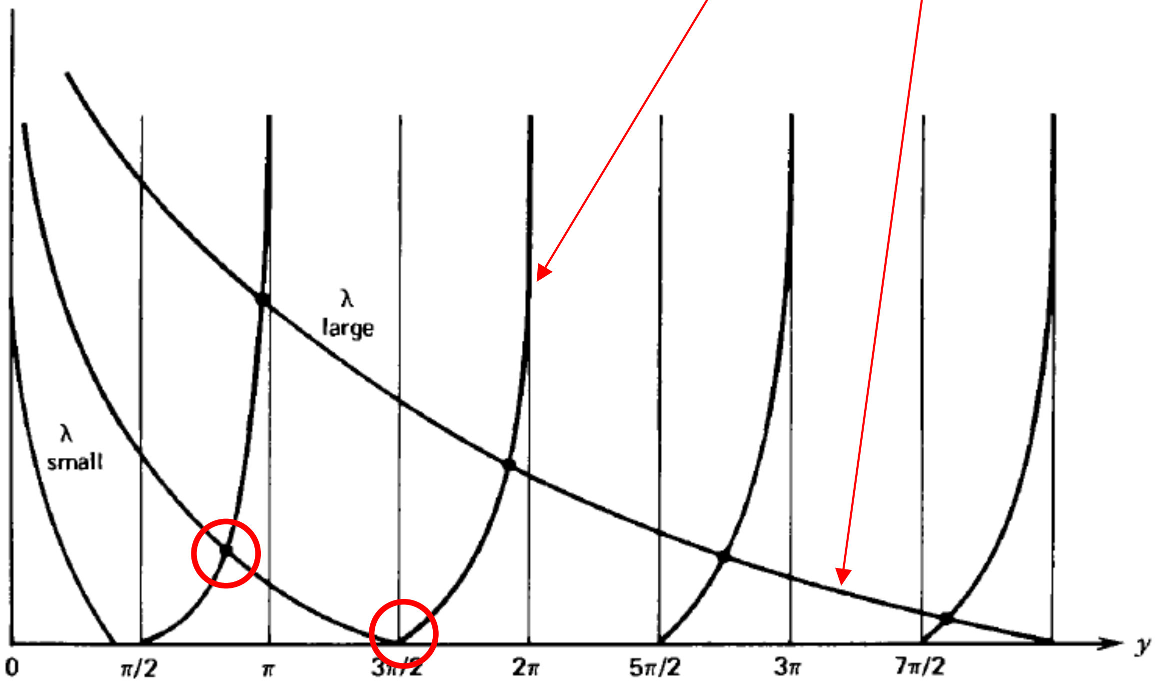
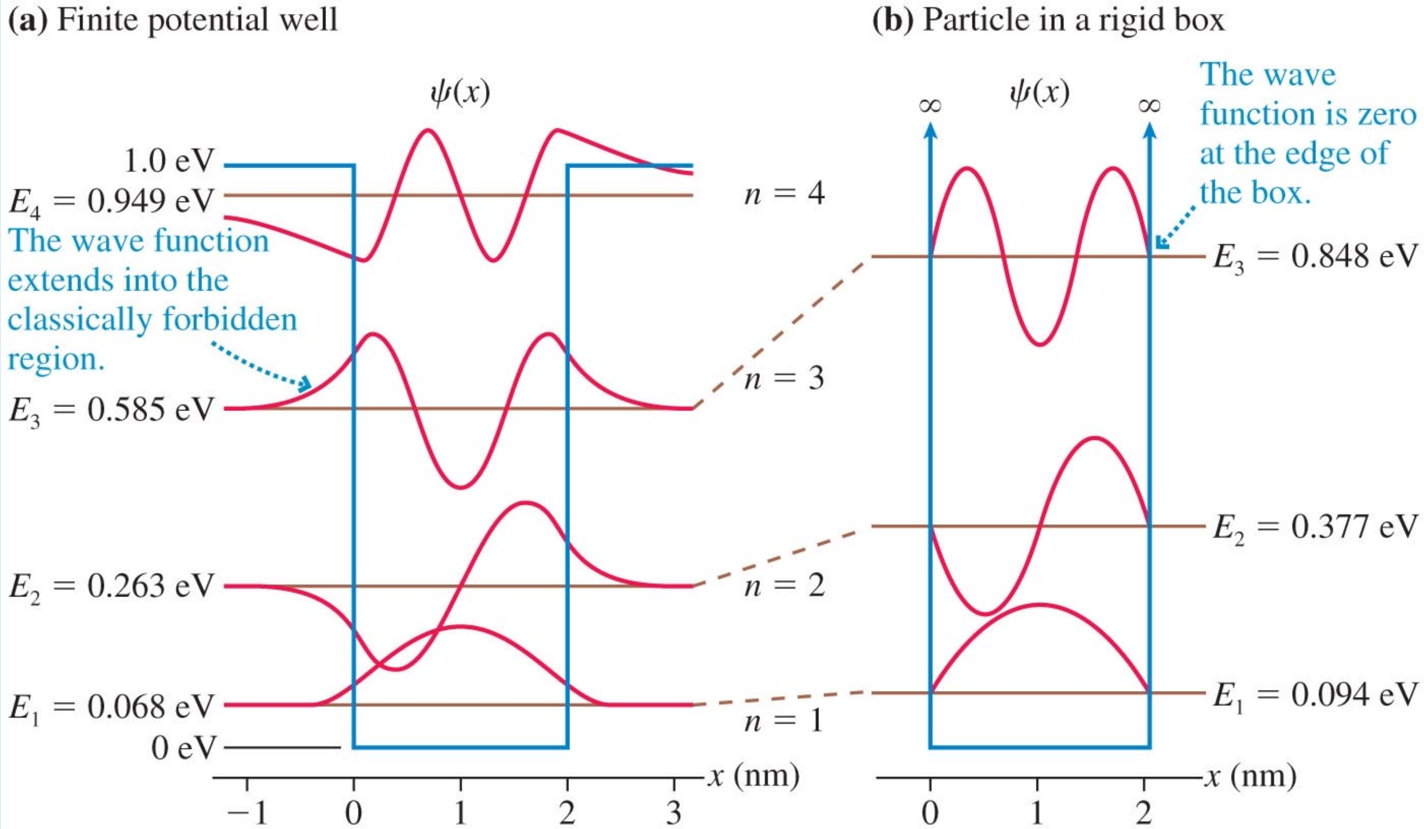
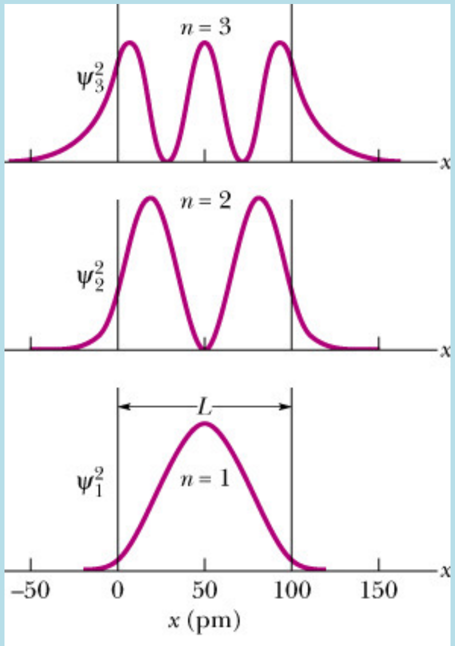


Figure 4-8 Location of discrete eigenvalues for odd solutions in a square well. The rising curves represent $-\cot y$; the falling curves are $\sqrt{\lambda - y^2}/y$ for different values of λ. Note that there is no eigenvalue for $\lambda < (\pi/2)^2$.

$qa \equiv y$　　由y的解即得到q，也就得到E。



(a) Finite potential well
(b) Particle in a rigid box
ψ(x)
1.0 eV
E4 = 0.949 eV
The wave function extends into the classically forbidden region.
E3 = 0.585 eV
E2 = 0.263 eV
E1 = 0.068 eV
0 eV
n = 4
n = 3
n = 2
n = 1
x (nm)
−1
0
1
2
3
∞
The wave function is zero at the edge of the box.
E3 = 0.848 eV
E2 = 0.377 eV
E1 = 0.094 eV



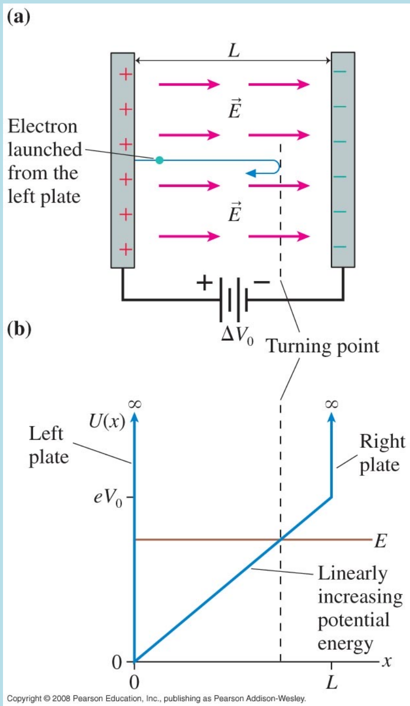
n = 3
ψ3²
n = 2
ψ2²
L
ψ1²
n = 1
x
–50
0
50
100
150
x (pm)

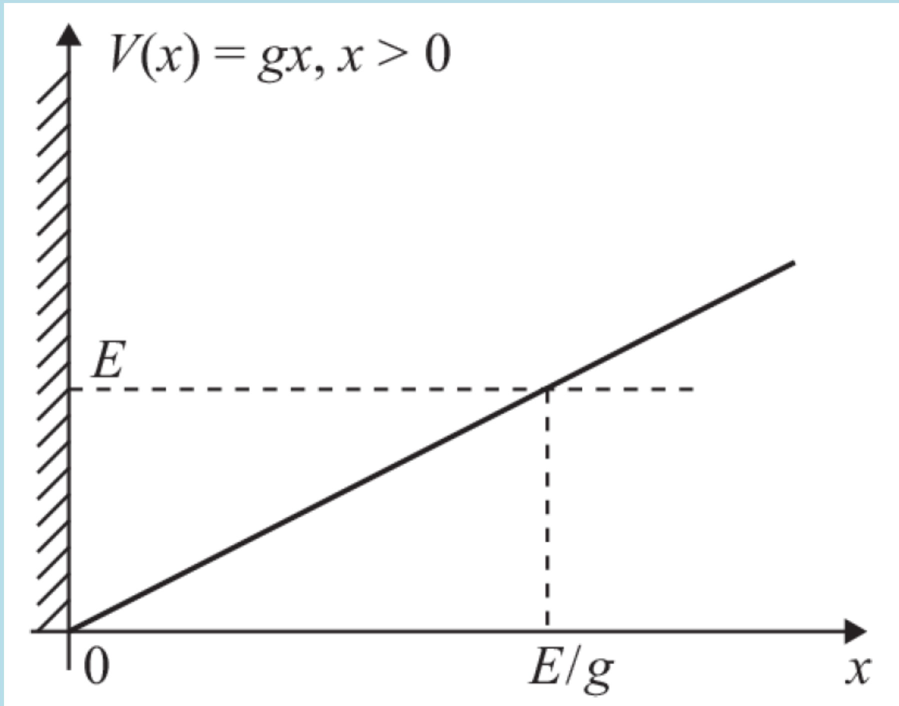
電容器中的電子

Linear Potential

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_E(x)}{dx^2}+V(x)\cdot\psi_E(x)=-\frac{\hbar^2}{2m}\frac{d^2\psi_E(x)}{dx^2}+\frac{eV_0}{L}x\cdot\psi_E(x)=E\cdot\psi_E(x)$$

The solution we have for step potential: $\psi_E = Ae^{ikx}+Re^{-ikx}$ *totally* cannot apply here. Some of you still copy here the formula $k\equiv\sqrt{\frac{2m(E-V(x))}{\hbar^2}}$. But it does not make sense.





定態方程式的解必須滿足在原點為零。

一邊是折返點，

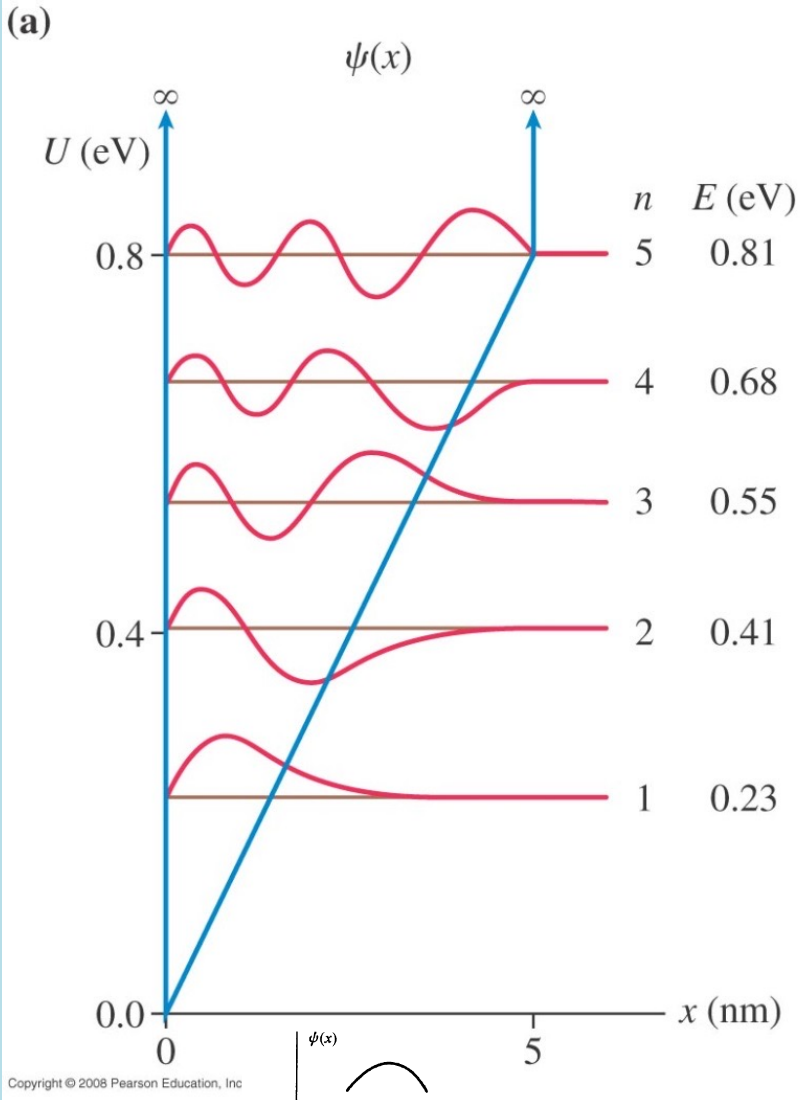
波函數指數遞減。

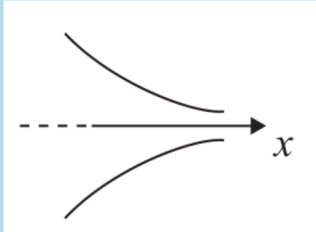
在容許區會來回振盪。

另一邊原點是無限大位能。

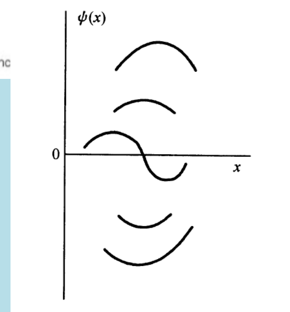
波函數必須降到零。

束縛態，能量量子化！





E_n能階定態解會有個$n-1$個Node節點。



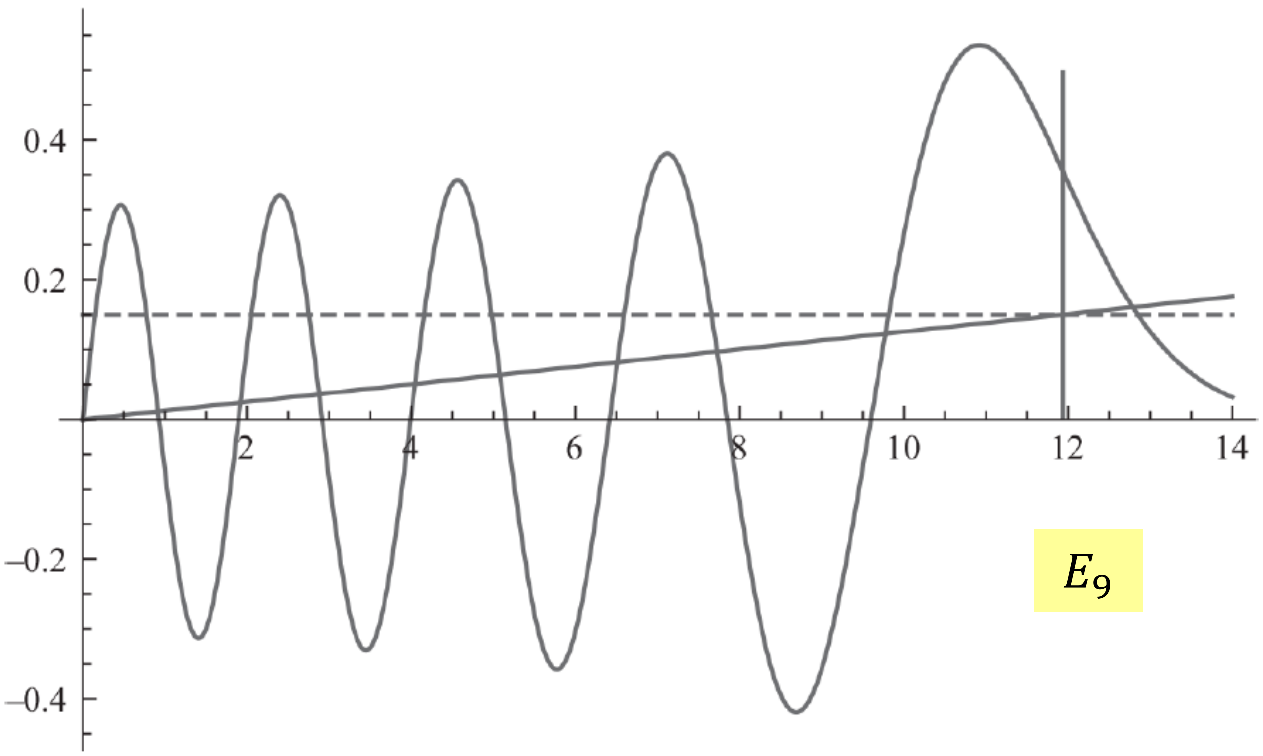


Figure 7.12
A wave function with eight nodes on a linear potential plus a wall at the origin. Both the de Broglie wavelength and the amplitude of the oscillation grow as we move to the right.

E_n能階定態解會有個$n-1$個Node節點。

這是一個可以證明的定理。

We can do better! Solving the Euqation!

1926. № 6.

ANNALEN DER PHYSIK.

VIERTE FOLGE. BAND 79.

1. *Quantisierung als Eigenwertproblem;*
von E. Schrödinger.

(Zweite Mitteilung.)[1]

1. Der Plancksche Oszillator. Die Entartungsfrage.

Wir behandeln zunächst den eindimensionalen Oszillator. Die Koordinate q sei die Elongation multipliziert mit der Quadratwurzel aus der Masse. Die beiden Formen der kinetischen Energie sind dann

(20) $$\bar{T} = {}^1/_2\,\dot{q}^2\,, \qquad T = {}^1/_2\,p^2\,.$$

Die potentielle Energie sei

(21) $$V(q) = 2\pi^2\nu_0^{\,2}q^2\,,$$

wo ν_0 die Eigenfrequenz im Sinne der Mechanik. Dann lautet Gleichung (18) für diesen Fall:

(22) $$\frac{d^2\psi}{dq^2} + \frac{8\pi^2}{h^2}(E - 2\pi^2\nu_0^{\,2}q^2)\psi = 0\,.$$

$$\psi_E(x) \equiv u(x)$$

$$\frac{d^2\psi_E}{dx^2} = \frac{2m}{\hbar^2}\left(\frac{1}{2}kx^2 - E\right)\psi_E \quad \Rightarrow \quad \frac{d^2u}{dx^2} = \frac{m^2\omega^2}{\hbar^2}x^2u - \frac{2mE}{\hbar^2}u$$

$$\omega = \sqrt{\frac{k}{m}}$$

$$\frac{d^2u}{dx^2} = \frac{m^2\omega^2}{\hbar^2}x^2u - \frac{2mE}{\hbar^2}u$$ 這些常數很繁雜！

很神奇又自然的：我們可以取任一個較方便的長度單位來解此方程式。

得到解後再換算回原單位！

$\frac{m\omega}{\hbar}$ 單位是長度平方的倒數。 $\sqrt{\frac{\hbar}{m\omega}} = 1$ 單位是長度。

我們可以選擇長度單位使此式的數值等於1。

$\frac{m\omega}{\hbar} = 1$ 那第一個常數 $\frac{m^2\omega^2}{\hbar^2}$ 也等於1。 $m = \frac{\hbar}{\omega}$

方程式簡化為：

$$\frac{d^2u}{dx^2} = x^2u - \frac{2E}{\hbar\omega}u$$

方程式只剩一個參數E，$\frac{2E}{\hbar\omega}$無單位，可以定義$\hbar\omega$為單位能量，引入： $\varepsilon \equiv \frac{2E}{\hbar\omega}$

$$\frac{d^2u}{dx^2} = x^2u - \varepsilon u \quad \longrightarrow \quad \frac{d^2u}{dy^2} = y^2u - \varepsilon u$$

給此單位制中的位置、新的名字y。

他們可以很容易換算回到原來的單位制的位置x。

$$x = y\sqrt{\frac{\hbar}{m\omega}}$$

薛丁格怎麼解這個方程式？ $\frac{d^2u}{dy^2} = (y^2 - \varepsilon)u$

Sei zur Abkürzung

(23) $$a = \frac{8\pi^2 E}{h^2}, \quad b = \frac{16\pi^4 \nu_0^2}{h^2}$$

also

(22′) $$\frac{d^2\psi}{dq^2} + (a - bq^2)\psi = 0 .$$

Wir führen als unabhängige Variable ein

(24) $$x = q\sqrt[4]{b}$$

und erhalten

(22″) $$\boxed{\frac{d^2\psi}{dx^2} + \left(\frac{a}{\sqrt{b}} - x^2\right)\psi = 0 .}$$

Die Eigenwerte und Eigenfunktionen dieser Gleichung sind *bekannt.*[1]) Die Eigenwerte sind in den hier benützten Zeichen

(25) $$\frac{a}{\sqrt{b}} = 1,\ 3,\ 5\ \ldots (2n+1) \ldots .$$

Die Eigenfunktionen sind die *Hermiteschen Orthogonalfunktionen*

(26) $$e^{-\frac{x^2}{2}} H_n(x) .$$

他直接知道答案！

$u_0(y) = e^{-\frac{y^2}{2}} \times$(一個特別的多項式)

這是一個指數遞減的高斯分佈函數，乘上一個Hermite多項式！

$$\frac{d^2u}{dy^2} - y^2u + \varepsilon u = 0$$

有限次多項式無法是此式的解，因為y^2u顯然比$\frac{d^2u}{dy^2}$及εu來得高階。
y^2u的最高次項沒有人可以抵消。
而且有限次多項式在無限遠處會發散，不符合定態的要求。

退而求其次，薛丁格猜想解可能是一個非多項式函數u_0乘上多項式$h(y)$。

$$u(y) \equiv u_0(y)\times h(y)$$

但薛丁格如何猜到正確的u_0呢？

$$u(y) = e^{-\frac{y^2}{2}}\times(\text{一個特別的多項式})$$

他的想法是：非多項式函數$u_0(y)$在無限遠處$y \to \infty$必須趨近於零。
而且在無限遠處u_0必須比多項式h重要。多項式相比之下如一個常數。

而在無限遠處$y \to \infty$，

$$y^2u - \varepsilon u \to y^2u$$

$$\frac{d^2u}{dy^2} - y^2u + \varepsilon u = 0 \quad \Rightarrow \quad \frac{d^2u_0}{dy^2} - y^2u_0 = 0$$

解出此方程式就可以得到u_0：

而u_0很容易就可以找到，就是一個高斯分佈函數，課本有細膩的推導 P86。

但直接代入即可驗證：

$$u_0(y) = e^{-\frac{y^2}{2}}$$

$$\frac{d^2 u_0}{dy^2} - y^2 u_0 = y u_0 \sim 0$$

$$\frac{d^2 \psi}{d x^2} + \left(\frac{a}{\sqrt{b}} - x^2\right) \psi = 0 \, .$$

nwerte und Eigenfunktionen dieser Gleichu

Die Eigenwerte sind in den hier benützten

$$\frac{a}{\sqrt{b}} = 1,\ 3,\ 5\ \ldots (2n+1) \ldots .$$

funktionen sind die *Hermiteschen Orthogonalfu*

$$e^{-\frac{x^2}{2}} H_n(x) \, .$$

因此如果這樣設定：

$$u(y) = e^{-\frac{y^2}{2}} \times h(y)$$

$h(y)$就可能得到有限次多項式的解！

$$\frac{d^2 u}{dy^2} = y^2 u - \varepsilon u \Rightarrow e^{-\frac{y^2}{2}} \frac{d^2 h}{dy^2} - 2y e^{-\frac{y^2}{2}} \frac{dh}{dy} + y^2 e^{-\frac{y^2}{2}} h - e^{-\frac{y^2}{2}} h = (y^2 - \varepsilon)\, e^{-\frac{y^2}{2}} h$$

$$\Downarrow$$

$$\frac{d^2 h}{dy^2} - 2y \frac{dh}{dy} + (\varepsilon - 1) h = 0$$

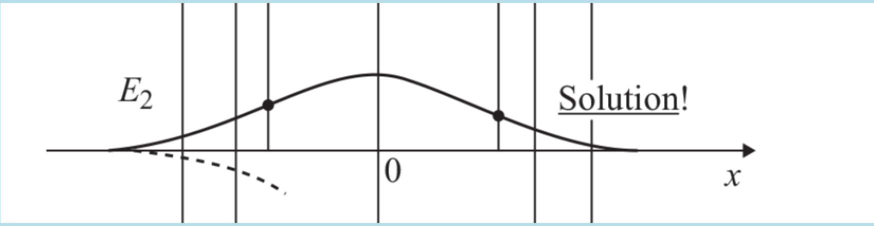
$y^2 h(y)$真的消失了。

後兩項是同次多項式，第一項則較低次，故後兩項的最高次項可以彼此抵消。

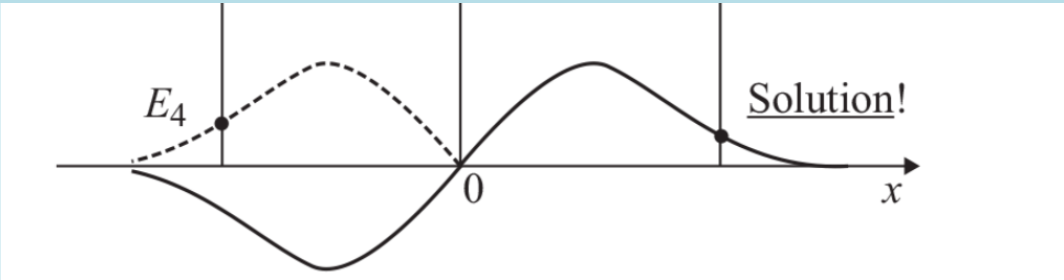
讓我們先感覺一下這個函數$u(y)$的特性：

$$u(y) = e^{-\frac{y^2}{2}} \times (\text{一個特別的多項式})$$

若式中(特別的多項式)是常數，此函數就是一個單純的高斯分佈：
在∞趨近指數遞減，在原點附近維持緩慢變化：

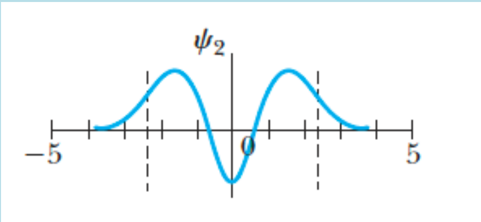


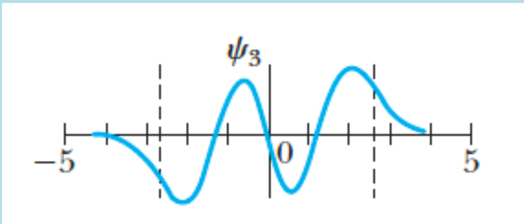
若(特別的多項式)是一次方x，此函數在遠處是高斯分佈：
在∞趨近指數遞減，在原點附近穿過x軸，在此函數需為零：



大膽猜想：在趨近∞處此解由高斯分佈控制，在原點附近則由多項式控制！

該多項式若是n次，則會穿過x軸n次，n越大能量越大。





以上是一個猜測的過程，是否可行，必須直接求解：

$$\frac{d^2h}{dy^2} - 2y\frac{dh}{dy} + (\varepsilon - 1)h = 0$$

這個方程式有有限次多項式解嗎？先讓我們假設$h(y)$為n次多項式：

$$h(y) = a_n y^n + a_{n-1}y^{n-1} + a_{n-2}y^{n-2} + \cdots$$

代入後先看各項的最高次的貢獻：

$$n(n-1)a_n y^{n-2} - 2na_n y^n + (\varepsilon - 1)a_n y^n$$

第一項的貢獻其實小兩次，在此可以先忽略。第二項與第三項必須抵消。

$$-2na_n y^n + (\varepsilon - 1)a_n y^n = 0$$

簡化後得到一個極漂亮的式子：

$$-2n + (\varepsilon - 1) = 0$$

n是多項式解的冪次，ε是該解對應的能量。

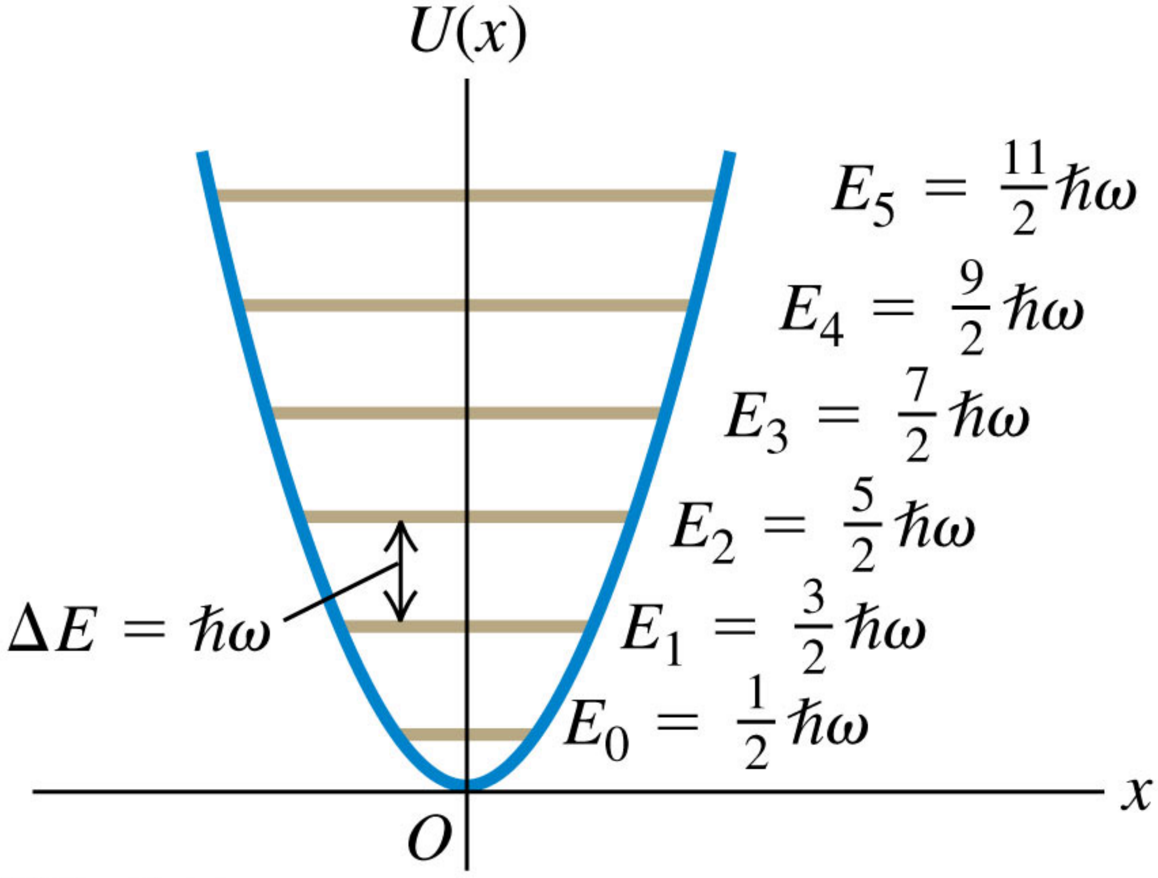
$$\varepsilon = 2n + 1 \equiv \frac{2E}{\hbar\omega}$$

只有當ε為奇整數時，方程式才有可歸一化的有限次多項式解！

$$E = \hbar\omega\left(n + \frac{1}{2}\right)$$

能量只有在這些值時，定態方程式才有解！

量子簡諧運動的能量是量子化的！



$$E = \hbar\omega\left(n + \frac{1}{2}\right)$$

完整的解可以以Recursion遞迴關係得到：

$$\frac{d^2h}{dy^2} - 2y\frac{dh}{dy} + (\varepsilon - 1)h = 0$$

已知$\varepsilon = 2n + 1$對應的解為n次多項式，記為：$h_n(y)$，寫成：

$$h_n(y) = a_n y^n + a_{n-1} y^{n-1} + a_{n-2} y^{n-2} + \cdots = \sum_{j=0\text{或}1}^{n} a_j y^j$$

$$\sum_{j=0\text{或}1}^{n} j(j-1)a_j y^{j-2} - 2\sum_{j=0\text{或}1}^{n} j a_j y^j + 2n\sum_{j=0\text{或}1}^{n} a_j y^j = 0$$

收集 y^i的項，係數必須為零：

$$(i+2)(i+1)a_{i+2} - 2ia_i + 2na_i = 0$$

$$a_{i+2} = \frac{2i - 2n}{(i+2)(i+1)} a_i$$

Recursion遞迴關係

$$a_{i+2} = \frac{2i - 2n}{(i+2)(i+1)} a_i$$

Recursion遞迴關係

注意多項式中偶數次項是偶函數，奇數次項是奇函數。

偶函數：n是偶數 $a_0 \to a_2 \to a_4 \cdots \to a_n$ 分子為零$a_{n+2} = 0$ 遞迴停止。

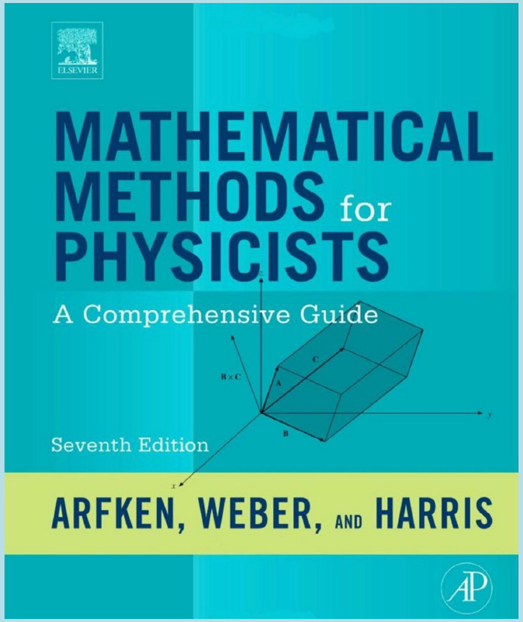
其餘奇數次項係數都為零。

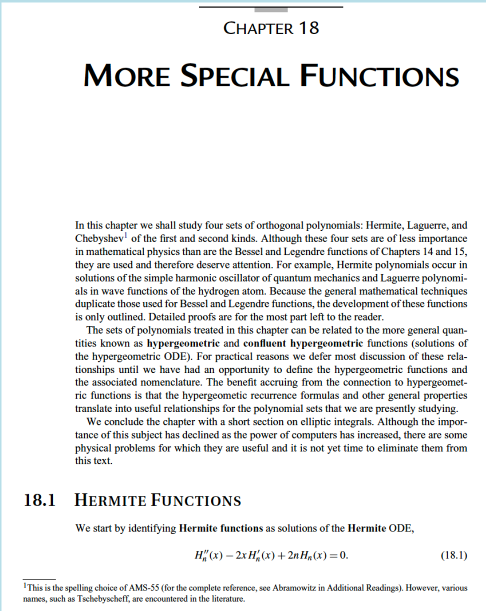
奇函數：n是奇數 $a_1 \to a_3 \to a_5 \cdots \to a_n$ $a_{n+2} = 0$ 遞迴會停止。

其餘偶數次項係數都為零。

這樣多項式正是Hermite polynomials。

若n不是整數，遞迴不會停止，多項式是無限次，可證明所得的解會發散。





Chapter 18

More Special Functions

In this chapter we shall study four sets of orthogonal polynomials: Hermite, Laguerre, and Chebyshev[1] of the first and second kinds. Although these four sets are of less importance in mathematical physics than are the Bessel and Legendre functions of Chapters 14 and 15, they are used and therefore deserve attention. For example, Hermite polynomials occur in solutions of the simple harmonic oscillator of quantum mechanics and Laguerre polynomials in wave functions of the hydrogen atom. Because the general mathematical techniques duplicate those used for Bessel and Legendre functions, the development of these functions is only outlined. Detailed proofs are for the most part left to the reader.

The sets of polynomials treated in this chapter can be related to the more general quantities known as **hypergeometric** and **confluent hypergeometric** functions (solutions of the hypergeometric ODE). For practical reasons we defer most discussion of these relationships until we have had an opportunity to define the hypergeometric functions and the associated nomenclature. The benefit accruing from the connection to hypergeometric functions is that the hypergeometic recurrence formulas and other general properties translate into useful relationships for the polynomial sets that we are presently studying.

We conclude the chapter with a short section on elliptic integrals. Although the importance of this subject has declined as the power of computers has increased, there are some physical problems for which they are useful and it is not yet time to eliminate them from this text.

18.1 Hermite Functions

We start by identifying **Hermite functions** as solutions of the **Hermite** ODE,

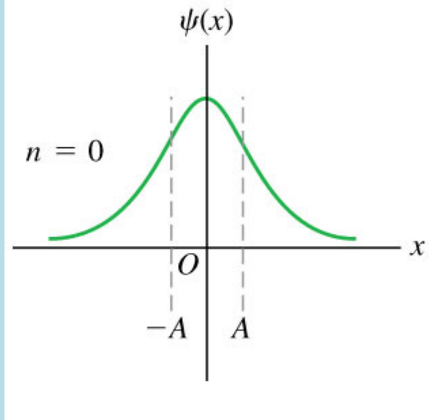
$$H_n''(x) - 2xH_n'(x) + 2nH_n(x) = 0. \quad (18.1)$$

[1] This is the spelling choice of AMS-55 (for the complete reference, see Abramowitz in Additional Readings). However, various names, such as Tschebyscheff, are encountered in the literature.

$$u(y) = e^{-\frac{y^2}{2}} \cdot y\text{的}n\text{次多項式}h_n$$

$$a_{i+2} = \frac{2i - 2n}{(i+2)(i+1)} a_i$$

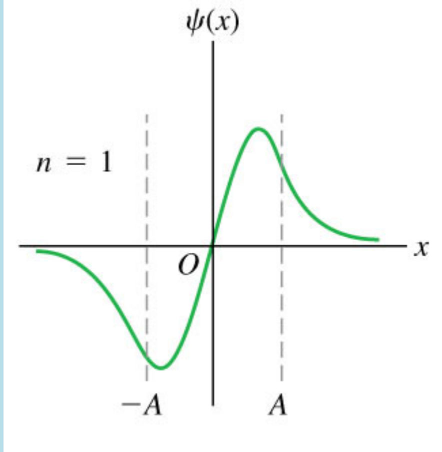
$$h_n(y) = \sum_{j=1}^{n} a_j y^j$$



前三個定態！

$n = 0$

$$h_0(y) = a_0, \qquad u_0(y) = a_0 e^{-\frac{y^2}{2}}$$



$$x = y\sqrt{\frac{\hbar}{m\omega}}$$

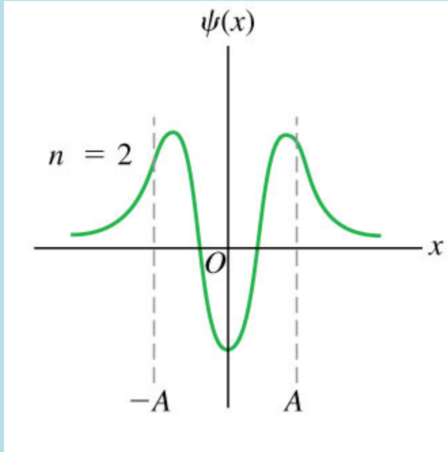
Ground state

$$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega x^2}{2\hbar}}$$

常數則由歸一化條件給定：

$n = 1$ 1st excited state

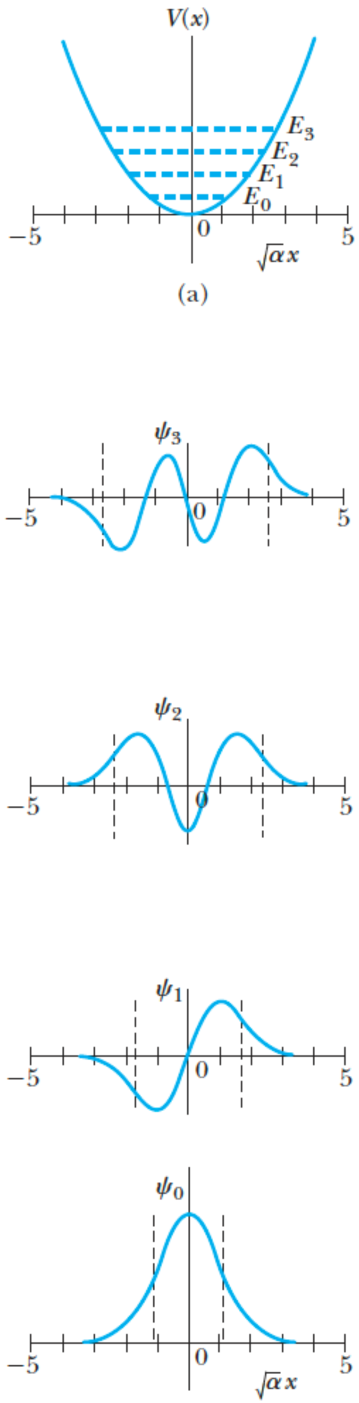
$$h_1(y) = a_1 y, \qquad u_1(y) = a_1 y e^{-\frac{y^2}{2}}$$



$n = 2$ 2nd excited state

$$a_2 = \frac{-4}{(2)(1)} a_0$$

$$h_2(y) = (a_0 - 2a_0 y^2), \qquad u_2(y) \sim (a_0 - 2a_0 y^2) e^{-\frac{y^2}{2}}$$



(a)

(b)

$$\alpha = \frac{m\omega}{\hbar}$$

Wave functions

$$\psi_3(x) = \left(\frac{\alpha}{\pi}\right)^{1/4} \frac{1}{\sqrt{3}} \left(\sqrt{\alpha}x\right)\left(2\alpha x^2 - 3\right) e^{-\alpha x^2/2}$$

$$\psi_2(x) = \left(\frac{\alpha}{\pi}\right)^{1/4} \frac{1}{\sqrt{2}} \left(2\alpha x^2 - 1\right) e^{-\alpha x^2/2}$$

$$\psi_1(x) = \left(\frac{\alpha}{\pi}\right)^{1/4} \sqrt{2\alpha}\; x e^{-\alpha x^2/2}$$

$$\psi_0(x) = \left(\frac{\alpha}{\pi}\right)^{1/4} e^{-\alpha x^2/2}$$

Equation 2.71 has solutions, of course, for *any* value of E (in fact, it has *two* linearly independent solutions for every E). But almost all of these solutions blow up exponentially at large x, and hence are not normalizable. Imagine, for example, using an E that is slightly *less* than one of the allowed values (say, $0.49\hbar\omega$), and plotting the solution: Figure 2.6(a). Now try an E slightly *larger* (say, $0.51\hbar\omega$); the "tail" now blows up in the *other* direction (Figure 2.6(b)). As you tweak the parameter in tiny increments from 0.49 to 0.51, the graph

"flips over" at precisely the value 0.5—only here does the solution escape the exponential asymptotic growth that renders it physically unacceptable.[36]

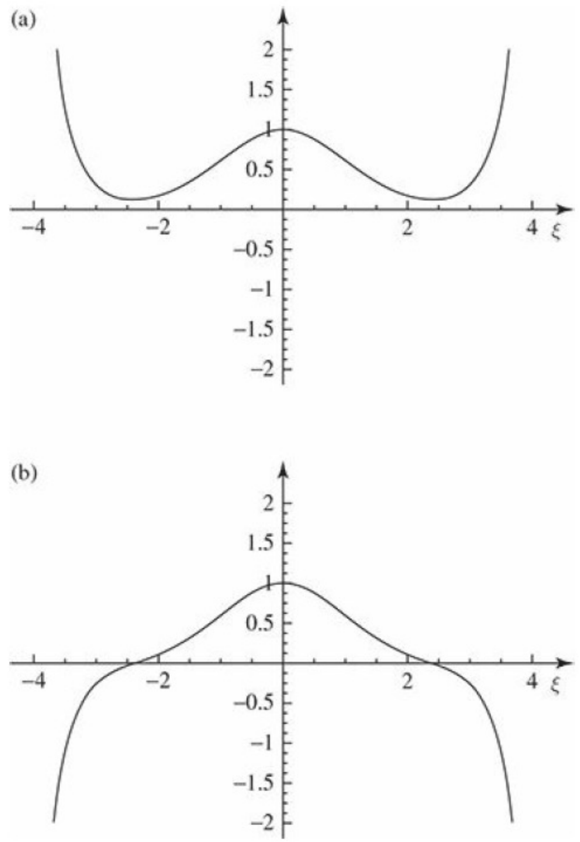
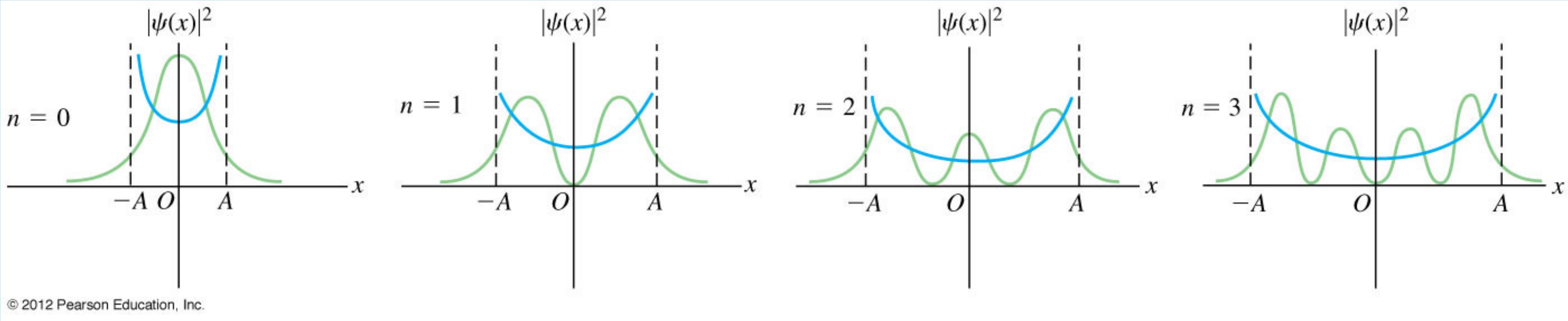
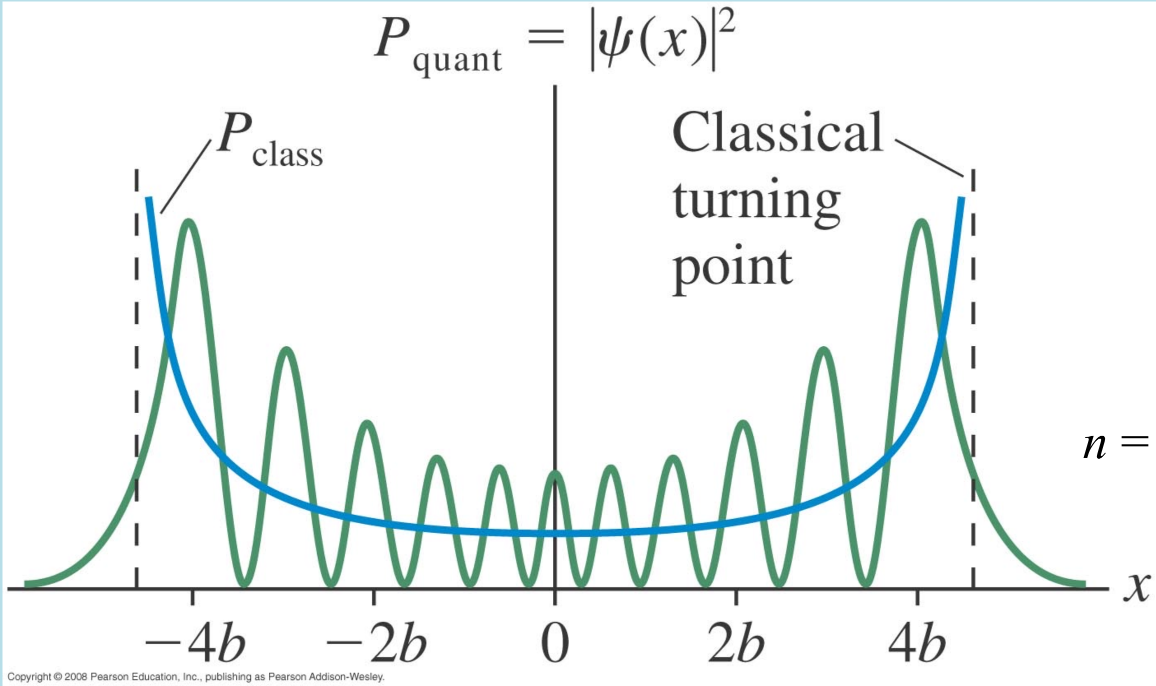


Figure 2.6: Solutions to the Schrödinger equation for (a) $E = 0.49\hbar\omega$, and (b) $E = 0.51\hbar\omega$.

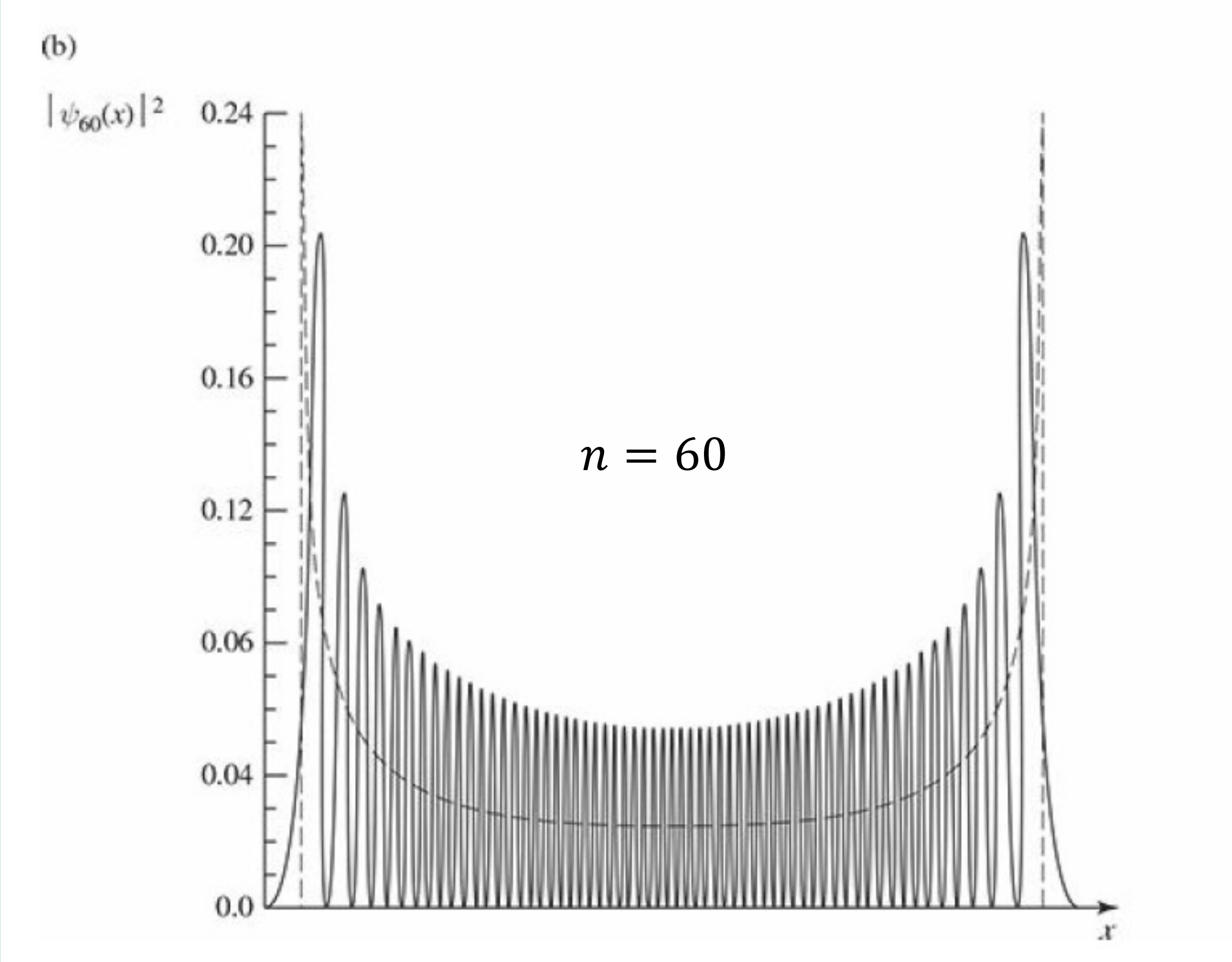


綠縣是量子機率分佈，藍線是對應古典振動的位置機率，兩端運動慢，出現機率高。



$n = 11$ State

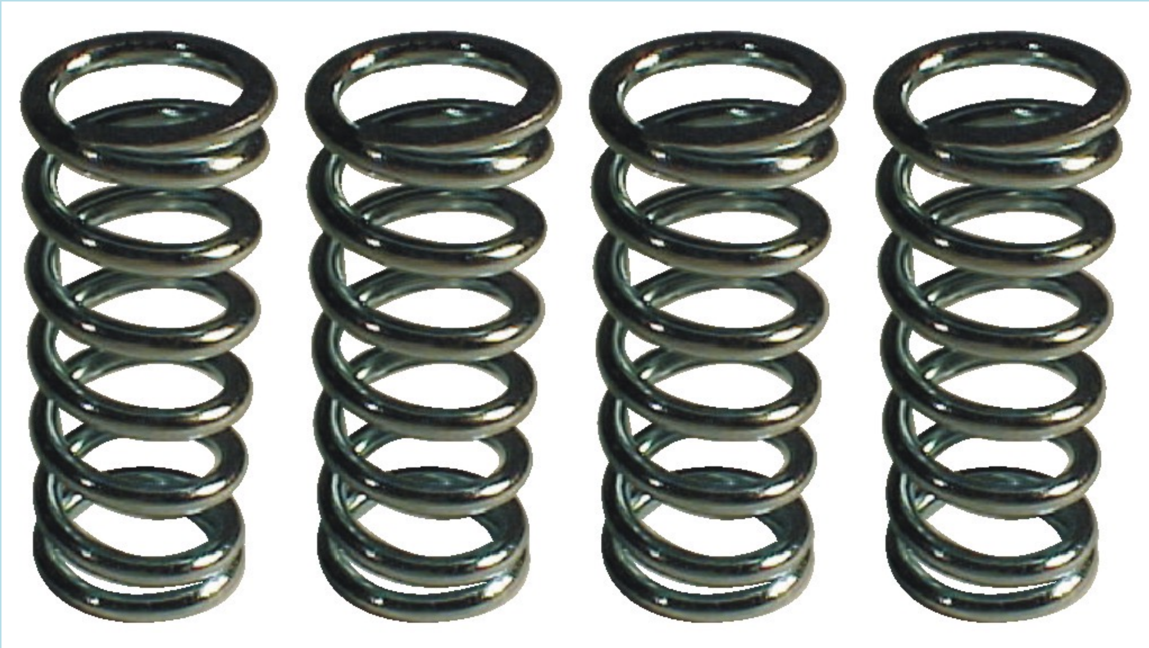
For large n, the quantum probability is similar to the classical one.



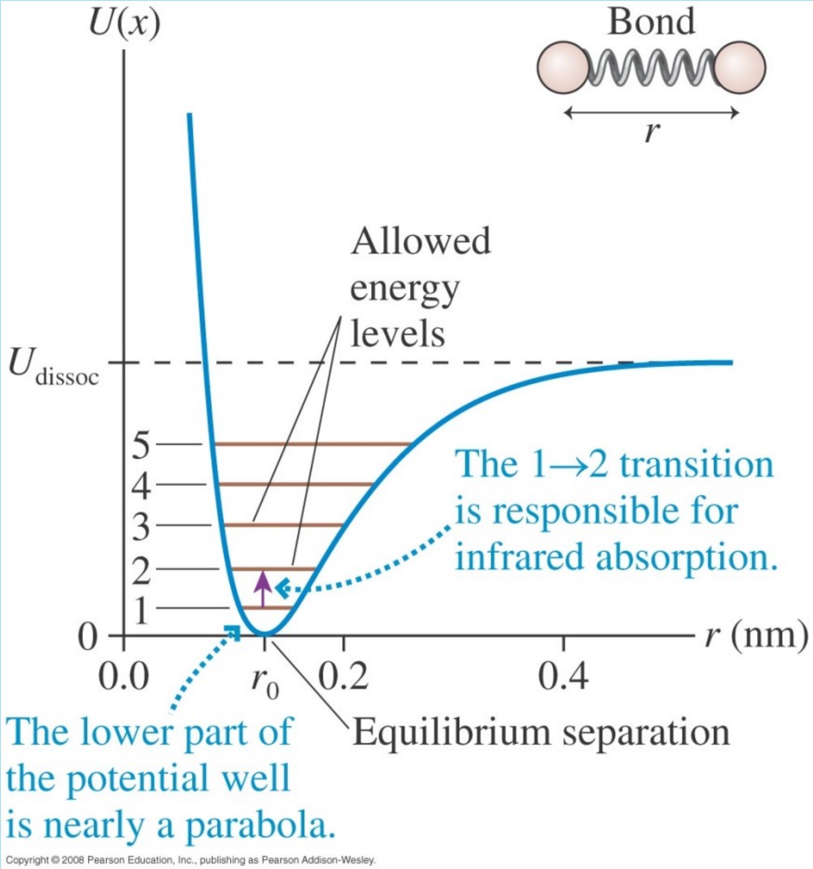
(b)
$|\psi_{60}(x)|^2$
0.24
0.20
0.16
0.12
0.06
0.04
0.0
$n = 60$
x

微觀世界有許多彈簧！

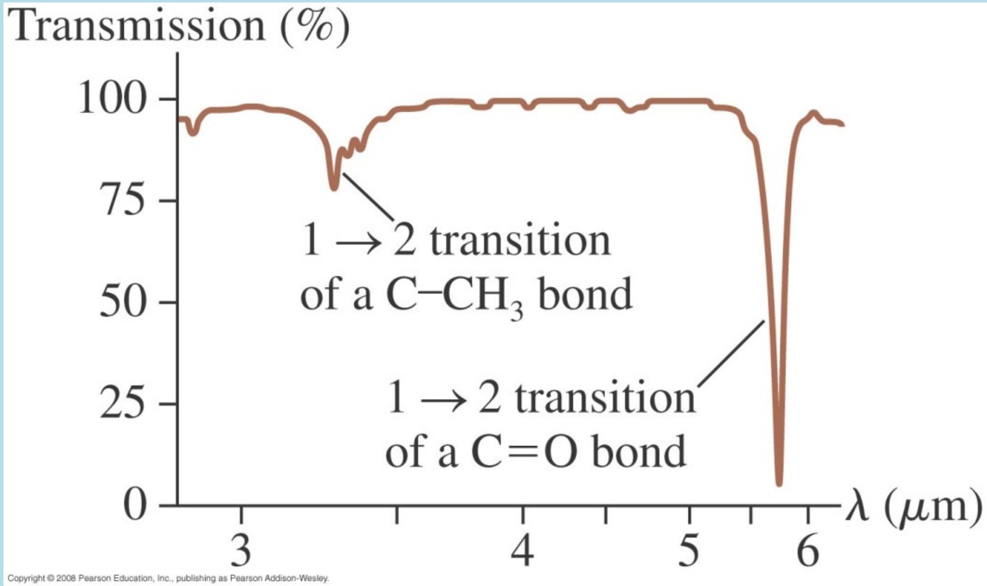
一個力學系統在平衡點附近的小範圍運動，都是簡諧運動！

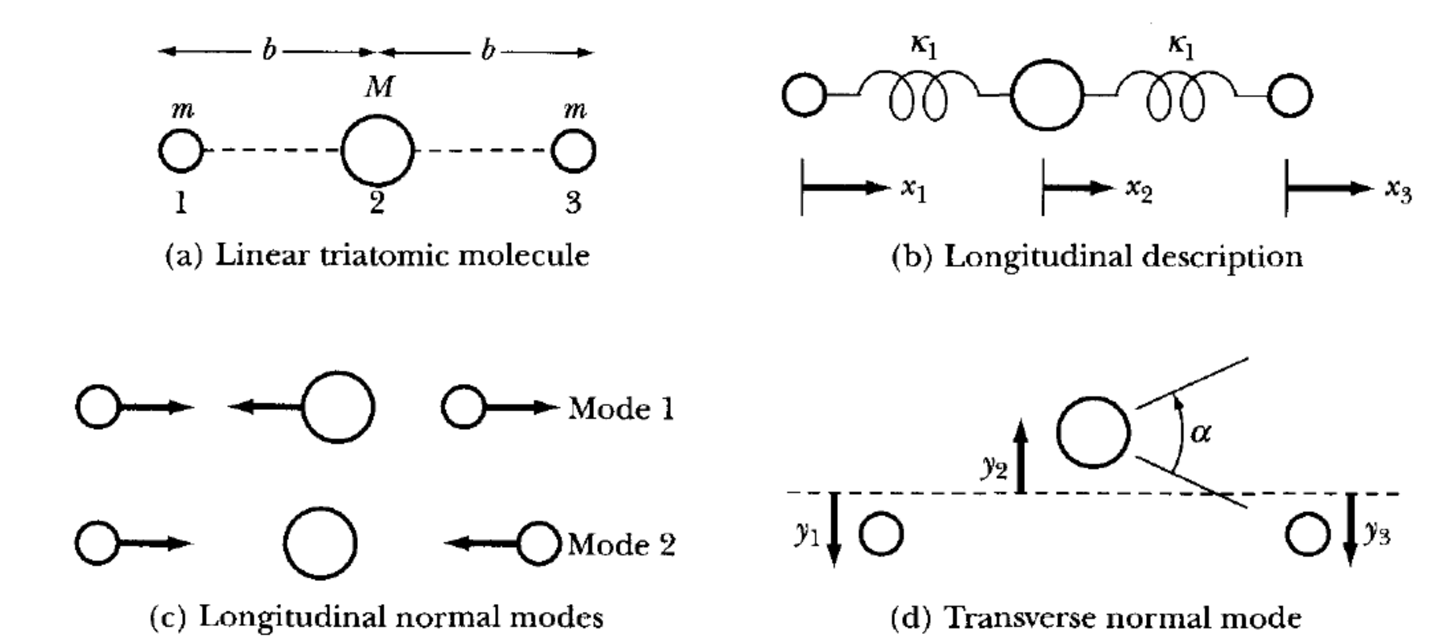


分子的束縛鍵就是一個彈簧！

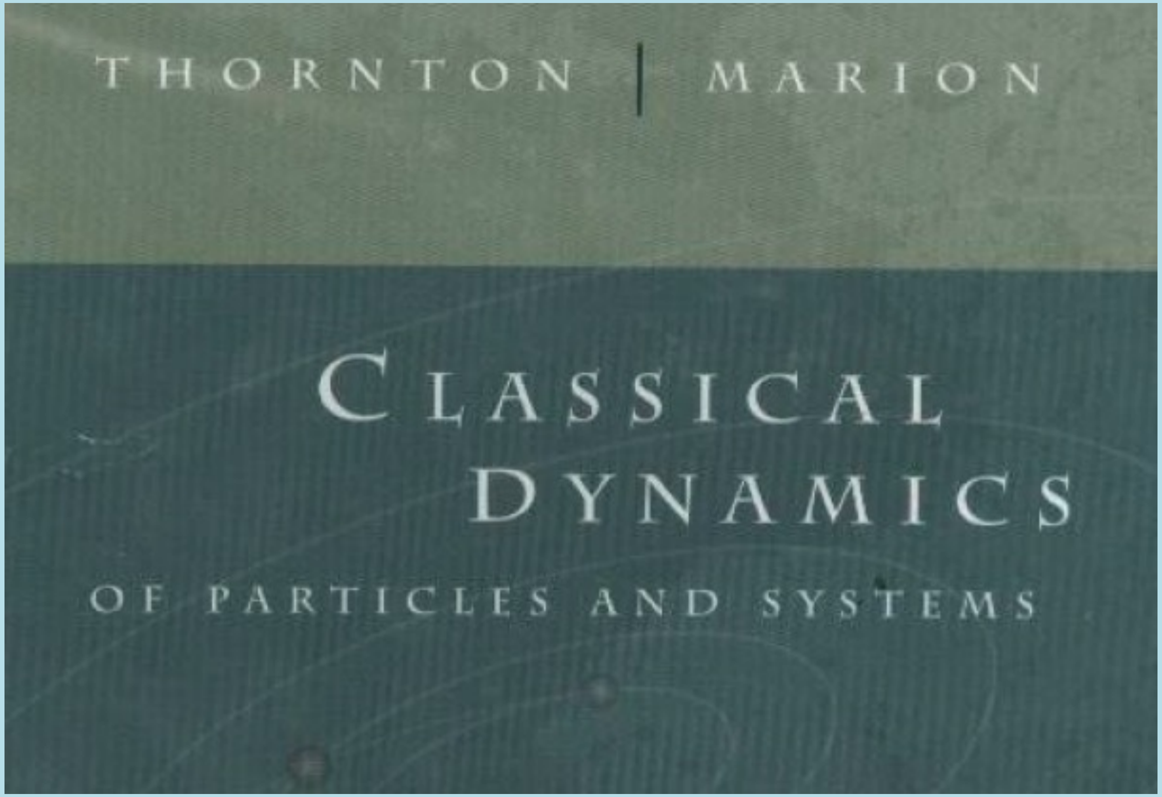


Molecular Vibration 分子光譜





三個原子組成的分子，可以有兩個振盪模式Mode，如同兩條獨立振動的彈簧。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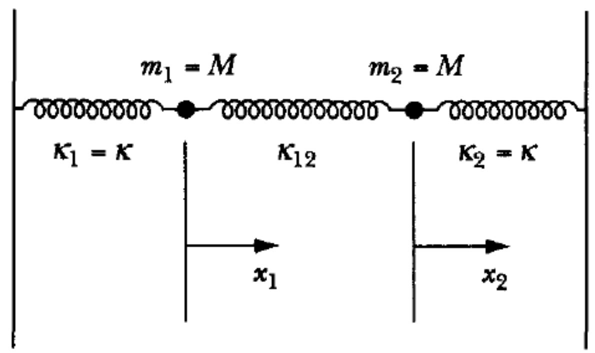
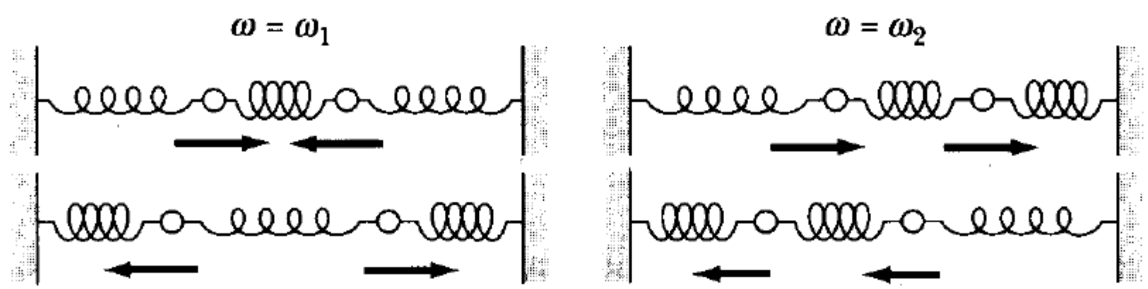
CLASSICAL DYNAMICS
OF PARTICLES AND SYSTEMS

CHAPTER 12

Coupled Oscillations





Antisymmetrical mode (out of phase)

Symmetrical mode (in phase)

有2個mode。

每一個振動mode對應一條彈簧。

$$\omega_1 = \sqrt{\frac{\kappa + 2\kappa_{12}}{M}}, \qquad \omega_2 = \sqrt{\frac{\kappa}{M}}$$

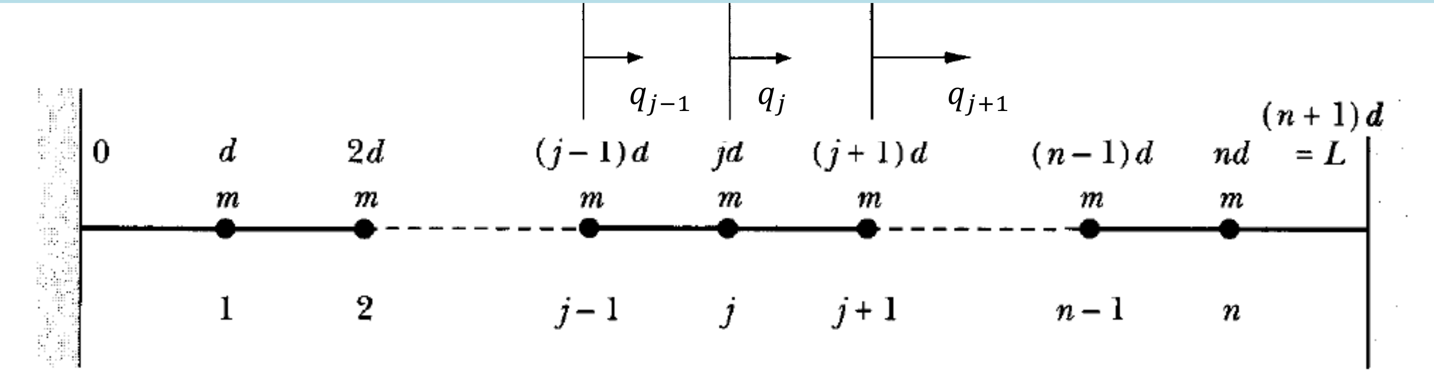
$$\left.\begin{aligned} x_1 &= \frac{1}{2}(\eta_2 + \eta_1) \\ x_2 &= \frac{1}{2}(\eta_2 - \eta_1) \end{aligned}\right\}$$

$$\boxed{\begin{aligned} T &= \frac{1}{2}\sum_{j,k} m_{jk}\dot{q}_j\dot{q}_k \\ U &= \frac{1}{2}\sum_{j,k} A_{jk}q_j q_k \end{aligned}}$$

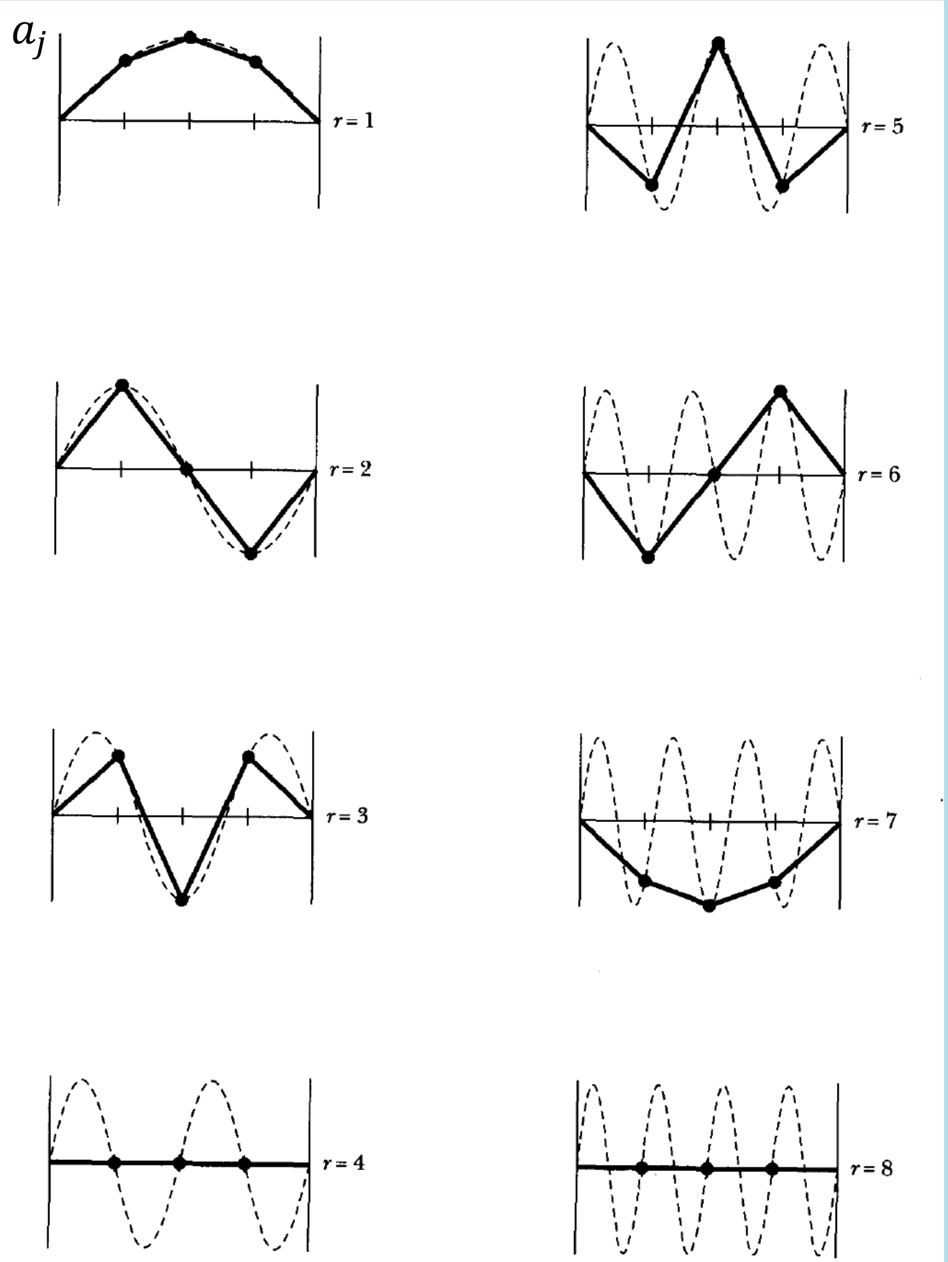
$$\left.\begin{aligned} M\ddot{\eta}_1 + (\kappa + 2\kappa_{12})\eta_1 &= 0 \\ M\ddot{\eta}_2 + \kappa\eta_2 &= 0 \end{aligned}\right\}$$

等於兩條獨立彈簧

12.9 The Loaded String* 原子晶格的振動波



晶格上原子的前後移動，可以改寫成一個一個獨立的振動模式mode。



每一個振動mode對應一條獨立彈簧。

第r個mode的角頻率為：$\omega_r \sim \sin\left[\dfrac{r\pi}{2(n+1)}\right]$

在第r個mode，第j個粒子的振幅可以寫成：

$$a_j \sim \sin\left(j\frac{r\pi}{n+1}\right) = \sin\left[jd\frac{r\pi}{(n+1)d}\right]$$

很像駐波。

重新定義變數：x為第j個粒子的位置。

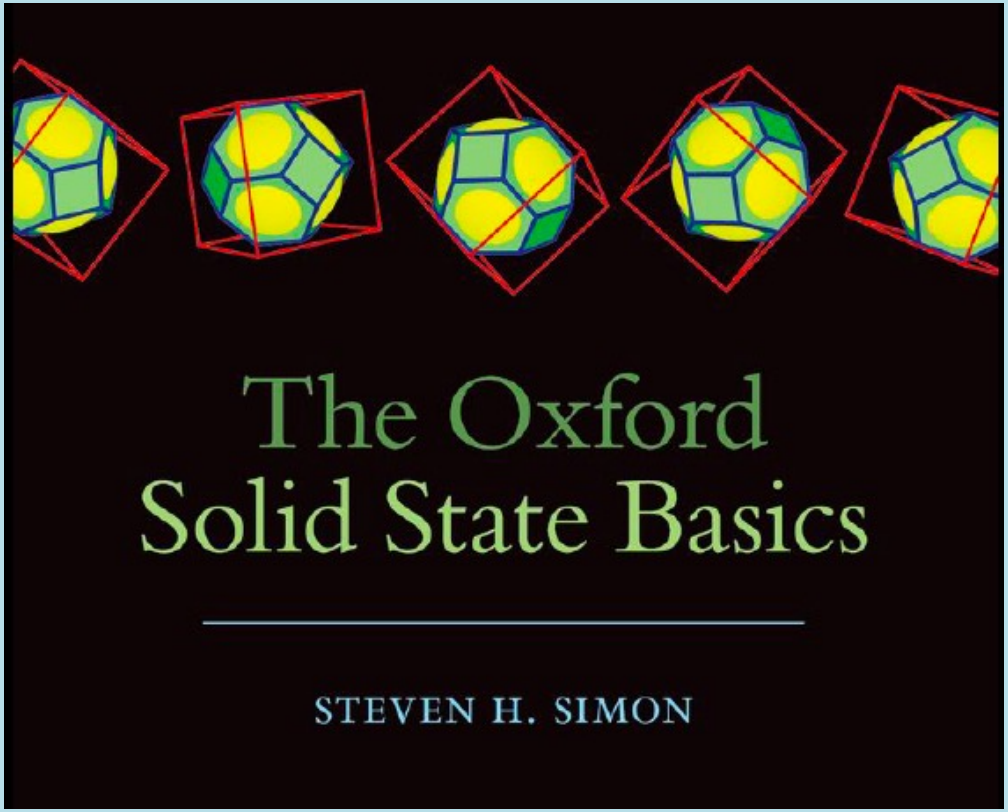
$x \equiv jd$ $\quad k \equiv \dfrac{r\pi}{(n+1)d}$ $\quad r$以k取代。

以上可以改寫成：

$$a_j \to \sin(kx)$$

$$\omega_r \sim \sin\left[\frac{r\pi}{2(n+1)}\right] \to \omega(k) \sim \sin\frac{kd}{2}$$

每一角波數k模式對應一條彈簧！



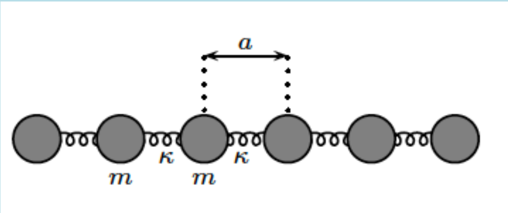
Vibrations of a One-Dimensional Monatomic Chain

9

In Chapter 2 we considered the Boltzmann, Einstein, and Debye models of vibrations in solids. In this chapter we will consider a more detailed model of vibration in a solid, first classically, and then quantum-

n很大時，k就成為連續變數。其實這就是角波數。

模式k時，在位置x的粒子的運動可以解出：



$$q(x,t)\sim \sin(kx)\, e^{i\omega(k)t}$$

$$\omega(k)\sim \sin\frac{kd}{2}$$ 晶格振動波的色散關係

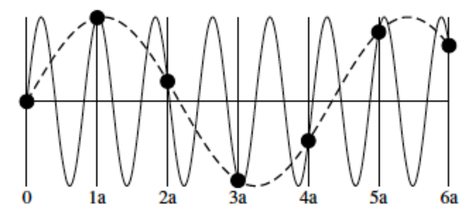
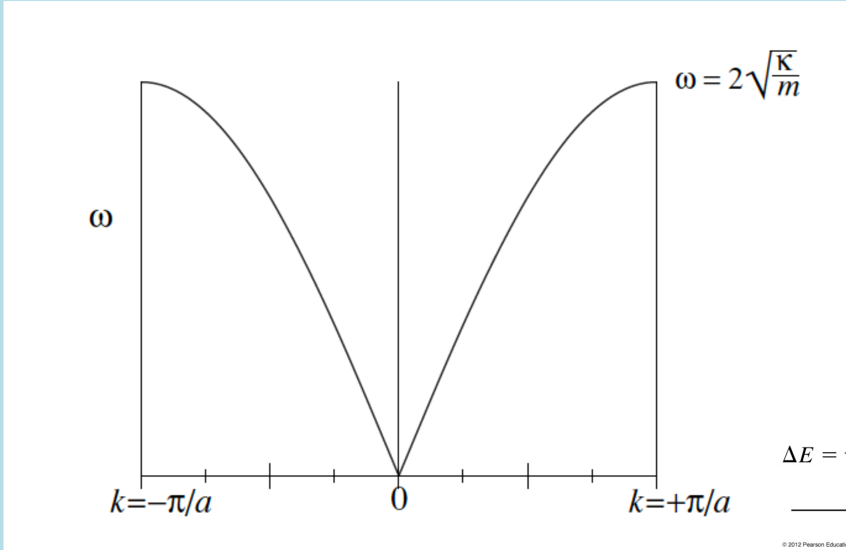
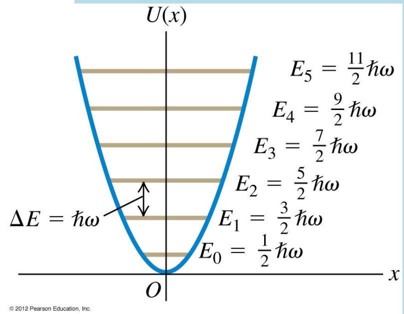


Fig. 9.3 Aliasing of waves. The dashed curve has wavevector k whereas the solid curve has wavevector $k + 2\pi/a$. These two waves have the same value (solid dots) at the location of the lattice points $x_n = na$, but disagree between lattice points. If the physical wave is only defined at these lattice points the two waves are fully equivalent.

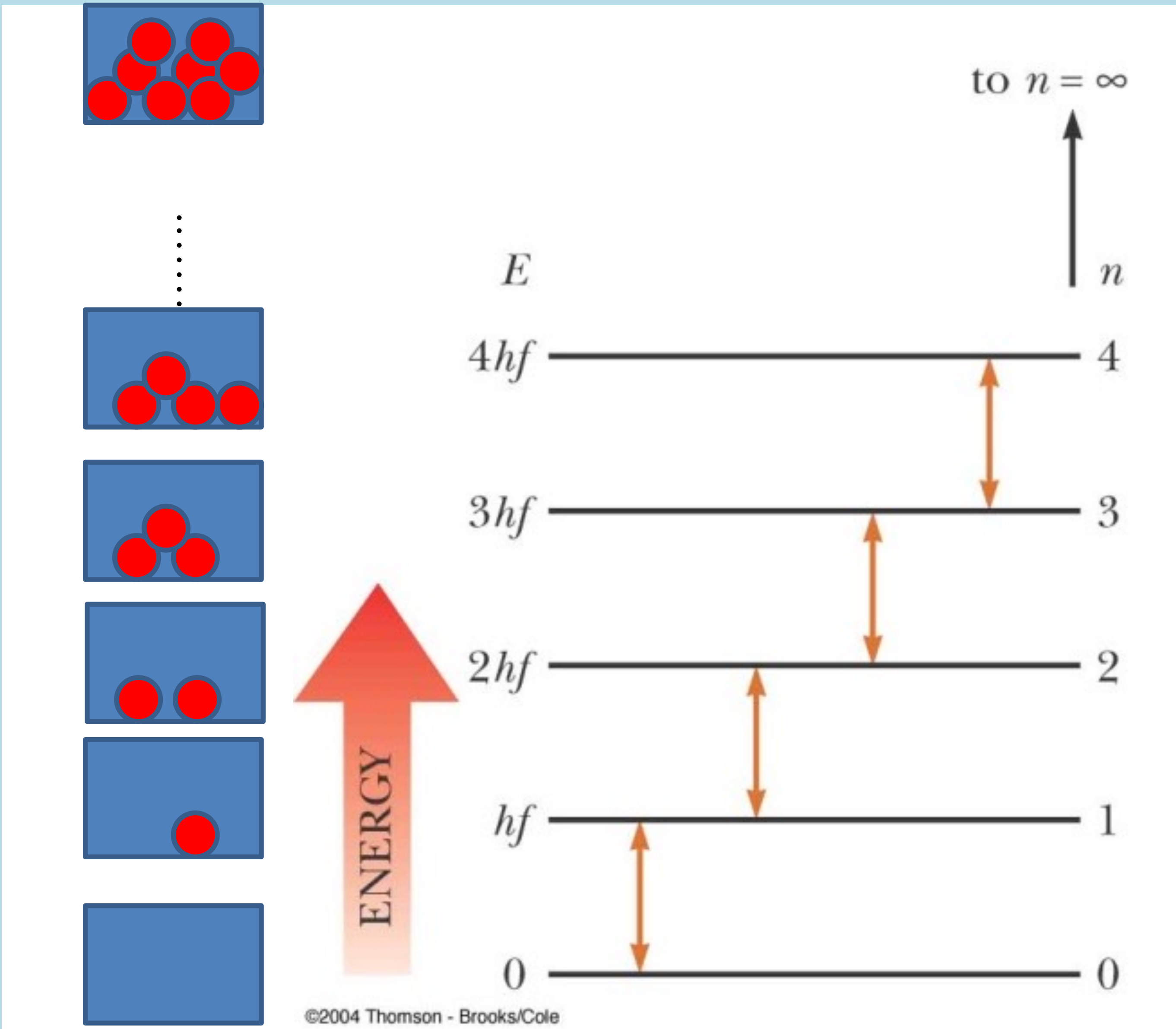




晶體中原子的振動，可以找到一系列如彈簧的模式。

這些模式一般如縱波平面波一般，有角波數k及對應的角頻率ω。

如同量子彈簧，每一模式的能量皆為量子化。



每一角波數k模式的能階像極了在盒子中一個個裝入能量相同的粒子。

量子 ⇨ 粒子 粒子數 $n = \dfrac{E}{\hbar\omega(k)}$

這就稱為聲子 phonon：量子彈簧的激發態！

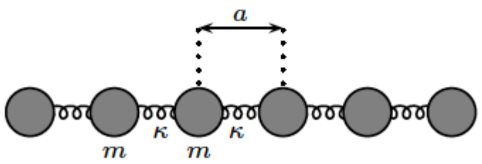


Fig. 9.1 The one-dimensional monatomic harmonic chain. Each ball has mass m and each spring has spring constant κ. The lattice constant, or spacing between successive masses at rest, is a.

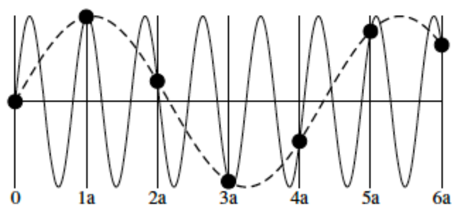
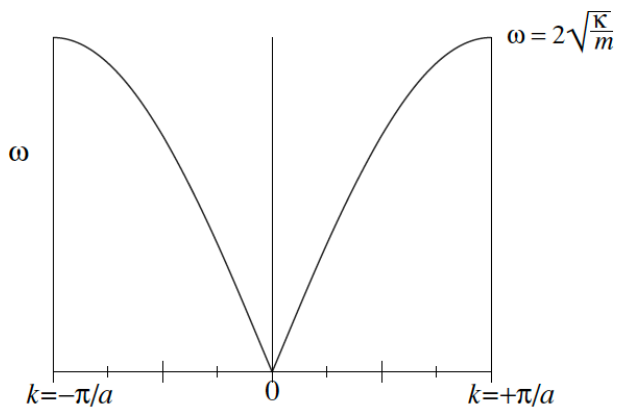


Fig. 9.3 Aliasing of waves. The dashed curve has wavevector k whereas the solid curve has wavevector $k + 2\pi/a$. These two waves have the same value (solid dots) at the location of the lattice



9.3 Quantum Modes: Phonons

We now make a rather important leap from classical to quantum physics.

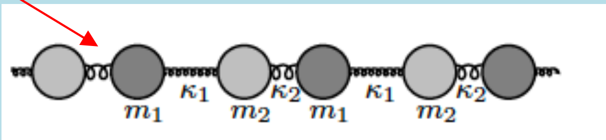
> **Quantum Correspondence:** If a classical harmonic system (i.e., any quadratic Hamiltonian) has a normal oscillation mode at frequency ω the corresponding quantum system will have eigenstates with energy
>
> $$E_n = \hbar\omega(n + \frac{1}{2}). \tag{9.7}$$

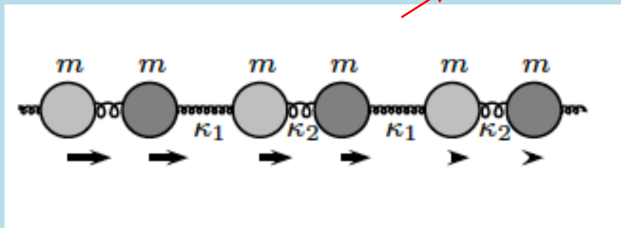
Presumably you know this well in the case of a single harmonic oscillator. The only thing different here is that our harmonic oscillator can be a collective normal mode not just the motion of a single particle. This quantum correspondence principle will be the subject of Exercises 9.1 and 9.7.

Definition 9.1 *A phonon is a discrete quantum of vibration.*[8]

This is entirely analogous to defining a single quantum of light as a photon. As is the case with the photon, we may think of the phonon as actually being a particle, or we can think of the phonon as being a quantized wave.

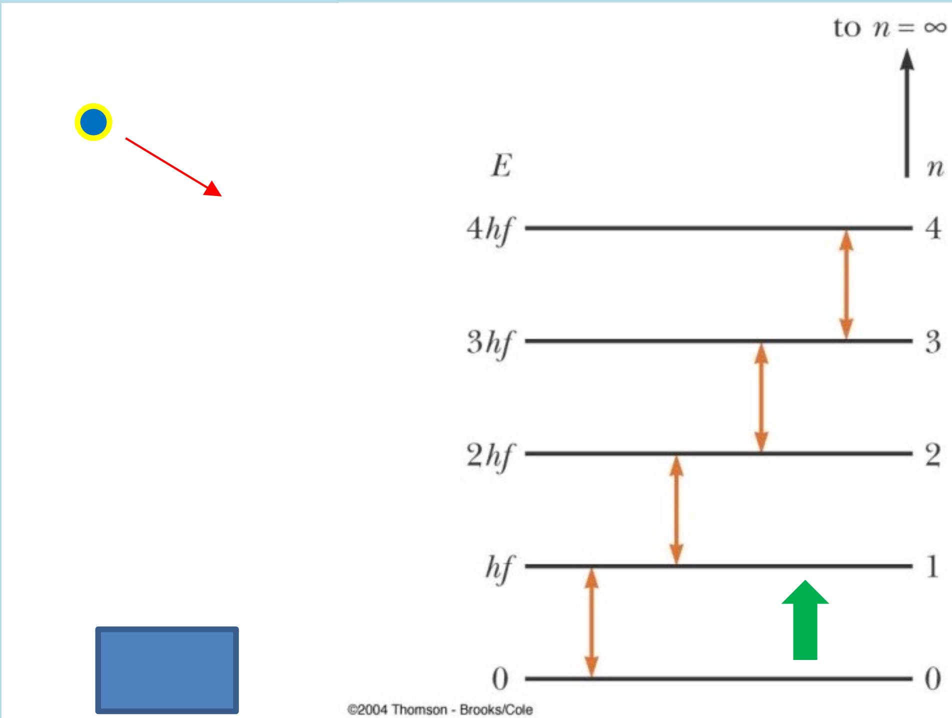
電子碰撞晶體中的原子鏈

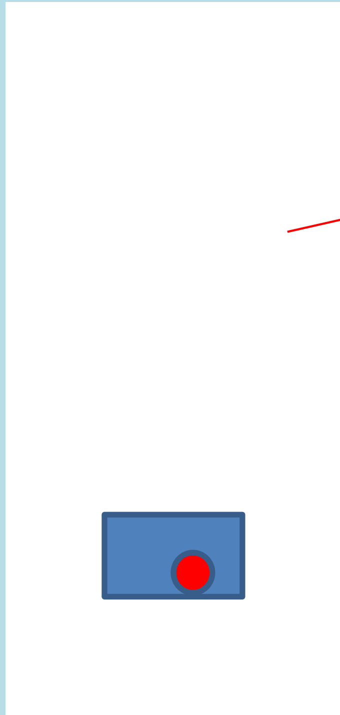




等同

電子碰撞激發某個模式k由$n = 1$定態躍遷到$n = 2$定態。



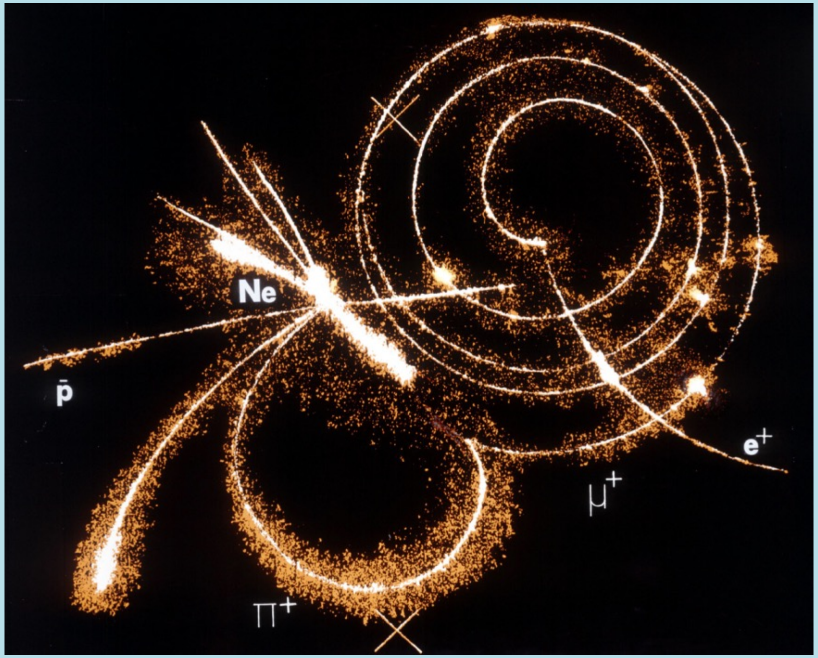


等同

電子移動中放出一個角波數為k的聲子

聲子好像一個基本粒子！

量子彈簧不是彈簧，而是可以產生、可以消滅的粒子的系統。

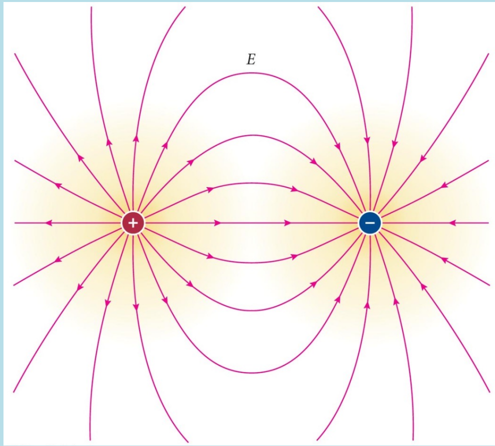


那基本粒子如電子，可不可能看成聲子呢？

基本粒子如電子，可不可能看成是量子彈簧的激發態呢？

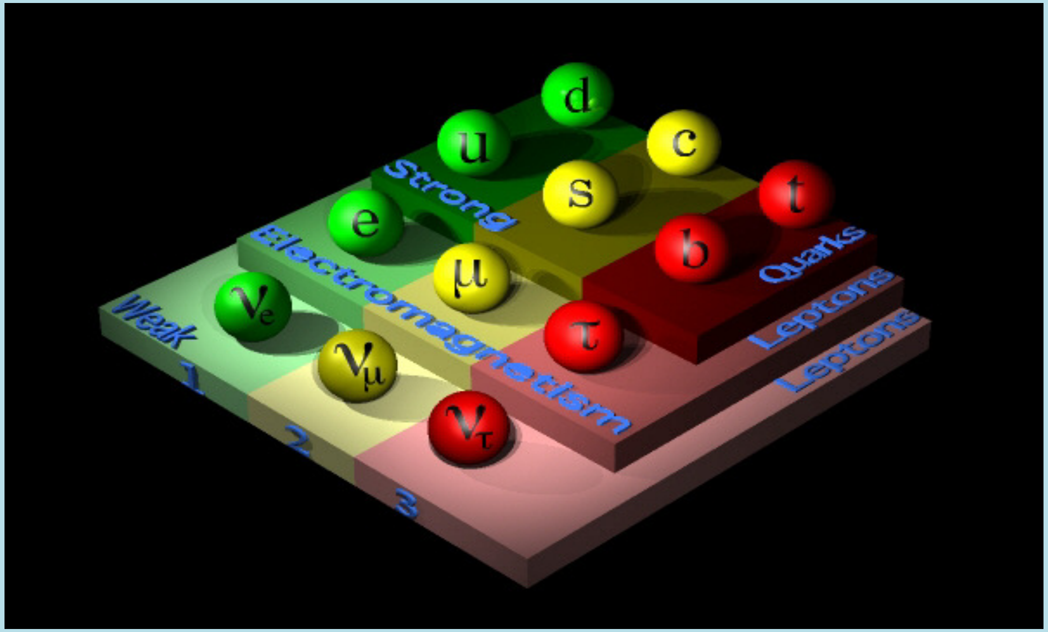
當然這時的彈簧就不能是原子的晶格。

但我們早已熟悉、真空中場的擾動，也可看成一個一個的彈簧的組合！



如果場也量子化了，這就稱為量子場，激發態就會是一個個基本粒子。

每一個基本粒子都對應一個量子場

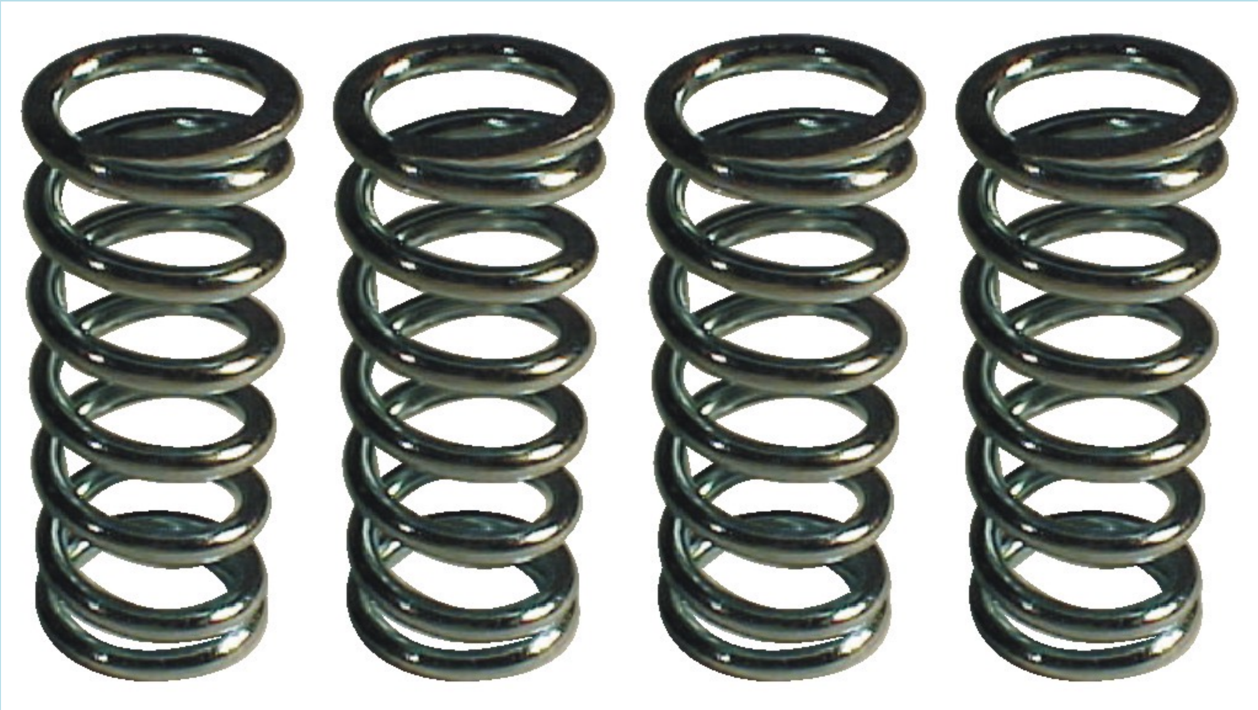


電子 ⟺ 電子場

u夸克 ⟺ u夸克場

描述可產生可消滅的粒子的理論：量子場論！

我們的宇宙是由彈簧組成的



Delta Potential

是否有$E < 0$的解？

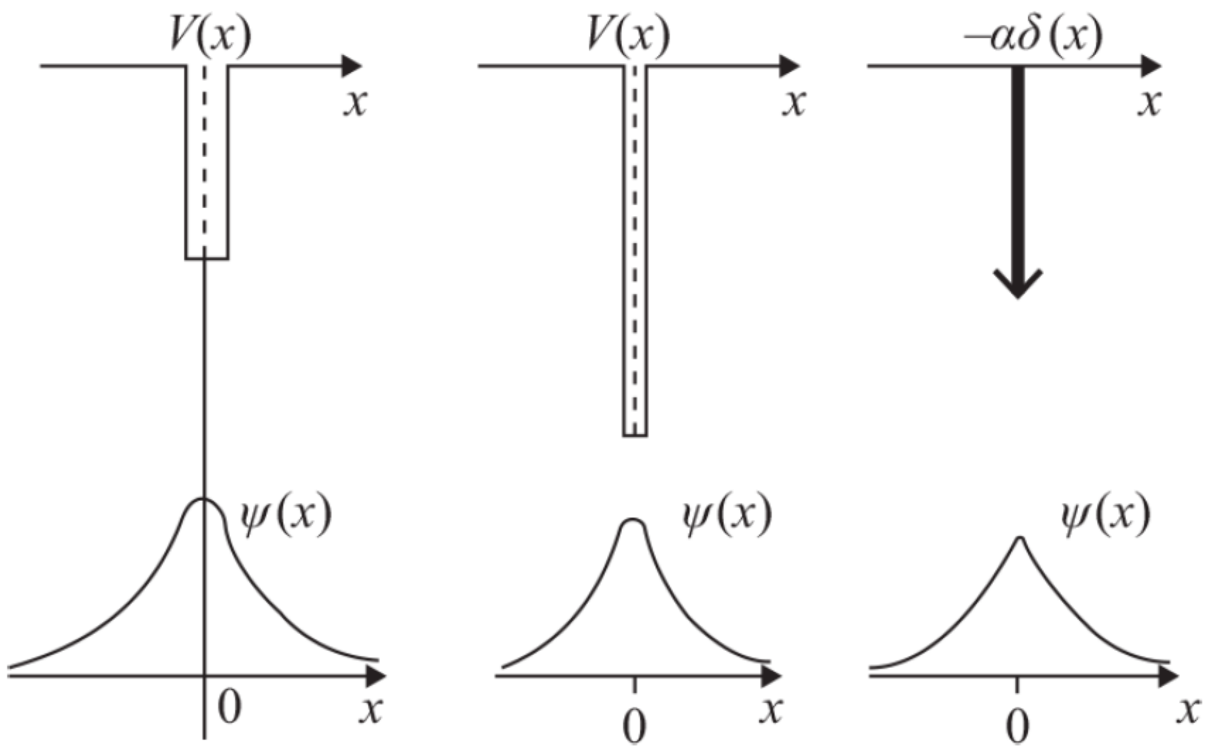
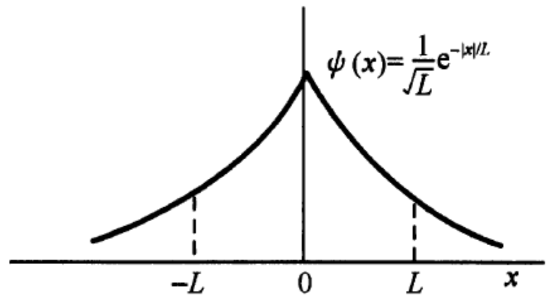


Figure 6.9
The delta function potential as the limit where the finite square well becomes narrower and deeper simultaneously. We expect to get a wave function with a discontinuous derivative.



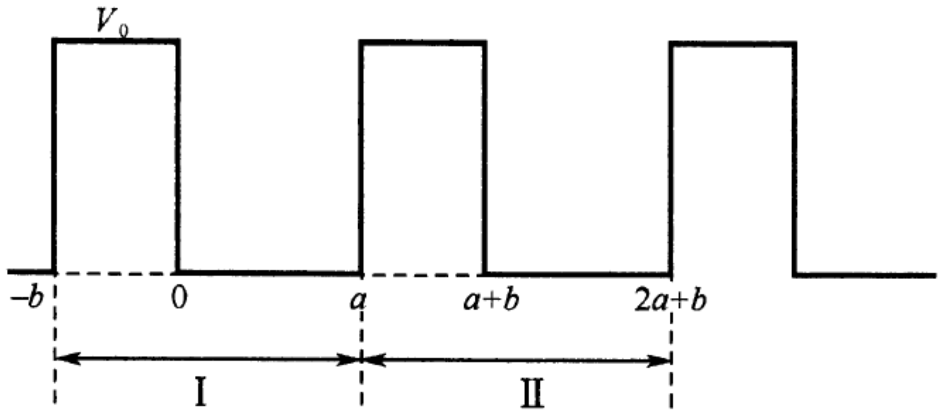
ψ'不連續。有一束縛態解。

$$\psi(x) = A e^{-\kappa |x|}.$$

Periodic Potential

例 考虑下列周期方势场(周期 $a+b$)中粒子(图 3.32)，

$$V[x+n(a+b)] = V(x)$$



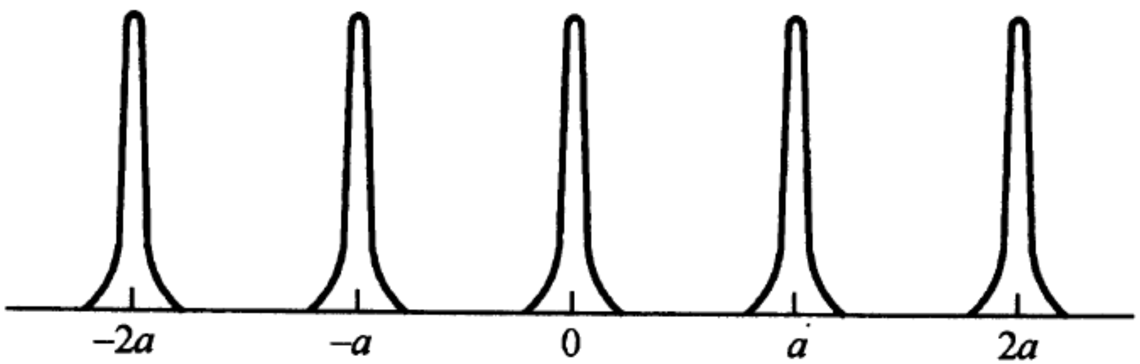


图 3.33 Dirac 梳