

量子力學
Quantum Mechanics

2006 年 10 月 15 日

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Motivation 動機

- 奈米科技 (Nanoscience) 是二十一世紀最重要的科學領域之一，2001 年美國與日本有關於本領域的科學預算分別為 US\$423 與 US\$396 Million，本領域的基礎研究攸關一個國家未來之全球競爭力。這是一個跨物理、化學、分子生物、材料、電子、以及數學等領域的整合性研究，量子力學是所有這些領域的共同基礎學科，計算數學是探討相關研究最基本的工具之一。
- 美國國家科學基金會 (NSF) 聲明：「跨入 21 世紀，奈米技術將對世界人類的健康、財富及安全產生重大影響，如同 20 世紀的抗生素、積體電路和人工合成聚合物一樣。」
- H. Rohrer (1986 物理諾貝爾獎) 「七十年代重視微米技術的國家如今都成為發達國家，現在重視奈米技術的國家很可能成為一下個世紀的先進國家！」
- IBM 2000 年 8 月發佈研發量子電腦。
- 日本電信電話公司 (NTT) 和 NEC 公司 2001 年 2 月決定聯合研發量子電腦。
- MagiQ Technologies, Inc. 1999 成立，研發 Quantum Information Technology。
- 量子電腦計算速度可望比超級電腦快 1 億倍，預估 2010 年前後實用化。
- 台積電年底進入 90 奈米時代 (2002.03.20 中國時報)
全球第一家以九十奈米製程的晶圓廠，領先國際半導體技術藍圖兩年的時間
- 0.25 微米 0.18 微米 0.13 微米 0.09 微米 (90 奈米)

1 Nanometer (nm 奈米) = 10^{-9} m = 10 Å

Atomic Size of Hydrogen: 1.58 Å (Atomic Radius)

References

- David J. Griffiths, **Introduction to Quantum Mechanics**, 2nd ed., Pearson Education, Inc., 2005.
- Paul C.W. Davies and David S. Betts, **Quantum Mechanics**, 2nd ed., Chapman & Hall, 1994.
- Richard Turton, **The Quantum Dot**, Oxford University Press, 1996.

Lecture 1

Schrödinger's Equation

1.0 Origins

Planck's Energy Quantization Formula (1900) : A natural fact.

The energy of *any* system that absorbs or emits electromagnetic radiation of frequency ν is an integer multiple of an energy quantum

$$E = h\nu = \hbar\omega \tag{1.1}$$

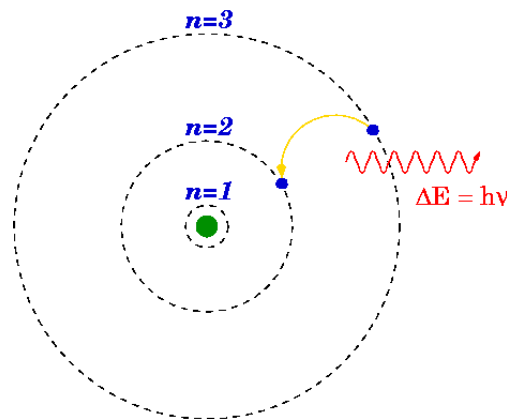


Fig. 1.1: Picture of the 1913 Bohr model of the hydrogen atom showing the Balmer transition from $n=3$ to $n=2$. The electronic orbitals (shown as dashed black circles) are drawn to scale, with 1 inch = 1 Angstrom; note that the radius of the orbital increases quadratically with n . The electron is shown in blue, the nucleus in green, and the photon in red. The frequency ν of the photon can be determined from Planck's constant h and the change in energy ΔE between the two orbitals. For the 3-2 Balmer transition depicted here, the wavelength of the emitted photon is 656 nm. [Photon](http://en.wikipedia.org/wiki/Photon) <http://en.wikipedia.org/wiki/Photon>

E : energy , $\omega = 2\pi\nu$ angular frequency
 h : Planck's constant (6.63×10^{-34} Js)
 $\hbar = h/2\pi$ (1.05×10^{-34} Js)

Discrete electromagnetic energies (Quanta, Photons).
 Light : $\nu \approx 10^{15}$ Hz , $E = 10^{-18}$ J.

The photon has zero rest mass and, in empty space, travels at a constant speed c ; in the presence of matter, it can be slowed or even absorbed, transferring energy and momentum proportional to its frequency. The photon has both wave and particle properties; it exhibits wave-particle duality.

Max Planck (1918 [Nobel Laureate in Physics](#))

"In recognition of the services he rendered to the advancement of Physics by his discovery of energy quanta."

Niels Bohr (1922 Nobel Laureate in Physics)

"for his services in the investigation of the structure of atoms and of the radiation emanating from them."

Einstein's Mass-Energy Equivalence Formula (1905)

$$E=mc^2$$

The relativistic expressions for the energy E of a particle with the rest mass m moving with a velocity v , i.e., with a momentum $p=mv$ can be manipulated into the fundamental *relativistic energy-momentum equation*:

$$E^2 - (pc)^2 = (mc^2)^2$$

Note that there is no relativistic mass in this equation; the m stands for the rest mass. This equation is a more general version of Einstein's famous equation " $E=mc^2$ ".

The equation is also valid for photons, which are massless (have no rest mass):

$$E^2 - (pc)^2 = 0$$

$$E = pc$$

$$p = E/c$$

Therefore a photon's momentum is a function of its energy; it is not analogous to the momentum in Newtonian mechanics.

Considering an object at rest, the momentum p , in the first equation above, is zero, and we obtain

$$E^2 = (mc^2)^2$$

which reduces to

$$E = mc^2$$

suggesting that this last well-known relation is only valid when the object is at rest, giving what is known as the *rest energy*. If the object is in motion, we have

$$E^2 = (mc^2)^2 + (pc)^2$$

From this we see that the total energy of the object E depends on its rest energy and momentum; as the momentum increases with the increase of the velocity v , so does the total energy. [Mass in special relativity](http://en.wikipedia.org/wiki/Relativistic_mass) http://en.wikipedia.org/wiki/Relativistic_mass

The fundamental relativistic energy-momentum equation for photons is

$$E = pc \tag{1.2}$$

c : speed of light

Albert Einstein (1921 Nobel Laureate in Physics)

"for his services to Theoretical Physics, and especially for his explanation of the photoelectric effect."

De Broglie's Particle – Wave Duality (1923) :

The wave-particle duality holds that light and matter exhibit properties of both waves and of particles.

$$p = \frac{h\nu}{c} = \frac{h}{\lambda} = \hbar k = \frac{h}{2\pi} \cdot \frac{2\pi}{\lambda}, \quad \boxed{p\lambda = h, p = \hbar k} \tag{1.3}$$

λ : wavelength

k : wave number

Photon - Photoelectric Effect - Coconut Shy.

One photon knocks out one electron.

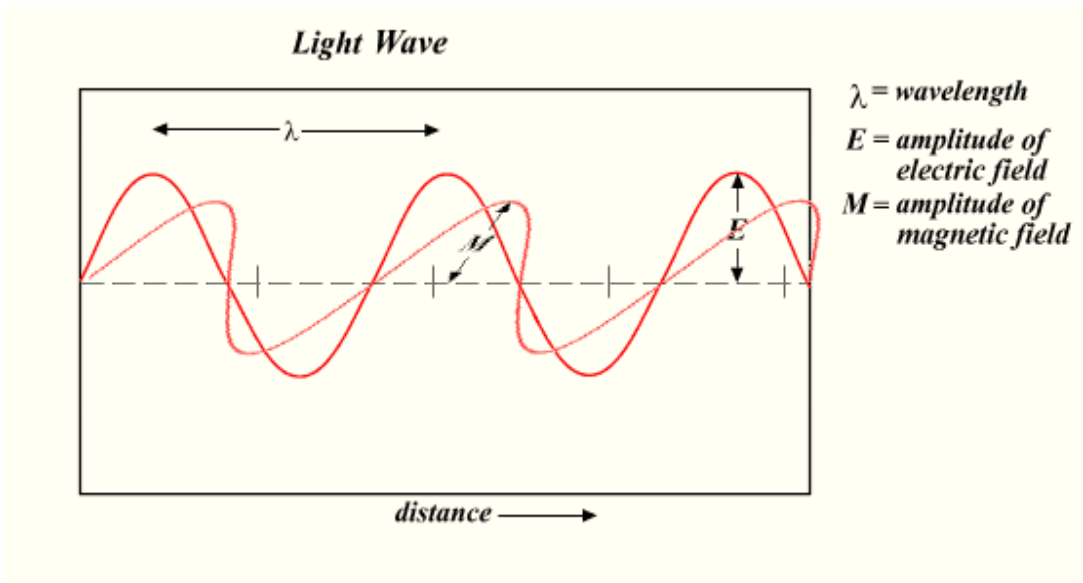
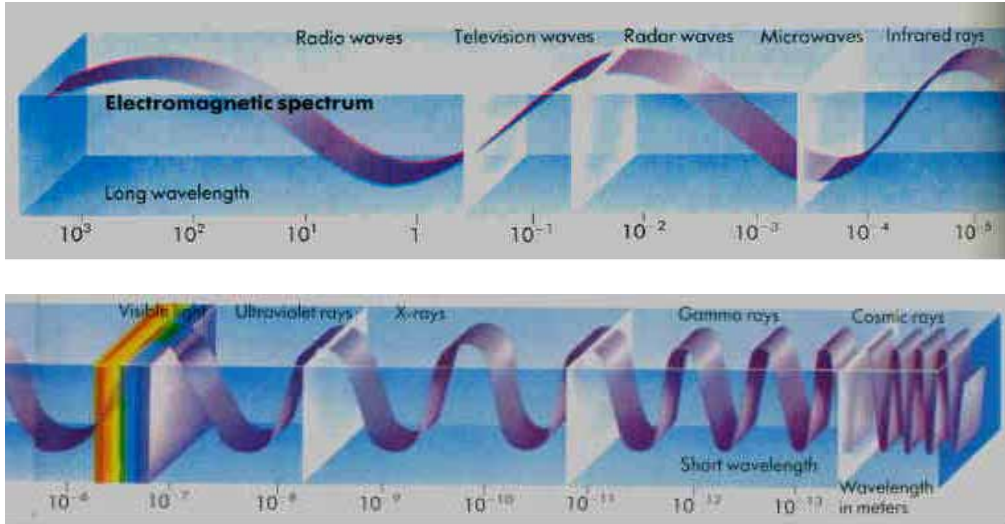
Photon $m = 0$ mass-less particle.

Louis de Broglie (1929 Nobel Laureate in Physics)

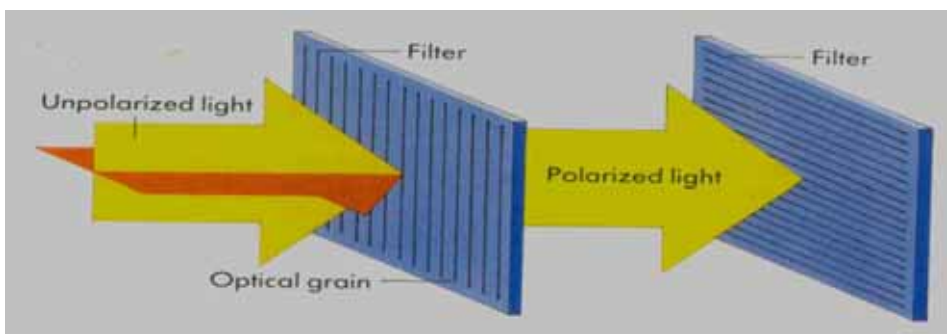
" for his discovery of the wave nature of electrons."

1.1 Collapse of Determinism (Probability)

Electromagnetic Wave



Polarized Wave : Electric or magnetic wave.



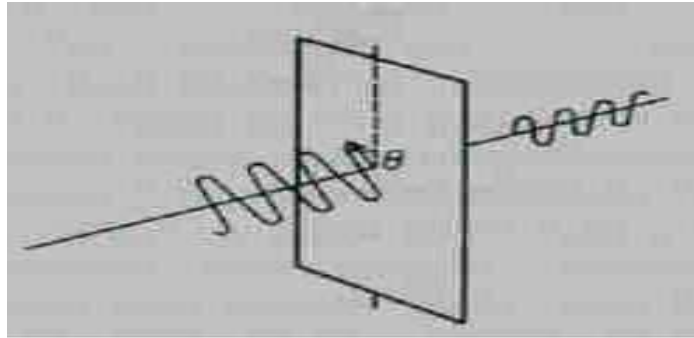


Fig. 1.2: A plane-polarized light encounters an obliquely oriented polarizer only a fraction $\cos^2 \theta$ of the intensity is transmitted.

$\theta = 0^\circ$: All the light is transmitted

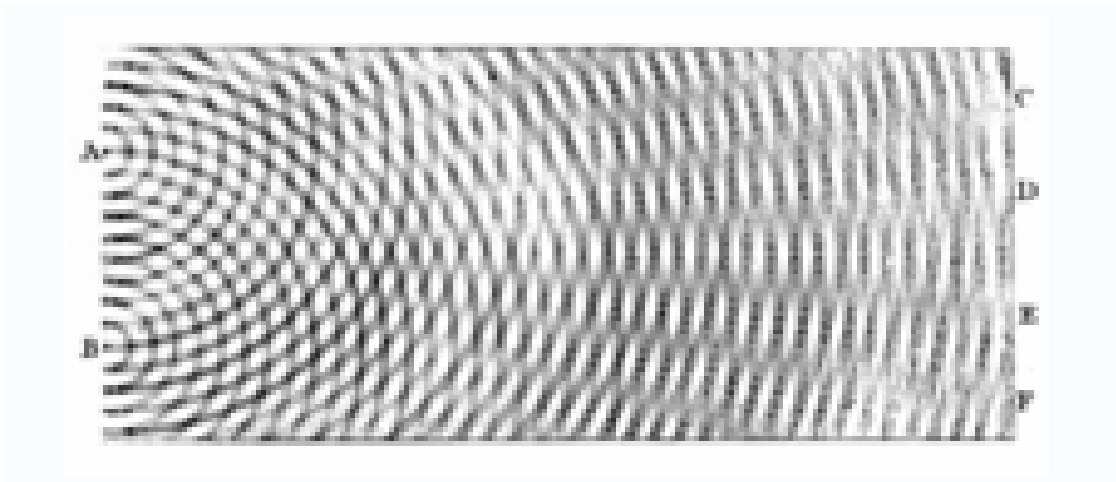
$\theta = 45^\circ$: Half gets through

$\theta = 90^\circ$: No transmission

Transmitted Fraction = Transmission Probability = $\cos^2 \theta$

- Weird Feature: Suppose the intensity of the light is reduced so that Only one photon at a time arrives at the polarizer.
- Photon cannot be chopped in half \Rightarrow Photon either does or does not get through the polarizer. (Who will get through?)
- The polarizer has no means of sorting photons into ‘sheep’ and ‘goats’.

1.2 When is a wave a particle?



[Thomas Young's double-slit experiment](#) in 1805 showed that light could act as a [wave](#), helping to defeat early [particle](#) theories of light.

- Physicists still regard an electron as a point-like entity but the precise location of that point may not be well-defined.
- Matter waves are abstract waves (crime waves, fashions, unemployment)
- Matter waves are also probability waves.

Waves vs. Particles

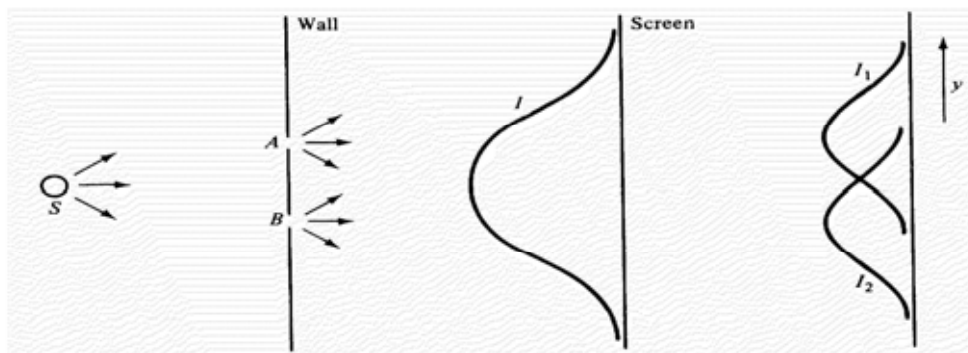


Fig. 1.3: Particle double-slit experiment. Particle intensities add.

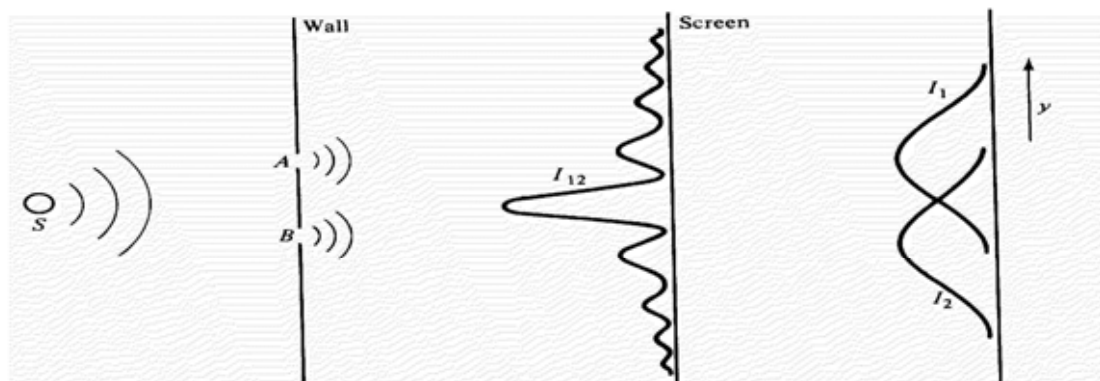


Fig. 1.4: Wave double-slit experiment. Amplitudes add.

$\psi = \psi(\vec{r}, t)$: wave function

$\psi = \psi(\vec{r}, t) = |\psi| e^{i\alpha}$ α : phase

$I = |\psi|^2$: Intensity

Superimposition:

$$\begin{aligned}
\psi &= \psi_1 + \psi_2 \\
I &= |\psi|^2 = |\psi_1 + \psi_2|^2 = (\psi_1 + \psi_2)(\overline{\psi_1 + \psi_2}) \\
&= |\psi_1|^2 + |\psi_2|^2 + |\psi_1\psi_2| [e^{i(\alpha_1 - \alpha_2)} + e^{-i(\alpha_1 - \alpha_2)}] \\
&= I_1 + I_2 + 2\sqrt{I_1 I_2} \cos(\alpha_1 - \alpha_2)
\end{aligned}$$

\Downarrow
Interference

The wave of each individual particle passes through both slits but the particle passes through only one.

1.3 Schrödinger's Wave Equation

Peter Debye (1926): If matter is a wave, there should be a wave equation to describe a matter wave.

A Traveling Sine Wave: $\psi(x, t) = A \sin \frac{2\pi}{\lambda} (x - vt)$

A Matter Wave:

$$\begin{aligned}
\psi(x, t) &= A \exp\left(\frac{2\pi i}{\lambda} (x - ct)\right) = A \exp\left(\frac{2\pi i}{\lambda} (x - \lambda vt)\right) \\
&= A \exp\left(2\pi i \left(\frac{p}{h} x - \frac{E}{h} t\right)\right) = A \exp\left(\frac{i}{\hbar} (px - Et)\right)
\end{aligned}$$

$$\frac{\partial \psi}{\partial x} = \frac{ip}{\hbar} \psi \quad \Rightarrow \quad p\psi = -i\hbar \frac{\partial \psi}{\partial x} \tag{1.4}$$

$$\frac{\partial^2 \psi}{\partial x^2} = -\frac{p^2}{\hbar^2} \psi \quad \Rightarrow \quad p^2 \psi = -\hbar^2 \frac{\partial^2 \psi}{\partial x^2} \tag{1.5}$$

$$\frac{\partial \psi}{\partial t} = -\frac{iE}{\hbar} \psi \quad \Rightarrow \quad E\psi = -i\hbar \frac{\partial \psi}{\partial t} \tag{1.6}$$

$$E = \frac{1}{2}mv^2 + V = \frac{p^2}{2m} + V = K + V$$

= Kinetic Energy + Potential Energy

Erwin Schrödinger (1926):

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

$$\boxed{i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi + V\psi} \quad (1.7)$$

- Key equation of the quantum theory.
- Must be accepted as a fundamental postulate.

$$\nabla^2 = \Delta = \nabla \cdot \nabla = \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}\right) \cdot \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}\right)$$

$$= \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \quad \text{or} \quad = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \quad (\text{Laplace operator})$$

$$V = V(\vec{r}, t), \quad \psi = \psi(\vec{r}, t)$$

How to interpret the wave function ψ (a complex function)?

Observables (position, speed, energy, ...) are real.

Max Born Postulate:

$|\psi(\vec{r}, t)|^2 = \psi^* \psi$ is the probability density for a particle to be located at point \vec{r} at time t .

$|\psi|^2 d\vec{r}$ is the probability it will be in the infinitesimal volume $d\vec{r}$ at time t .

ψ is not an observable quantity \Rightarrow the phase of ψ is arbitrary (changing) without changing the observable quantity $|\psi|^2$.

Normalization Condition: $\int_{\mathbb{R}^3} |\psi(\vec{r}, t)|^2 d\vec{r} = 1$

1D : $I = (x_1, x_2)$

$$\frac{\partial}{\partial t} \int_{x_1}^{x_2} |\psi(x, t)|^2 dx = \int_{x_1}^{x_2} \left(\psi^* \frac{\partial \psi}{\partial t} + \psi \frac{\partial \psi^*}{\partial t} \right) dt$$

↓

Rate of
change
of prob. for a
particle to be
in I.

$$\begin{aligned}
 &= \frac{i\hbar}{2m} \int_{x_1}^{x_2} \left(\psi^* \frac{\partial^2 \psi}{\partial x^2} - \psi \frac{\partial^2 \psi^*}{\partial x^2} \right) dx \\
 &= \frac{i\hbar}{2m} \left(\psi^* \frac{\partial \psi}{\partial x} - \psi \frac{\partial \psi^*}{\partial x} \right) \Big|_{x_1}^{x_2} \quad (1.8)
 \end{aligned}$$

Define $j(\vec{r}, t) = -\frac{i\hbar}{2m} (\psi^* \nabla \psi - \psi \nabla \psi^*)$ the probability current

density.

(1.8) \Rightarrow rate of increase of probability that particle is in I

$$= j(x_1, t) - j(x_2, t)$$

= flow into I from left + flow into I from right

= total flow in I.

Average (or expectation) value of the particle's position:

$$\langle \vec{r} \rangle = \int \vec{r} |\psi(\vec{r}, t)|^2 d\vec{r}$$

Similarly, expectation value of other quantity $f(\vec{r})$

$$\langle f(\vec{r}) \rangle = \int f(\vec{r}) |\psi(\vec{r}, t)|^2 d\vec{r}$$

Erwin Schrödinger (1933 Nobel Laureate in Physics)

" for the discovery of new productive forms of atomic theory."

Max Born (1954 Nobel Laureate in Physics)

"for his fundamental research in quantum mechanics, especially for his statistical interpretation of the wavefunction."

Lecture 2

Solutions of Schrödinger's Equation

2.1 Time-Independent Schrödinger's Equation

$V = V(\vec{r})$ static (time-independent) potential.

The energy of a particle moving in a static potential is conserved.

Separation of variable:

$$\psi(\vec{r}, t) = u(\vec{r})f(t)$$

(1.10) \Rightarrow

$$\frac{1}{u} \left[-\frac{\hbar^2}{2m} \nabla^2 u + V(\vec{r})u \right] = \frac{i\hbar}{f} \frac{\partial f}{\partial t} \quad (2.1)$$

$$-\frac{\hbar^2}{2m} \nabla^2 u + Vu = Eu \quad (2.2)$$

$$i\hbar \frac{\partial f}{\partial t} = Ef(t) \quad (2.3)$$

$$(2.3) \Rightarrow f(t) = e^{\frac{-iEt}{\hbar}}$$

$$\psi(\vec{r}, t) = u(\vec{r})e^{\frac{-iEt}{\hbar}} \quad (2.4)$$

$e^{\frac{-iEt}{\hbar}}$: a pure phase factor

The probability density is independent of the phase, i.e.,

$$|\psi(\vec{r}, t)|^2 = |u(\vec{r})|^2 \quad (2.5)$$

What is E ?

Consider a free particle by putting $V = 0$ in (2.2), i.e.,

$$\nabla^2 u = -\frac{2mE}{\hbar^2} u$$

Which has solutions of the form

$$u \propto e^{i\vec{k}\cdot\vec{r}} \quad (2.6)$$

$$k^2 = |\vec{k}|^2 = \frac{2mE}{\hbar^2}$$

$$E = \frac{k^2 \hbar^2}{2m} = \frac{p^2}{2m} = \frac{1}{2} m v^2 \quad \text{by (1.3)}$$

E is the kinetic energy of the particle.

When $V \neq 0$,

$$E = \text{Kinetic Energy} + \text{Potential Energy} = \text{Total Energy}$$

Hence (2.2) is an energy equation.

1D Time-Independent Schrödinger's Equation:

$$-\frac{\hbar^2}{2m} \frac{d^2 u(x)}{dx^2} + V(x)u(x) = Eu(x) \quad (2.7)$$

An eigenvalue problem : Given V , find E and u .

To be physically acceptable, a wave function must satisfy the following important conditions :

- (1) ψ is a single-valued function of position and time.
- (2) ψ is normalizable.
- (3) ψ and $\nabla \psi$ will be continuous everywhere except where

V has an infinite discontinuity.

2.2 Infinite Square-Well Potential

Example 2.1.

$$V(x) = \begin{cases} \infty & |x| > a \\ 0 & |x| < a \end{cases}$$

$$-\frac{\hbar^2}{2m} \frac{d^2 u}{dx^2} = Eu \quad |x| < a$$

Solutions :

$$\begin{aligned} u(x) &= A \sin \alpha x + B \cos \alpha x & |x| < a & \quad (2.8) \\ &= 0 & |x| > a & \end{aligned}$$

A, B : constants

$$\alpha = \left(\frac{2mE}{\hbar^2} \right)^{1/2}$$

Continuity Condition on Boundary

Since u must be continuous at $x = \pm a$, we have

$$\left. \begin{aligned} + A \sin \alpha a + B \cos \alpha a &= 0 \\ - A \sin \alpha a + B \cos \alpha a &= 0 \end{aligned} \right\} \quad (2.9)$$

Hence, either

$$\left. \begin{aligned} A = \cos \alpha a = 0 &\Rightarrow \alpha = \frac{n\pi}{2a}, n = 1, 3, 5 \dots \\ \text{or} \\ B = \sin \alpha a = 0 &\Rightarrow \alpha = \frac{n\pi}{2a}, n = 2, 4, 6 \dots \end{aligned} \right\} \quad (2.10)$$

$$\Rightarrow E \equiv E_n = n^2 \pi^2 \hbar^2 / 8ma^2 \quad (2.11)$$

Note: (2.8) \Rightarrow Continuity Condition on Boundary \Rightarrow (2.9)
 \Rightarrow Restriction on α (2.10)
 $\Rightarrow E_n$ Discrete energy levels (2.11)
 \Rightarrow Energy is Quantized!

Classical limit $\hbar \rightarrow 0 \Rightarrow E_n$ is continuous

$E_n a \approx \hbar^2$ m : electron mass

Atom : $a \approx 10^{-10}$ m $\Rightarrow E_n, n=1, 2$ will be spaced out
 by several electron volts (eV).

Ground state energy ($n = 1$) :

$$E_1 = \frac{\pi^2 \hbar^2}{8ma^2} \neq 0$$

$$= 0 \text{ (could be classically)}$$

Heisenberg's Principle :

$$\Delta p \approx \hbar/a \quad \Delta x = a$$

$$\frac{(\Delta p)^2}{2m} \approx \frac{\hbar^2}{2ma^2} \approx E_1$$

$$a \rightarrow \infty \Rightarrow E_1 \rightarrow 0$$

Normalization Condition

$$\int_{-\infty}^{\infty} |\psi|^2 dx = \int_{-a}^a |u|^2 dx = A^2 \int_{-a}^a \sin^2(n\pi x / 2a) dx = 1 \quad n : \text{even}$$

$$\Rightarrow A = \sqrt{\frac{1}{a}}$$

Similarly, $B = \sqrt{\frac{1}{a}}$. Thus

$$u(x) = \begin{cases} \sqrt{\frac{1}{a}} \sin(n\pi x / 2a) & n : \text{even} \\ \sqrt{\frac{1}{a}} \cos(n\pi x / 2a) & n : \text{odd} \end{cases} \quad (2.12)$$

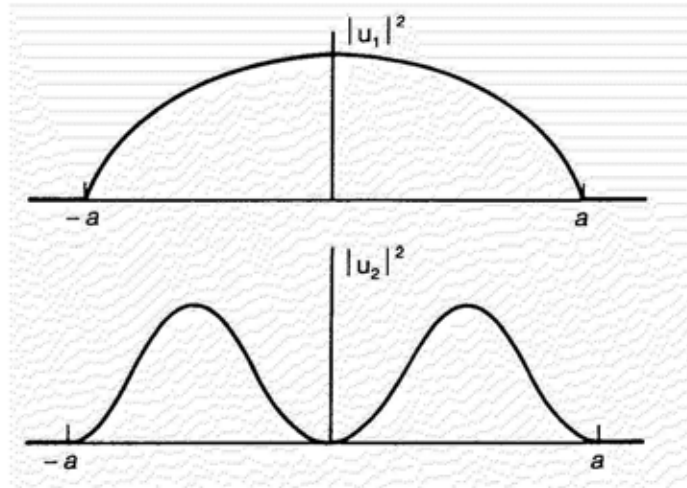


Fig. 2.1. Position probability densities for the ground state ($n = 1$) and first excited state ($n = 2$) of a particle trapped in a 1D impenetrable box of length $2a$. Note the symmetry about the origin.

Classical standing waves with discrete frequencies of vibration

$$\langle x \rangle = \frac{1}{a} \int_{-a}^a x \sin^2(n\pi x / 2a) dx = 0 \quad (\text{by symmetry})$$

2.3 Finite Square Well

Example 2.2.

$$V(x) = \begin{cases} V_0 > 0 & |x| > a \\ 0 & |x| < a \end{cases} \quad (2.7) \Rightarrow$$

$$-\frac{\hbar^2}{2m} \frac{d^2 u}{dx^2} = Eu \quad |x| < a$$

$$-\frac{\hbar^2}{2m} \frac{d^2 u}{dx^2} + V_0 u = Eu \quad |x| > a$$

$$\alpha = \sqrt{\frac{2mE}{\hbar^2}}, \quad \beta = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$$

For $E < V_0$:

$$\frac{d^2 u}{dx^2} = -\alpha^2 u \quad |x| < a$$

$$\frac{d^2 u}{dx^2} = \beta^2 u \quad |x| > a$$

Solution :

$$u = \begin{cases} A \sin \alpha x + B \cos \alpha x & |x| < a \\ C e^{-\beta x} + D e^{\beta x} & |x| > a \end{cases} \quad (2.13)$$

(i) Even parity \Rightarrow

$$u = \begin{cases} B \cos \alpha x & 0 < x < a \\ C e^{-\beta x} & x > a \end{cases}$$

$$\text{Continuity at } x = a \quad \Rightarrow \quad \tan \alpha a = -\beta / \alpha$$

(ii) Odd Parity + Continuity $\Rightarrow \quad \cot \alpha a = -\beta / \alpha$

$$\text{Let } \gamma = \sqrt{\frac{2mV_0 a^2}{\hbar^2}} \quad \theta = \gamma \sqrt{\frac{E}{V_0}}$$

$$\text{Then } \beta / \alpha = \sqrt{[(\gamma / x)^2 - 1]} \quad -\cot \alpha a = -\cot \theta$$

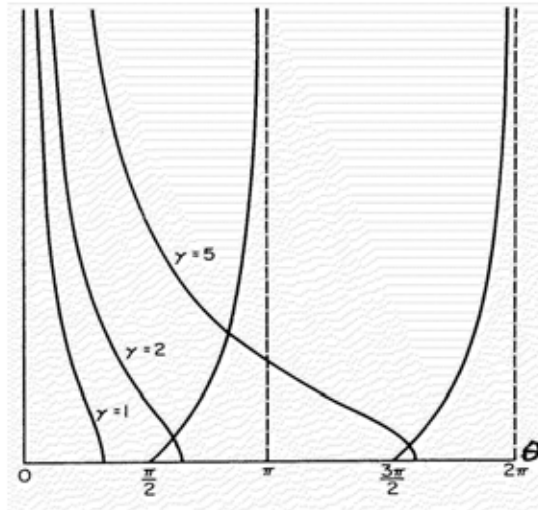


Fig. 2.2. Graphs of $-\cot \theta$ and $\sqrt{\left(\frac{\gamma}{\theta}\right)^2 - 1}$ are shown. As

γ is increased so the latter curves reach out farther to the right. The points of intersection determine the values of E , which correspond to the allowed energy levels

$$(E_1 = \theta_1^2 V_0 / \gamma^2, E_2 = \theta_2^2 V_0 / \gamma^2, E_3 = \theta_3^2 V_0 / \gamma^2).$$

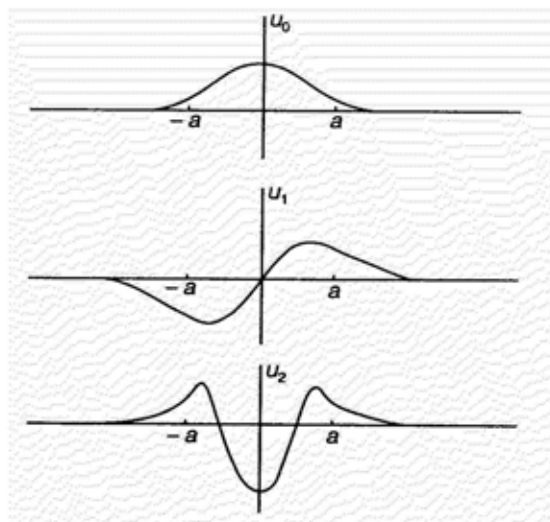


Fig. 2.3. Wave functions for the first three energy levels of the finite square-well system.

2.4 Tunneling

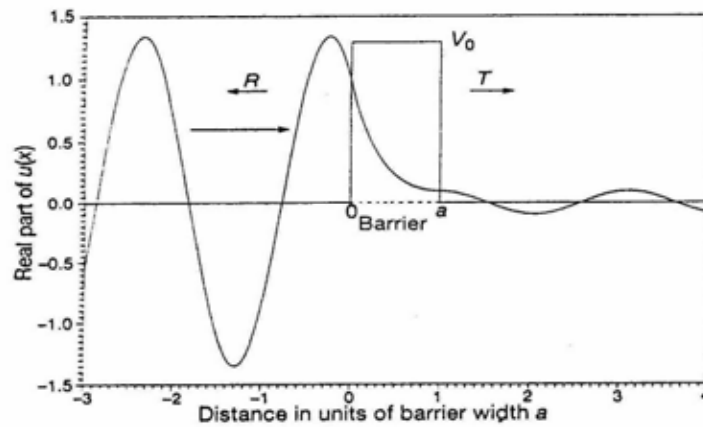


Fig. 2.4. A steady stream of particles from the left encounters a 'square-hill' potential barrier with energy $E < V_0$. Quantum penetration of the barrier allows the wave to emerge weakened on the remote side of the barrier, representing a finite probability that a given particle will quantum mechanically 'tunnel' through the barrier. There will thus be a transmitted fraction T and a reflected fraction R . The wave function shown decays rapidly inside the barrier so the tunnel effect is small except for low thin barriers.

2.5 Finite Difference Approximation

$$\frac{-\hbar^2}{2m^*} u''(x) + V(x)u(x) = \lambda u(x) \quad \forall x \in (a, b) \quad (2.14)$$

$$u(a) = 0, \quad u(b) = 0$$

Central Difference Formulas:

Partition: $h = \frac{b-a}{N+1}$: mesh size, $x_i = a + ih$, $i = 0, 1, \dots, N+1$.

$$u'(x_i) \approx \frac{u\left(x_i + \frac{1}{2}h\right) - u\left(x_i - \frac{1}{2}h\right)}{h} =: \frac{u_{i+\frac{1}{2}} - u_{i-\frac{1}{2}}}{h}, \quad i = 1, \dots, N.$$

$$u''(x_i) \approx \frac{u_{i+1} - 2u_i + u_{i-1}}{h^2} \approx \frac{U_{i+1} - 2U_i + U_{i-1}}{h^2}$$

$u(x_i) = u_i \approx U_i$, i.e., the unknown scalar U_i is an approximate value of the unknown wave function $u(x)$ at x_i .

代入原式(2.14)，可以得到

$$\frac{-\hbar^2}{2m^*} \left(\frac{U_{i+1} - 2U_i + U_{i-1}}{h^2} \right) + V_i U_i = \lambda U_i, \quad i = 1, \dots, N.$$

$$i = 1 \Rightarrow \left(\frac{\hbar^2}{m^* h^2} + V_1 \right) U_1 + \left(\frac{-\hbar^2}{2m^* h^2} \right) U_2 = \lambda U_1$$

$$i = 2 \Rightarrow \left(\frac{-\hbar^2}{2m^* h^2} \right) U_1 + \left(\frac{\hbar^2}{m^* h^2} + V_2 \right) U_2 + \left(\frac{-\hbar^2}{2m^* h^2} \right) U_3 = \lambda U_2$$

⋮

$$i = N \Rightarrow \left(\frac{-\hbar^2}{2m^* h^2} \right) U_{N-1} + \left(\frac{\hbar^2}{m^* h^2} + V_N \right) U_N = \lambda U_N$$

$$\begin{pmatrix}
\frac{\hbar^2}{m^*h^2} + V_1 & \frac{-\hbar^2}{2m^*h^2} & 0 & 0 & 0 & \dots & \dots & 0 & 0 \\
\frac{-\hbar^2}{2m^*h^2} & \frac{\hbar^2}{m^*h^2} + V_2 & \frac{-\hbar^2}{2m^*h^2} & 0 & 0 & \vdots & \vdots & 0 & 0 \\
0 & \frac{-\hbar^2}{2m^*h^2} & \frac{\hbar^2}{m^*h^2} + V_3 & \frac{-\hbar^2}{2m^*h^2} & 0 & \vdots & \vdots & \vdots & \vdots \\
\vdots & 0 & \ddots & \ddots & \ddots & \vdots & \vdots & \vdots & \vdots \\
\vdots & \vdots & \vdots & \ddots & \ddots & \ddots & \ddots & \vdots & \vdots \\
\vdots & \vdots & \vdots & \vdots & \ddots & \ddots & \ddots & \vdots & 0 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \ddots & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & \frac{-\hbar^2}{2m^*h^2} & \frac{\hbar^2}{m^*h^2} + V_{N-1} & \frac{-\hbar^2}{2m^*h^2} \\
0 & 0 & 0 & 0 & 0 & 0 & \frac{-\hbar^2}{2m^*h^2} & \frac{\hbar^2}{m^*h^2} + V_N & \frac{-\hbar^2}{2m^*h^2}
\end{pmatrix}
\begin{pmatrix} U_1 \\ U_2 \\ U_3 \\ \vdots \\ \vdots \\ \vdots \\ U_{N-2} \\ U_{N-1} \\ U_N \end{pmatrix}
= \lambda
\begin{pmatrix} U_1 \\ U_2 \\ U_3 \\ \vdots \\ \vdots \\ \vdots \\ U_{N-2} \\ U_{N-1} \\ U_N \end{pmatrix}$$

⇒ Eigenvalue Problem:

$$AU = \lambda U \quad (2.15)$$