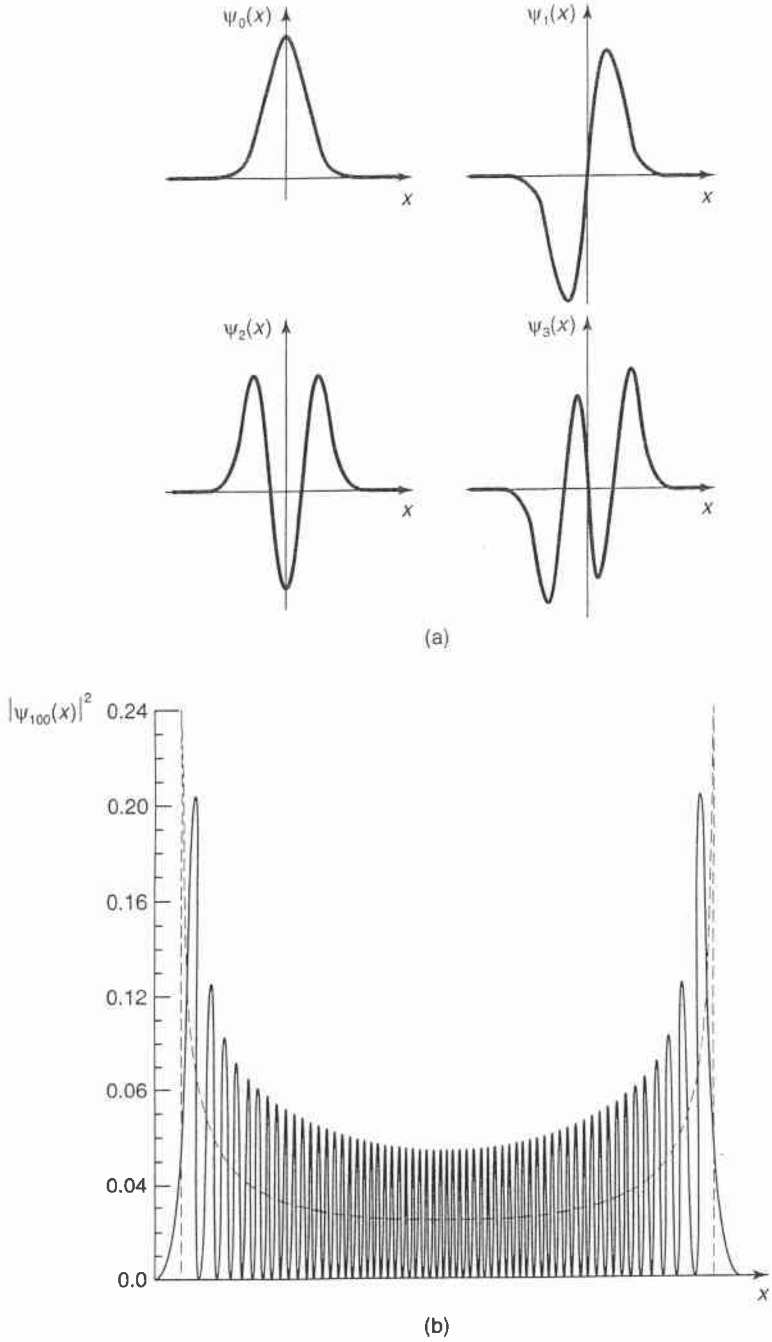
Nov. 7

Lecture 1

Simple harmonic oscillator figure
classical limit

Heisenberg's Uncertainty Principle

Comment on harmonic oscillator
wave function, classical limit



(a) The first four stationary states of the harmonic oscillator.
(b) Graph of $|\psi_{100}|^2$, with the classical distribution (dashed curve) superimposed.

Operator

$$\hat{a} = \left(\frac{\hbar\omega}{2}\right)^{1/2}\left(y + \frac{\partial}{\partial y}\right) \quad \text{annihilation}$$

operators

$$\hat{a}^{+} = \left(\frac{\hbar\omega}{2}\right)^{1/2}\left(y - \frac{\partial}{\partial y}\right) \quad \text{creation}$$

$\hat{a}$, $\hat{a}^{+}$ are the "normalized" annihilation and creation operator

Show $[\hat{a}, \hat{a}^{+}] = \hbar\omega$

$$\hat{a}\hat{a}^{+} = \hat{H} + \frac{1}{2}\hbar\omega$$

$$\hat{a}^{+}\hat{a} = \hat{H} - \frac{1}{2}\hbar\omega$$

$$H = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2$$

Heisenberg's Uncertainty Relation.

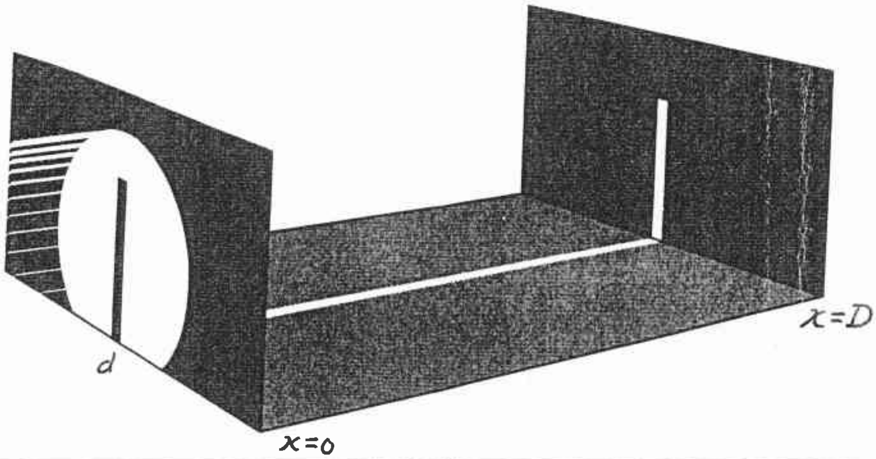
Relation with particle-wave duality

$$[x, P_x] = i\hbar \Rightarrow \Delta x \Delta P_x \geq \frac{\hbar}{2}$$

Applications

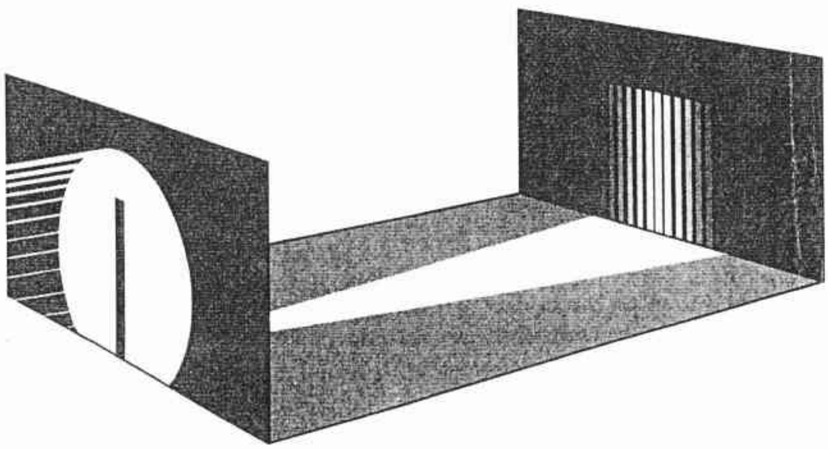
Uncertainty relation and wave-particle duality

Classical particle



According to classical mechanics, the image of a slit upon which a beam of particles is incident is the geometric projection of the slit.

A beam of particle of momentum P_x emerges from the slit $x=0$, $\Delta y = d$ they will strike the screen at $x = D$ within a marrow strip of width d.



If a slit is illuminated by waves (e.g., light), a diffraction pattern is seen on the screen.

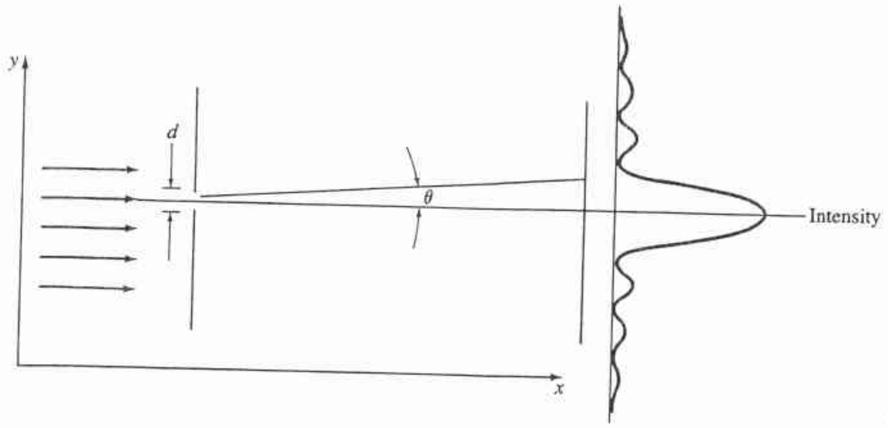
Wave $\Rightarrow$ the intensity of the wave will exhibit the typical diffraction pattern

The width of the pattern is defined by the angular seperation between the two minima bordering the central maximum. $= 2\theta$

$$\sin\theta = \theta = \frac{\lambda}{d} = \frac{\lambda}{\Delta y} \quad \text{for } \theta \ll 1 \quad (\lambda \ll d)$$

See P. 701 of Alonso and Finn

$\Rightarrow$ the more we try to delimit the position of the wave at $x = 0$ by reducing the width of the slit the more we broaden the diffraction pattern



Particles exhibit wavelike behavior, we can use above equation and the de Broglie relation to determine ΔP_y (the spread in P_y)

$$\frac{\Delta P_y}{P_x} = \frac{\delta y}{D} = \tan\theta \sim \theta = \frac{\lambda}{\Delta y}$$

$$\frac{h}{P} \sim \frac{h}{P_x} = \lambda$$

$$\frac{\Delta P_y}{P_x} = \frac{h/P_x}{\Delta y}$$

$\Rightarrow \quad \Delta P_y \, \Delta y \simeq h \quad \rightarrow$ consistent with the uncertainty relation

Remark:

Uncertainty relation is a direct and necessary consequences of the wave nature of particles.

The uncertainty relation is independent of λ.

The beam of electrons is moving only in the x direction so before passing the slit it has no momentum component in the y direction ($P_y = 0$)

Since we know P_y exactly ($\Delta P_y = 0$)

$\Delta = \infty$

we have no knowledge at all about the particles along the y direction.

The diffraction (spreading) of a beam following passage through a slit is the effect of the uncertainty principle on our attempt to specify the location of the particle.

As we make the slit narrower P_y increases and the beam spread even more

The trade-off between observations of position and momentum is the core of the Heisenberg uncertainty principle.

分類：
編號： 9-18
總號：

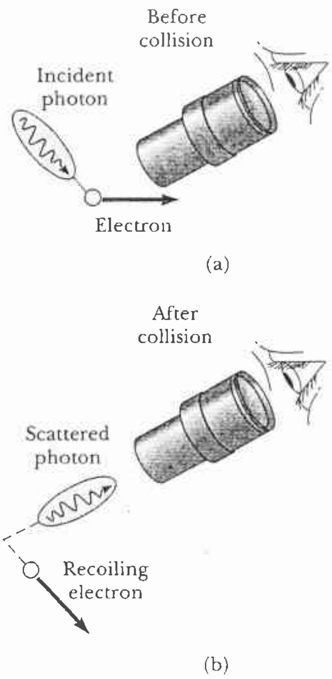
Heisenberg's microscope

This photograph of Werner Heisenberg was taken around 1924 (University of Hamburg). Heisenberg obtained his PhD in 1923 at the University of Munich where he studied under Arnold Sommerfeld and became an enthusiastic mountain climber and skier. Later, he worked as an assistant to Max Born at Göttingen and Niels Bohr in Copenhagen. While physicists such as de Broglie and Schrödinger tried to develop pictorialized models of the atom, Heisenberg, with the help of Born and Pascual Jordan, developed an abstract mathematical model called matrix mechanics to explain the wavelengths of spectral lines. The more successful wave mechanics by Schrödinger announced a few months later was shown to be equivalent to Heisenberg's approach. Heisenberg made many other significant contributions to physics, including his famous uncertainty principle, for which he received the Nobel prize in 1932, the prediction of two forms of molecular hydrogen, and theoretical models of the nucleus. During World War II he was director of the Max Planck Institute at Berlin where he was in charge of German research on atomic weapons. Following the war, he moved to West Germany and became director of the Max Planck Institute for Physics at Göttingen.

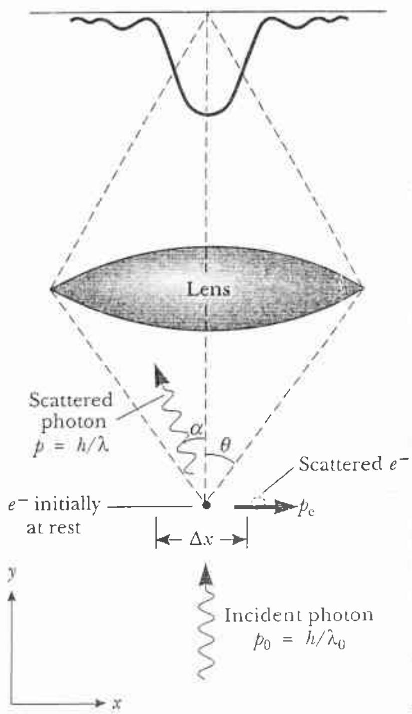
B I O G R A P H Y

WERNER HEISENBERG
(1901–1976)

(Photo courtesy of the University of Hamburg)



A thought experiment for viewing an electron with a powerful microscope. (a) The electron is shown before colliding with the photon. (b) The electron recoils (is disturbed) as a result of the collision with the photon.



The Heisenberg microscope. Conservation of momentum requires $p_{e^-} = (h \sin \alpha)/\lambda$. Because of diffraction by the lens opening, the electron may be anywhere in the region Δx.

Use the photon to measure the position of an electron.

Photon as wave
↓
resolving the position to Δx
with wavelength λ, then

$$\Delta x = \frac{\lambda}{2\sin\theta}$$

where 2θ is the angle subtended by the object lens

To be collected by the lens, the photon may be scattered through an angle from $-\theta$ to $+\theta$

$$\Delta p_x = 2p\sin\theta = 2\frac{h}{\lambda}\sin\theta$$

↕
the uncertainty of p_x imparts to the electron
(momentum conservation)

$$\Rightarrow \quad \Delta p_x \Delta x = \frac{2h}{\lambda}\sin\theta \cdot \frac{\lambda}{2\sin\theta}$$

$$= h.$$

· Again, we see that it is a consequence of particle-wave duality

· The result is independent of λ.

分類：
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Uncertainty relation

$$(\Delta A)^2 = \langle A^2\rangle - \langle A\rangle^2 = \langle (A - \langle A\rangle)^2\rangle$$

$$(\Delta B)^2 = \langle B^2\rangle - \langle B\rangle^2 = \langle (B - \langle B\rangle)^2\rangle$$

Define $U = A - \langle A\rangle$
$V = B - \langle B\rangle$

Consider $\phi = U\psi + i\lambda V\psi$

$$I(\lambda) = \int dx\, \phi^* \phi \geq 0$$

$$= \int dx\, (U\psi + i\lambda V\psi)^* (U\psi + i\lambda V\psi)$$

$$= \int dx\, (U\psi)^*(U\psi) + \lambda^2 \int dx\, (V\psi)^*(V\psi)$$
$$\cancel{+ i\lambda \int dx\, \{(U\psi^*)(V\psi) - (V\psi)^*(U\psi)\}}$$

U, V are Hermitian

$$= \int dx\, \psi^* (U^2 + \lambda^2 V^2 + i\lambda [U, V])\psi$$

commutator

$$= (\Delta A)^2 + \lambda^2 (\Delta B)^2 + i\lambda \int dx\, \psi^* [U, V]\psi$$

$[U, V] = [A, B]$

$$= (\Delta A)^2 + \lambda^2 (\Delta B)^2 + i\lambda \langle [A, B]\rangle \geq 0$$

Minimum occur at $\frac{dI(\lambda)}{d\lambda} = 0$

$$2\lambda (\Delta B)^2 + i\langle [A, B]\rangle = 0$$

$$\Rightarrow \quad \lambda = -i \frac{\langle [A, B]\rangle}{2(\Delta B)^2}$$

Substitute into $I(\lambda)$

$$\Rightarrow \quad (\Delta A)^2 - \frac{\langle [A, B]\rangle^2}{4(\Delta B)^2} + \frac{\langle [A, B]\rangle^2}{2(\Delta B)^2} \geq 0$$

$$\Rightarrow \quad (\Delta A)^2 (\Delta B)^2 \geq \frac{1}{4} \langle i[A, B]\rangle^2$$

this is the "uncertainty relation

$A \rightarrow x_{op}$, $B \rightarrow P_{op}$

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$$[A, B] \rightarrow [x, p_x] = i\hbar$$

$$\Delta x \, \Delta p_x \geq \frac{\hbar}{2}$$

this is the uncertainty relation of Heisenberg.

It asserts that a state of finite duration Δt cannot have a precisely defined energy in E specified by

$$\Delta E \Delta t \geq \frac{\hbar}{2}$$

Applying the uncertainty principle

- It is a useful tool, not a just a negative statement
- It is a great help in understanding many phenomena in quantum level.
- It gives a qualitative estimates
- The lower limit of $\frac{\hbar}{2}$ for $\Delta x \Delta p_x$ is rarely attained.

- The uncertainty principle changing nothing for macroscopic objects

  racquetball 100 g confined to a room of 15 m on a side. the ball is moving at 2 m/sec along x axis

$$\Delta p_x \geq \frac{\hbar}{2\Delta x} = \frac{1.05 \cdot 10^{-34}\,J\cdot sec}{2\cdot 10m}$$

$$= 3.5 \cdot 10^{-36}\,kg\,m/sec$$

$$\Delta v_x = \frac{\Delta p_x}{m} \sim 3.5 \cdot 10^{-35}\,m/sec.$$

$$\frac{\Delta v_x}{v_x} = 1.8 \cdot 10^{-35}$$

↳ certainly unmeasurable.

- Estimate the minimum kinetic energy of an electron confined by the electromagnetic force to be inside an atom

$$\Delta x \simeq 0.1\,nm \rightarrow \text{atomic radius}$$

$$m = 0.5\ MeV/c^2$$

$$\langle E_k \rangle_{min} = \frac{\hbar^2}{8m(\Delta x)^2} \sim 1\,eV$$

Estimate the minimum kinetic energy of the proton to be inside the nucleus

$$\Delta x \simeq 2\,fm \rightarrow \text{nuclear radius}$$

$$\Rightarrow \langle E_k \rangle_{min} \sim 1\,MeV.$$

· Do electron exist within the nucleus

Nuclear size is take to be $1 \cdot 10^{-14} m$

$$\Rightarrow \quad \Delta p = \underset{\substack{\downarrow \\ 20\ MeV/c}}{2 \cdot 10^{7}} \frac{eV}{c} \sim p \quad \sim 20\ MeV/c$$

Need relativity

$$E^2 = p^2c^2 + (m_e e)^2$$

$$E \geq 20\ MeV \qquad K = E - m_e c^2 \geq 19.2\ MeV$$

Since electron emitted in radioactive decay of the nucleus (β decay) have energies much less than 19.2 MeV (about 1 MeV or less) and is known no other mechanism could carry off an internuclear electron's energy during the decay process

$\Rightarrow$ electrons observed in β-decay do not come from within the nucleus but are actually created at the instant of decay.

· "Zero-point" energy of a harmonic oscillator

$$(\Delta p)^2 = \langle (p - \langle p \rangle)^2 \rangle = \langle (p^2 - 2p\underset{0}{\langle p \rangle} + \underset{0}{\langle p \rangle^2}) \rangle = \langle p \rangle^2$$

$$\langle K.E. \rangle = \frac{\langle p^2 \rangle}{2m} = \frac{(\Delta p)^2}{2m}$$

Same argument $\quad \langle P.E. \rangle = \frac{1}{2} m\omega^2 (\Delta x)^2$

$$\Rightarrow \quad E = \frac{1}{2} m\omega^2 (\Delta x)^2 + \frac{(\Delta p)^2}{2m}$$

$$\Delta p\, \Delta x \geq \frac{\hbar}{2}$$

$$\Rightarrow \quad E \geq \frac{1}{2} m\omega^2 (\Delta x)^2 + \frac{\hbar^2/8m}{(\Delta x)^2}$$

$$\frac{\partial E}{\partial (\Delta x)} = 0 \quad \Rightarrow \quad (\Delta x)_{min} = \sqrt{\frac{\hbar}{2m\omega}}$$

$$\Rightarrow E_{min} = \frac{1}{2} \hbar \omega$$

Exercise Estimate the size of hydrogen atom

$$E = \frac{p^2}{2m} - \frac{ke^2}{r} \qquad k = \frac{1}{4\pi\epsilon_0}$$

$\Delta x = r$

$(\Delta p)^2 = \langle p^2 \rangle \geq \frac{\hbar^2}{r^2}$

$E = \frac{\hbar^2}{2mr^2} - \frac{ke^2}{r}$

$\frac{dE}{dr} = 0 \Rightarrow r_{min} = \frac{\hbar^2}{ke^2 m} = a_0$

↳ Bohr radius

$\Rightarrow E_{min} = -\frac{k^2 e^4 m}{2\hbar^2} = -13.6\ eV$

Unstable particle

Many elementary particles are unstable
For example, the Δ has an average lifetime of only $3 \cdot 10^{-24}$ sec.
The average mass of the Δ is $1232\ MeV/c^2$
What is the uncertainty in the measurement of the mass of the Δ?

$\Delta E \geq \frac{\hbar}{2\Delta t} \simeq 110\ MeV$

↓ the uncertainty in its rest energy

$\Rightarrow m_\Delta = 1232 \pm 110\ MeV/c^2$

Width of atomic spectral lines.
When an atom is raised to an excited state, it usually decays to the ground state in about $\Delta t \sim 10^{-8}$ sec.
Consequently, there is an uncertainty in the short-lived excited state and a corresponding uncertainty in the wavelength of the radiation emitted as the atom returns to the ground state

$$\lambda = \frac{hc}{E_i - E_f}$$

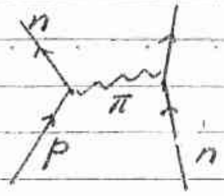
$E_i \rightarrow$ initial, excited state
$E_f \rightarrow$ final, ground state

$$\frac{d\lambda}{dE_i} = -\frac{hc}{(E_i - E_f)^2} = -\frac{\lambda}{E_i - E_f}$$

$$\Rightarrow \frac{\Delta\lambda}{\lambda} = -\frac{\Delta E}{E_i - E_f}$$

$$\Delta E \geq \frac{\hbar}{2\Delta t}$$

Range of the Forces



In order to produce π meson

$$\Delta E \gtrsim 140 \text{ MeV} = m_\pi c^2$$

It can "live"

$$\Delta t = \frac{h}{2\Delta E} = \frac{h}{2m_\pi c^2}$$

It at most travel a distance

$$R = c\Delta t = \frac{hc}{2\Delta E} = \frac{\hbar}{2m_\pi c^2}$$

$\downarrow$

mass - range relation

Nuclear force has a range $\sim 1-2\,fm \Rightarrow m_\pi$ can be estimated

$\downarrow$

Yukawa.

Operator

Physical Observable $\longrightarrow$ Linear, Hermitian operator

$$\langle \hat{A} \rangle_t = \int_{-\infty}^{\infty} \psi^*(x,t)\ \hat{A}\ \psi(x,t)\, dx$$

Eigenfunctions and Eigenvalues

The Physical Meaning of Eigenfunctions and Eigenvalues of $\hat{H}\psi_n = E_n \psi_n$

E_n , ψ_n

Orthonormality

$\hat{A}\ \psi_n = a_n \psi_n$

$\hat{A}\ \psi_m = a_m \psi_m$

$\hat{A}$ is Hermitian

a_n , a_m are real

If $a_n \neq a_m$, then

$$\int \psi_n^*(x) \psi_m(x)\, dx = 0 \quad \text{orthogonal.}$$

If $a_n = a_m$, then

$$\hat{A}\ (\alpha \psi_n + \beta \psi_m) = \underset{\substack{\downarrow \\ a_n = a_m}}{a_n}\ (\alpha \psi_n + \beta \psi_m)$$

we can choose a linear combination) of ψ_n , ψ_m such that ψ_n', ψ_m' are orthogonal

If ψ_n is an eigenfunction of $\hat{A}$, i.e.,

$$\hat{A}\ \psi_n = a_n \psi_n$$

then $\lambda_n \psi_n$ is also an eigenfunction of $\hat{A}$ with an eigenvalue a_n

$$\int \psi_n^*(x) \psi_n(x)\, dx < \infty$$

Then we can choose $u_n(x) = \lambda_n \psi_n(x)$

such that

$$\int u_n^*(x) \underset{\downarrow}{u_m}(x)\, dx = \delta_{nm}$$

orthormal

$\{u_n(x); E_n\}$ form an

orthonormal set

Example infinite potential well.

$$u_n(x) = \sqrt{\frac{2}{L}} \sin(n\pi \frac{x}{a})$$

with $E_n = \dfrac{\hbar^2\pi^2}{2mL^2} n^2$

Completeness

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

c_n can be determined by

$$\int u_m^*(x)\psi(x)\, dx = \sum_n \int u_m^*(x) u_n(x)\, dx \cdot c_n$$

$$= \sum_n \delta_{mn} c_n = c_m.$$

Put back the t-dependence

$$\psi(x,t) = \sum_n c_n u_n(x) e^{iE_n t/\hbar}$$

with

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

time-independent Schrodinger equation.

$$\int u_n^*(x) u_m(x)\, dx = \delta_{nm}$$

c_n can be determined from initial condition $\psi(x, 0)$

$$\psi(x,0) = \sum_n c_n u_n(x)$$

$$\Rightarrow \quad c_n = \int_{-\infty}^{\infty} u_n^*(x)\, \psi(x,0)\, dx$$

$$\Rightarrow \quad \psi(x,t) = \sum c_n u_n(x)\, e^{iE_n t/\hbar}$$

Physical meaning of $|C_n|^2$

$$\underset{\langle E\rangle}{\overset{\parallel}{\langle \hat{H} \rangle}} = \int \psi^*(x,t)\, \hat{H}\, \psi(x,t)\, dx$$

$$= \int \sum_m c_m^* u_m^*(x)\, e^{-iE_m t/\hbar}\ \hat{H} \sum_n c_n u_n(x) e^{iE_n t/\hbar}\, dx$$

$$\hat{H} u_n = E_n u_n$$

$$= \sum_m \sum_n c_m^* c_n\, e^{-iE_m t/\hbar}\, e^{iE_n t/\hbar} \underline{\int u_m^*(x) \hat{H} u_n(x)\, dx}$$

$$\downarrow$$

$$\int u_m^*(x) E_n u_n(x)\, dx$$

$$\Downarrow$$

$$E_n \int u_m^*(x) u_n(x) dx$$

$$\overset{\parallel}{E_n \delta_{nm}}$$

$$= \sum_m \sum_n c_m^* c_n\, e^{-iE_m t}\, e^{iE_n t/\hbar}\, E_n \delta_{nm}$$

$$= \sum_n |C_n|^2 E_n \qquad (A)$$

$|C_n|^2$ = probability of finding the state in an energy eigenstate with energy eigenvalue E_n

Meaning of $u_n(x)$

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

In state $u_n(x)$

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

$$\updownarrow$$

$$\langle E \rangle = E_n \int_{-\infty}^{\infty} u_n^*(x) u_n(x)\, dx$$

$$= E_n$$

$$\langle H^2 \rangle = \int u_n^*(x)\, \hat{H}^2\, u_n(x)\, dx$$

$$\langle E^2 \rangle = \int u_n^*(x)\, \hat{H}\, \hat{H}\, u_n(x)\, dx$$

$$= \int u_n^*(x)\, E_n\, \hat{H}\, u_n(x)\, dx$$

$$= E_n^2$$

$$(\Delta E)^2 = \langle E^2 \rangle - \langle E \rangle^2 = E_n^2 - E_n^2 = 0$$

If we measure the energy of $u_n(x)$, we will definitely get E_n!

$\downarrow$

compare with (A)

For any Hermitian operator $\hat{A}$

$$\hat{A}\, u_\alpha = \alpha\, u_\alpha$$

A measurement $\leftrightarrow$ $\hat{A}$

$\Rightarrow$ definite value of α

Energy is such an example.

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

$\hat{H}\, u_m(x) = E_m\, u_n(x)$

u_n, u_m are independent functions

but with the same energy, i.e., E_n. E_m

then u_n, u_m are said to be degenerate

Number of states (independent) with the same energy are said to be degree of degeneracy.

Comment

Normalization

$$\psi(x,t) = \sum_n c_n u_n(x) e^{iE_n t/\hbar} \qquad \{u_n(x) ; E_n\}$$

orthonormal set

$$\int \psi^*(x,t)\,\psi(x,t)\,dx$$

$$= \int \sum_m c_m^* \; u_m(x) e^{-iE_m t/\hbar} \sum_n c_n u_n(x) e^{iE_m t/\hbar} dx$$

$$= \sum_m \sum_n c_m^* c_n e^{-iE_m t/\hbar} e^{iE_n t/\hbar} \underbrace{\int_{-\infty}^{\infty} u_m(x) u_n(x)\, dx}_{\delta_{mn}}$$

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

$$= 1$$

Collape of the wave function

$\psi(x,t)$

measure E

$|c_n|^2$ = probability of finding it with energy E_n

right afterwards

[illegible]

: $u_n(x)$

Lecture 2

Simultaneous eigenfunction of $\hat{A}$, $\hat{B}$

Momentum Space Wave Function.

δ - function

Further Comments

The eigenfunction u_a corresponding to the eigenvalue a of the operator A

$$A u_a(x) = a u_a(x)$$

will be simultaneous eigenfunctions of another B when

$$B u_a(x) = b u_b(x)$$

$$\Rightarrow \quad AB u_a(x) = Ab u_a(x) = bA u_a(x) = ab u_a(x)$$

$$BA u_a(x) = Ba u_a(x) = aB u_a(x) = ab u_a(x)$$

$$\Rightarrow \quad (AB - BA)\, u_a(x) = 0$$

$$\psi(x) = \sum_a C_a u_a(x)$$

$$(AB - BA)\,\psi(x) = (AB - BA) \sum_a C_a u_a(x)$$

$$= \sum_a C_a (AB - BA)\, u_a(x) = 0$$

valid for any $\psi(x)$ $\Rightarrow$ $AB - BA = 0$
$\Rightarrow$ A, B commute

Conversely if A, B are two Hermitian operators

$$[A, B] = 0$$

$$A \underline{B u_a(x)} = Ba u_a(x) = a \underline{B u_a(x)}$$

$B u_a(x)$ is also an eigenfunction of A corresponding to eigenfunction of A corresponding to the eigenvalue a.

If there is only eigenfunction of A corresponding to eigenvalue a, then $B u_n(x)$ must be proportional to $u_a(x)$

$$\Rightarrow \quad B u_a(x) = b u_a(x)$$

$\Rightarrow$ $u_a(x)$ is a simultaneous eigenfunction of A and B

If there is only eigenfunction of A with eigenvalue a, then the eigenfunctions of A are not degenerate. (definition)

If there are two eigenfunctions of A corresponding to the eigenvalue a, i.e., we have two-fold degeneracy

$$A u_n^{(1)}(x) = a u_n^{(1)}(x)$$
$$A u_n^{(2)}(x) = a u_n^{(2)}(x)$$

$\Rightarrow$ $B u_a^{(1)}(x)$ and $B u_n^{(2)}(x)$ must be linear combination of $u_a^{(1)}(x)$ and $u_a^{(2)}(x)$

$$B u_a^{(1)}(x) = b_{11} u_a^{(1)}(x) + b_{12} u_a^{(2)}(x)$$

$$B u_a^{(2)}(x) = b_{21} u_a^{(1)}(x) + b_{22} u_a^{(2)}(x)$$

$$B(\underline{u_a^{(1)}(x) + \lambda u_a^{(2)}}) = (b_{11} + \lambda b_{21}) u_a^{(1)} + (b_{12} + \lambda b_{22}) u_a^{(2)}$$

Choose $\lambda = \dfrac{b_{12} + \lambda b_{22}}{b_{11} + \lambda b_{21}}$ (A)

$$= (b_{11} + \lambda b_{21}) \Big[\underbrace{u_a^{(1)} + \frac{b_{12} + \lambda b_{22}}{b_{11} + \lambda b_{12}} u_a^{(2)}}_{\underline{u_a^{(1)} + \lambda u_a^{(2)}}} \Big]$$

Find λ by solving equation (A) $\Rightarrow$ two λ's

λ_1 $\quad u_a^{(1)} + \lambda_1 u_a^{(2)}$
$\downarrow$
eigenfunction of B
with eigenvalue $b_{11} + \lambda_1 b_{21}$
it is also an eigenfunction of
A with eigenvalue a

λ_2 $\quad u_a^{(1)} + \lambda_2 u_a^{(2)}$
eigenfunction of B
with eigenvalue $b_{11} + \lambda_2 b_{21}$
it is also eigenfunction of
A with eigenvalue a.

Thus we have found simultaneous eigenfunctions of A, B.

The procedure can be extended to higher degeneracy.

For a set of mutually commuting operators $A, B, C, \cdots M$ we can find a set of functions which are simultaneous eigenfunctions of $A, B, C, \cdots M$

These set of common eigenfunctions is called a complete set of commuting observable.

Take the case of $H = \frac{p^2}{2m}$ in one dimension

It can be readily show that $[H, P] = 0$

$\Rightarrow$ one can find simultaneous eigenfunctions of H, P

Eigenvalue problem for momentum operator

$$-i\hbar \frac{d}{dx} \quad u_p(x) = p\, u_p(x)$$

$$\Rightarrow \quad \underset{\substack{\downarrow \\ \text{eigenfunction}}}{u_p(x)} = A e^{ipx/\hbar}$$

It is a plane wave solution

$$\underbrace{\int_{-\infty}^{\infty} u_p^*(x)\, u_p(x)\, dx}_{\text{it cannot be normalized.}} = |A|^2 \int_{-\infty}^{\infty} dx$$

Solution exists for all real p

$\downarrow$

continuous spectrum

Localized particle $\rightarrow$ wave packet.

$$\psi_n(x,t) = u_n(x)\, e^{-iE_n t}$$

$$\psi(x,t) = \sum_n c_n u_n(x)\, e^{-iE_n t}$$

$$\rightarrow \int A(p)\, e^{i(px - Et)/\hbar}\, dp$$

$\downarrow$

this is equation (7.12) of the textbook

Look at the situation at $t = 0$

$$\psi(x) = \int A(p)\, e^{ipx/\hbar}\, dp$$

Next we want to find the meaning of $A(p)$

$$\int e^{-ip'x/\hbar}\, \psi(x)\, dx = \iint A(p)\, e^{ipx/\hbar}\, e^{-ip'x/\hbar}\, dx\, dp$$

$$\int e^{ipx/\hbar}\, e^{-ip'x/\hbar}\, dx = 2\pi\hbar\,\delta(p-p')$$

See notes on Dirac δ-function

$$\int_{-\infty}^{\infty} e^{i(p-p')y}\, dy = \delta(p-p')$$

$$\int e^{-ip'x/\hbar}\,\psi(x)\,dx = \int A(p)\, 2\pi\hbar\,\delta(p-p')\, dp = 2\pi\hbar A(p')$$

$$\langle p \rangle = \int dx\, \psi^*(x)\, \frac{\hbar}{i}\frac{\partial \psi(x)}{\partial x}$$

$$= \int dx\, \psi^*(x)\, \frac{\hbar}{i}\frac{\partial}{\partial x}\int A(p)\, e^{ipx/\hbar}\, dp$$

$$= \int dp\, A(p)\, p \int dx\, \psi^*(x)\, e^{ipx/\hbar}$$

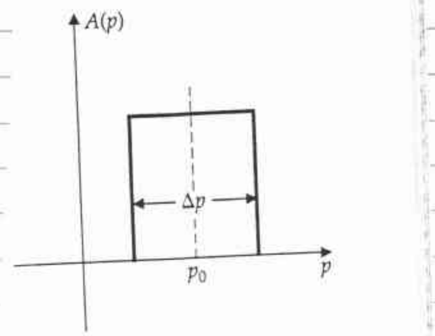
$$= 2\pi\hbar \int dp\, A(p)\, p\, A^*(p)$$

$\Rightarrow$ $2\pi\hbar\, |A(p)|^2 dp$ = probability that the momentum will be found between p and $p+dp$

(7-15) of the textbook.

Example

$$A(p) = \begin{cases} 0 & \text{for} \quad p < p_0 - \Delta p/2 \\ C & \text{for} \quad p_0 - \frac{\Delta p}{2} < p < p_0 + \frac{\Delta p}{2} \\ 0 & \text{for} \quad p > p_0 + \Delta p/2 \end{cases}$$



The weight function $A(p)$ for Eq. (7–16).

$$\psi(x) = \int_{-\infty}^{\infty} A(p)\, e^{ipx/\hbar}\, dp = C \int_{p_0-\Delta p/2}^{p_0+\Delta p/2} e^{ipx}\, dx$$

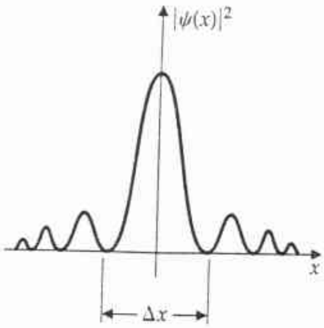
$$q = p - p_0$$

$$= C\, e^{ip_0/\hbar} \int_{-\Delta p/2}^{\Delta p/2} e^{iqx/\hbar}$$

$$= c\, e^{ip_0x/\hbar}\, \frac{\hbar}{ix} \left[e^{x\Delta p/2\hbar} - e^{-ix\Delta p/2\hbar} \right]$$

$$= 2c\, e^{ip_0x}\, \frac{\hbar}{x} \sin\frac{x\Delta p}{2\hbar}$$

$$|\psi(x)|^2 = \frac{4c^2\hbar^2}{x^2} \sin^2\frac{x\Delta p}{2\hbar}$$



The probability density $|\psi(x)|^2$ obtained in Eq. (7–18) that results from the superposition of plane waves with the weight function $A(p)$ of Eq. (7–16). Our choice of "width"—the distance between the first two minima of the distribution—is shown in the figure.

The first minimum occur at $x = \pm x_0$

$$\frac{x_0\Delta p}{2\hbar} = \pi$$

$$x_0 = \frac{2\pi\hbar}{\Delta p}$$

$$\Rightarrow \quad \Delta x = 2x_0 = \frac{4\pi\hbar}{\Delta p} \quad \Rightarrow \quad \Delta p\, \Delta x = 2h$$

From the correspondence

$$p \leftrightarrow E$$
$$x \leftrightarrow t$$

$$\Rightarrow \quad \Delta E\, \Delta t \geq \frac{\hbar}{2}$$

time - energy uncertainty relation

Eigenstate of position operator

$$x\, u_{x_0}(x) = x_0\, u_{x_0}(x)$$

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

$$[L_x, L_y] = i\hbar L_z$$

$$\Downarrow$$

$$\Delta L_x \, \Delta L_y \gtrsim \langle \hbar L_z \rangle$$

If a state is in the eigenstate of $L_x \Rightarrow \Delta L_x = 0$

But for this state, we can prove $\langle L_z \rangle = 0$

The uncertainty relation is still valid.

Dirac

Definition of δ-function

$$\int_{a_0}^{a_1} f(x)\delta(x-a)\mathrm{d}x = \begin{cases} f(a) & \text{if} \quad a \in [a_0, a_1] \subset \mathbb{R}, \\ 0 & \text{if} \quad a \notin [a_0, a_1]. \end{cases}$$

The Dirac delta function is *not* an ordinary well-behaved map $\mathbb{R} \longrightarrow \mathbb{R}$, but a distribution, also known as an *improper* or *generalized function*. Physicists express its special character by stating that the Dirac delta function makes only sense as a factor in an integrand ("under the integral"). Mathematicians say that the delta function is a linear functional on a space of test functions.

Properties

Most commonly one takes the lower and the upper bound in the definition of the delta function equal to $-\infty$ and ∞, respectively. From here on this will be done.

$$\begin{aligned}
\int_{-\infty}^{\infty} \delta(x)\mathrm{d}x &= 1, \\
\frac{1}{2\pi}\int_{-\infty}^{\infty} e^{ikx}\mathrm{d}k &= \delta(x) \\
\delta(x-a) &= \delta(a-x), \\
(x-a)\delta(x-a) &= 0, \\
\delta(ax) &= |a|^{-1}\delta(x) \quad (a \neq 0), \\
f(x)\delta(x-a) &= f(a)\delta(x-a), \\
\int_{-\infty}^{\infty} \delta(x-y)\delta(y-a)\mathrm{d}y &= \delta(x-a)
\end{aligned}$$

The physicist's proof of these properties proceeds by making proper substitutions into the integral and using the ordinary rules of integral calculus. The delta function as a Fourier transform of the unit function $f(x) = 1$ (the second property) will be proved below. The last property is the analogy of the multiplication of two identity matrices,

$$\sum_{j=1}^{n} \delta_{ij}\,\delta_{jk} = \delta_{ik}, \quad i,k = 1,\ldots,n.$$

APPENDIX 8

DIRAC δ-FUNCTIONS

One-Dimensional δ functions. Definition:

$$\int F(x)\,\delta(x - x_0)\,dx = F(x_0) \tag{A8-1}$$

provided the integration includes $x = x_0$.
Properties:

$$\delta(x' - x) = \delta(x - x'), \tag{A8-2}$$

$$x\,\delta x = 0, \tag{A8-3}$$

$$\delta(\alpha x) = \frac{1}{|\alpha|}\,\delta(x), \tag{A8-4}$$

$$f(x)\,\delta x = f(0)\,\delta(x), \tag{A8-5}$$

$$\delta[(x - x_1)(x - x_2)] = \frac{\delta(x - x_1) + \delta(x - x_2)}{|x_1 - x_2|}, \tag{A8-6}$$

$$\delta(x^2 - a^2) = \frac{1}{2a}\,[\delta(x - a) + \delta(x + a)] \qquad (a > 0), \tag{A8-7}$$

$$\delta(x - x_1)\,\delta(x - x_2) = \delta(x - x_1)\,\delta(x_1 - x_2) = \delta(x - x_2)\,\delta(x_1 - x_2), \tag{A8-8}$$

$$\int_{-\infty}^{\infty} \delta(x)\,dx = 1, \tag{A8-9}$$

$$\delta'(-x) = -\delta'(x), \tag{A8-10}$$

$$x\,\delta'(x) = -\delta(x), \tag{A8-11}$$

$$x^2\,\delta'(x) = 0, \tag{A8-12}$$

$$\int \delta^{(n)}(x) f(x)\,dx = (-1)^n f^{(n)}(0). \tag{A8-13}$$

If $u_n(x)$ form a complete set,

$$\begin{aligned} f(x) &= \sum_n c_n u_n(x) \\ &= \sum_n u_n(x) \int u_n{}^*(x') f(x')\,dx' \\ &= \int \left[\sum_n u_n{}^*(x') u_n(x) \right] f(x')\,dx' \\ &= \int \delta(x' - x) f(x')\,dx'. \end{aligned}$$

We then have the *closure* property

$$\sum_n u_n{}^*(x') u_n(x) = \delta(x' - x). \tag{A8-14}$$

Representations:

$$\delta(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ikx}\,dk \tag{A8-15}$$

$$= \frac{1}{2\pi} \int_{-\infty}^{\infty} \cos(kx)\,dk \tag{A8-16}$$

$$= \lim_{\alpha \to \infty} \frac{\sin(\alpha x)}{\pi x} \tag{A8-17}$$

$$= \lim_{\alpha \to \infty} \frac{1 - \cos(\alpha x)}{\pi \alpha x^2} = \lim_{\alpha \to \infty} \frac{\sin^2 \alpha(x/2)}{2\pi\alpha(x/2)^2} \tag{A8-18}$$

$$= \lim_{\alpha \to 0} \frac{\alpha}{\pi(\alpha^2 + x^2)} \tag{A8-19}$$

$$= \lim_{\alpha \to 0} \frac{e^{-x^2/4k\alpha}}{\sqrt{4\pi k\alpha}} \qquad (k > 0) \tag{A8-20}$$

$$= \lim_{\alpha \to \infty} \frac{\alpha e^{-\alpha^2 x^2}}{\sqrt{\pi}} \tag{A8-21}$$

$$= \lim_{\alpha \to 0} \frac{1}{\pi} \int_0^{\infty} e^{-\alpha t} \cos kx\,dk. \tag{A8-22}$$

Three-dimensional δ functions:

$$\delta(\mathbf{r}) = \delta(x)\,\delta(y)\,\delta(z) \tag{A8-23}$$

$$= \begin{cases} \dfrac{1}{2\pi} \dfrac{\delta(r)}{r^2} & \text{(A8-24)} \\[2ex] -\dfrac{1}{2\pi} \dfrac{\delta'(r)}{r} & \text{(A8-25)} \\[2ex] \dfrac{1}{(2\pi)^3} \displaystyle\int_{-\infty}^{\infty} e^{i\mathbf{k}\cdot\mathbf{r}}\,d^3k, & \text{(A8-26)} \end{cases}$$

$$\delta(\mathbf{r}_1 - \mathbf{r}_2) = \frac{1}{r_1{}^2}\,\delta(r_1 - r_2)\,\delta(\cos\theta_1 - \cos\theta_2)\,\delta(\varphi_1 - \varphi_2), \tag{A8-27}$$

$$\delta(\mathbf{k} - \mathbf{k}') = \frac{1}{(2\pi)^3} \int e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}}\,d\mathbf{r}, \tag{A8-28}$$

$$\int f(\mathbf{r}')\,\delta(\mathbf{r} - \mathbf{r}')\,d\mathbf{r}' = f(\mathbf{r}) \qquad \text{(closure)}, \tag{A8-29}$$

$$\nabla^2(1/r) = -4\pi\,\delta(\mathbf{r}). \tag{A8-30}$$

Chapter 8

Barriers and Wells

The quantum mechanical nature of matter has some surpising consequences

The behaviors seen in realistic experiments and applications can be illustrated in highly simplified systems which contains one - dimensional potentials with sharp edges

General Discussions

Time - dependent Schrodinger equation

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

$V(x)$ is assumed to be real and independent of time.

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

$\psi^* \cdot (A) - \psi \cdot (B)$

$$\Rightarrow \quad i\hbar\left[\psi^* \frac{\partial}{\partial t}\psi + \psi \frac{\partial}{\partial t}\psi^*\right] = -\frac{\hbar^2}{2m}\left[\psi^* \frac{\partial^2 \psi}{\partial x^2} - \psi \frac{\partial^2 \psi^*}{\partial x}\right]$$

$$\frac{\partial}{\partial t}\psi^*\psi = \frac{1}{i\hbar}\left(\frac{\hbar^2}{2m}\frac{\partial^2 \psi^*}{\partial x^2}\psi - \frac{\hbar^2}{2m}\psi^*\frac{\partial^2 \psi}{\partial x^2}\right)$$

$$= -\frac{\partial}{\partial x}\left[\frac{\hbar}{2im}\left(\psi^*\frac{\partial \psi}{\partial x} - \frac{\partial \psi^*}{\partial x}\psi\right)\right]$$

Define the probability flux $S(x,t) = \frac{\hbar}{2im}\left(\psi^*\frac{\partial \psi}{\partial x} - \frac{\partial \psi^*}{\partial x}\psi\right)$

$$\Rightarrow \quad \frac{\partial}{\partial t}P(x,t) + \frac{\partial}{\partial x}S(x,t) = 0$$

[Going to three dimensional case

$$\frac{\partial}{\partial t}P(\vec{r},t) + \nabla \cdot \vec{S}(\vec{r},t) = 0 \qquad (C)$$

$$\vec{S}(\vec{r},t) = \frac{\hbar}{2im}\left[\psi^*(\vec{r},t)\nabla\psi(\vec{r},t) - \nabla\psi^*(\vec{r},t)\psi(\vec{r},t)\right]$$

It is similar to the continuity equation

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \vec{j} = 0 \quad \longleftrightarrow \quad \text{conseration of charge}$$

Equation (C) $\rightarrow$ conservation of probability.]

$$\frac{\partial}{\partial t}\int_a^b dx\, P(x,t) = -\int_a^b dx \frac{\partial}{\partial x} S(x,t)$$

$$= S(a,t) - S(b,t)$$

$\Rightarrow$ $S(x,t) \longrightarrow$ probability flux.
(probability / time cross point x)

Remark. (C) is a consequence of $V(x)$ is real.

When $V(x)$ is independent of time $\rightarrow$ seperation of variable method can be used.

$$\psi(x,t) = \psi_E(x)\, e^{-iEt/\hbar} = \psi_E(x)\, e^{-\omega t}$$

with

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

$\psi_E(x) \equiv \psi(x)$ — time independent Schrodinger equation.

Requirements for acceptible solutions

(i) $\psi(x)$ is square integrable*

(ii) (a) $\psi(x)$ must be finite
(b) $\psi(x)$ must be continuous
(c) $\frac{d\psi(x)}{dx}$ must be finite
(d) $\frac{d\psi(x)}{dx}$ must be continuous

*for unbound motion, we shall discuss this point further

(a), (c) follows from the requirement that $P(x,t)$, $S(x,t)$ are well-defined

(b) follows from requirement (c)

Requirement (d) $\leftrightarrow$ Schrodinger equation

Time-independent Schrodinger equation

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

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

Integrate the above equation from $a-\epsilon$ to $a+\epsilon$

$$\left(\frac{d\psi}{dx}\right)_{a+\epsilon} - \left(\frac{d\psi}{dx}\right)_{a-\epsilon} = \int_{a-\epsilon}^{a+\epsilon}\frac{2m}{\hbar^2}[V(x)-E]\psi(x)dx$$

$\longrightarrow 0$ as $\epsilon \to 0$
if V is finite

分類:
編號: 8-3
總號:

Note: If potential V has an infinite discontinuity, then the right-hand side may or may not vanish

Example $\quad V(x) = V_0\,\delta(x-a)$

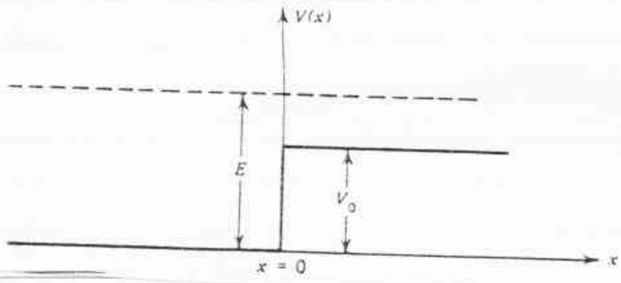
$$\Rightarrow \quad \left(\frac{d\psi}{dx}\right)_{a+\epsilon} - \left(\frac{d\psi}{dx}\right)_{a-\epsilon} = \int_{a-\epsilon}^{a+\epsilon} \frac{2m}{\hbar^2}\left[V_0\,\delta(x-a) - E\right]\psi(x)\,dx$$

$$= \frac{2m}{\hbar^2} V_0\,\psi(a)$$

The Potential Step

$E > V_0 > 0$

$$V(x) = \begin{cases} 0 & \text{for } x<0 \\ V_0 & \text{for } x>0 \end{cases}$$



The Schrodinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi_1 = E\psi_1 \quad \text{in I } (x<0)$$

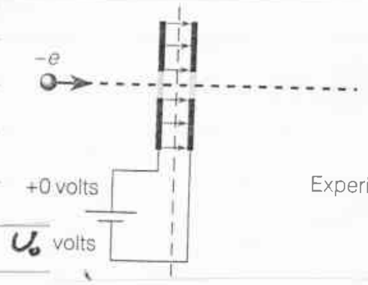
$$\Rightarrow \frac{d^2}{dx^2}\psi_1 = -\frac{2mE}{\hbar^2}\psi_1 = -k_1^2\psi_1$$

$$k_1 = \sqrt{2mE}/\hbar$$

$$\Rightarrow \psi_1(x) = Ae^{ik_1x} + Be^{-ik_1x}$$

$$\psi_1(x,t) = \psi_1 e^{-i\omega t}$$

$$= A\underbrace{e^{ik_1x - i\omega t}}_{\text{incident plane wave}} + B\underbrace{e^{-ik_1x-i\omega t}}_{\text{reflected plane wave}}$$



Experimental setup

$V_0 = eU_0$

Experimental setup

The Schrodinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_2}{dx^2} + V_0\psi_2(x) = E\psi_2(x) \quad \text{in II } (x>0)$$

$$\Rightarrow \frac{d^2}{dx^2}\psi_2 = -\frac{2m}{\hbar^2}(E-V_0)\psi_2 = -k_2^2\psi_2$$

$$k_2 = \frac{\sqrt{2m(E-V_0)}}{\hbar}$$

$$\Rightarrow \psi_2(x) = Ce^{ik_2x} + De^{-ik_2x}$$

$D = 0$ (no new potential to reflect the wave from the right)

$$\psi(x) = \begin{cases} \psi_1(x) = Ae^{ik_1x} + Be^{-ik_1x}, & x<0 \\ \psi_2(x) = Ce^{ik_2x}, & x>0 \end{cases}$$

Continuity equation at $x = 0$

$$\psi_1(x=0) = \psi_2(x=0) \Rightarrow A + B = C$$

$$\left(\frac{d\psi_1}{dx}\right)_{x=0} = \left(\frac{d\psi_2}{dx}\right)_{x=0} \Rightarrow k_1(A-B) = k_2 C$$

$$\Rightarrow \quad B = \frac{k_1 - k_2}{k_1 + k_2} A$$

$$C = \frac{2k_1}{k_1 + k_2} A$$

$$\Rightarrow \quad \psi(x) = \begin{cases} A e^{ik_1 x} + A \dfrac{k_1 - k_2}{k_1 + k_2} e^{-ik_1 x} & x < 0 \\ A \dfrac{2k_1}{k_1 + k_2} e^{ik_2 x} & x \geq 0 \end{cases}$$

$$\psi(x,t) = \psi(x) e^{-i\omega t}$$

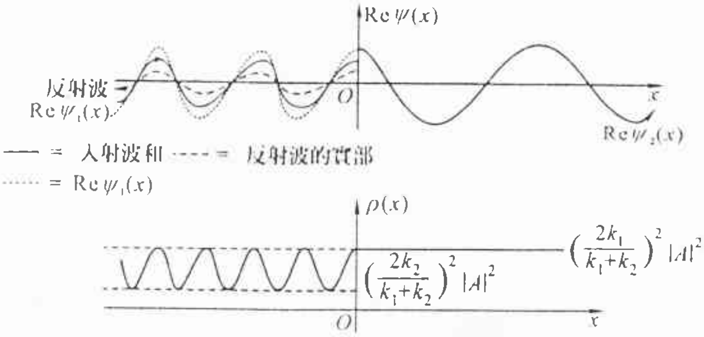
$$\rho(x,t) = \psi^*(x,t)\,\psi(x,t)$$

$$= \begin{cases} \dfrac{4}{(k_1+k_2)^2} |A|^2 (k_1 \cos k_1 x - i k_2 \sin k_1 x)(k_1 \cos k_1 x + i k_2 \sin k_1 x) & [x \leq 0] \\ \dfrac{2k_1}{(k_1+k_2)^2} |A|^2 & x \geq 0 \end{cases}$$

$\rho(x,t)$ is positive definite and independent of time.

$$\rho_I(x) = \frac{4|A|^2}{(k_1+k_2)^2}(k_1^2 \cos^2 k_1 x + k_2^2 \sin^2 k_1 x)$$

$$\rho_{II}(x) = \frac{4k_1^2}{(k_1+k_2)^2} |A|^2$$



$$\rho(x<0) = \frac{4|A|^2}{(k_1+k_2)^2}(k_1^2 \cos^2 k_1 x + k_2^2 \sin^2 k_1 x) \qquad \rho(x \geqslant 0) = \frac{4k_1^2}{(k_1+k_2)^2}|A|^2$$

$\psi(x)$= 能量本徵函數，$\rho(x)$= 機率密度

Reflection Coefficient and Transmission Coefficient

$$R = \frac{\text{reflected probability flux}}{\text{incident probability flux}}$$

$\downarrow$
reflection coefficient

$$= \frac{\left(\frac{k_1-k_2}{k_1+k_2}\right)^2 |A|^2 \frac{\hbar}{2im}\left(e^{ik_1x}\frac{d}{dx}e^{-ik_1x} - e^{-ik_1x}\frac{d}{dx}e^{ik_1x}\right)}{|A|^2 \frac{\hbar}{2im}\left(e^{-ik_1x}\frac{d}{dx}e^{ik_1x} - e^{ik_1x}\frac{d}{dx}e^{-ik_1x}\right)}$$

$$= \left(\frac{k_1-k_2}{k_1+k_2}\right)^2 = \left\{\frac{1-\sqrt{1-\frac{V_0}{E}}}{1+\sqrt{1-\frac{V_0}{E}}}\right\}^2$$

$$T = \frac{\text{transmitted probability flux}}{\text{incident probability flux}}$$

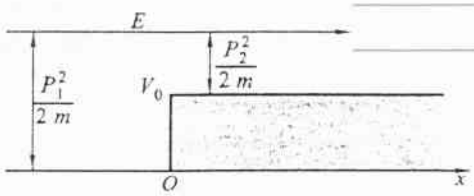
$$= \frac{\left(\frac{2k_1}{k_1+k_2}\right)^2 |A|^2 \frac{\hbar}{2im}\left(e^{-ik_2x}\frac{d}{dx}e^{ik_2x} - e^{ik_2x}\frac{d}{dx}e^{-ik_2x}\right)}{|A|^2 \frac{\hbar}{2im}\left(e^{-ik_1x}\frac{d}{dx}e^{ik_1x} - e^{ik_1x}\frac{d}{dx}e^{-ik_1x}\right)}$$

$$= \frac{4k_1k_2}{(k_1+k_2)^2}$$

Remarks

- For classical mechanics, when $E > V_0$, the particle only change its momentum at $x=0$

  $R \neq 0$, the presence of reflected wave, is due to the wave property of particle
  $\downarrow$
  quantum effect.



- Probability density $\rho(x)$ is real, positive-definite.
  $\rho(x)\,dx \sim$ probability of finding the particle in the interval dx

- $\rho(x,t)$ is independent of time
  Probability conservation

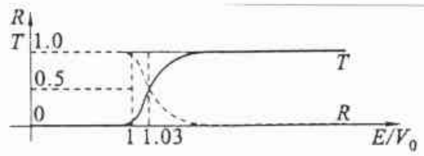
$$\frac{\partial S}{\partial x} + \frac{\partial \rho}{\partial t} = 0$$

$\Rightarrow$ $S(x)$ is a constant

Furthermore, $R + T = 0$

$\downarrow$

can be seen from the following figure
(R, T are plotted as a function of $\frac{V_0}{E}$)



$E < V_0$

In region (I)

$$\psi_1(x) = A e^{ik_1x} + B e^{-ik_1x}$$

$$k_1 = \frac{\sqrt{2mE}}{\hbar}$$

In region (II)

Schrodinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi_2 + V_0\psi_2 = E\psi_2$$

$$\Rightarrow \frac{d^2}{dx^2}\psi_2 = \frac{2m(V_0-E)}{\hbar^2}\psi_2 = k_2^2\psi_2$$

$$k_2 = \frac{\sqrt{2m(V_0-E)}}{\hbar}$$

$$\Rightarrow \psi_2(x) = Ce^{k_2x} + De^{-k_2x}$$

cannot increase exponentially as $x \to \infty$

$\Rightarrow C = 0$

$$\Rightarrow \psi_2(x) = De^{-k_2x}$$

Continuity equation at $x = 0$

$$\psi_1(x=0) = \psi_2(x=0) \qquad \Rightarrow \quad A + B = D$$

$$\left(\frac{d\psi_1}{dx}\right)_{x=0} = \left(\frac{d\psi_2}{dx}\right)_{x=0} \qquad \Rightarrow \quad ik_1(A-B) = -k_2 D$$

$$\Rightarrow A = \frac{D}{2}\left(1 + \frac{ik_2}{k_1}\right)$$

$$B = \frac{D}{2}\left(1 - \frac{ik_2}{k_1}\right)$$

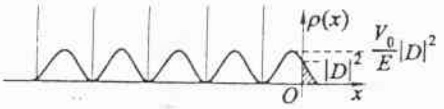
$$\Rightarrow \psi(x,t) = \psi(x)e^{-i\omega t}$$

$$= \begin{cases} \left(D\cos k_1x - D\frac{k_2}{k_1}\sin\frac{k_2}{k_1}\sin k_1x\right)e^{-i\omega t} & x<0 \\ De^{-k_2x}e^{-i\omega t} & x>0 \end{cases}$$

$$\rho(x,t) = \begin{cases} |D|^2\left(\cos k_1x - \frac{k_2}{k}\sin k_1x\right)^2 & x<0 \\ |D|^2 e^{-2k_2x} & x>0 \end{cases}$$

$\rho(x,t)$ is independent of time, positive-definite

The $\rho(x)$ can be plotted



Penetrating depth.

$$\rho(x>0) = |D|^2 e^{-2k_2 x}$$

The particle can penerate into $x>0$ region (classically forbidden region)

The penetrating depth

$$\Delta x = \frac{1}{2k_2} \sim \frac{1}{k_2} = \frac{\hbar}{\sqrt{2m(V_0-E)}}$$

$$\Delta p \sim \frac{\hbar}{\Delta x} = \sqrt{2m(V_0-E)}$$

$$\Rightarrow \quad \Delta E \sim \frac{(\Delta p)^2}{2m} = V_0 - E$$

↳ the energy deficit

Reflection coefficient

$$R = \frac{\text{reflected probability flux}}{\text{incident probability flux}}$$

$$= \frac{\frac{1}{4}|D|^2\left(1+\frac{ik_2}{k_1}\right)\left(1-\frac{ik_2}{k_1}\right)}{\frac{1}{4}|D|^2\left(1-\frac{ik_2}{k_1}\right)\left(1+\frac{ik_2}{k_1}\right)} = 1$$

Transmission coefficient

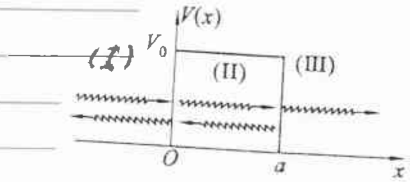
$$T = \frac{\text{transmitted probability flux}}{\text{incident probability flux}}$$

$$\text{Transmitted probability flux} = \underbrace{\frac{\hbar}{2im}|D|^2\left(e^{-k_2 x}\frac{d}{dx}e^{-k_2 x} - e^{-k_2 x}\frac{d}{dx}e^{-k_2 x}\right)}_{=0}$$

$$\Rightarrow \quad T = 0 \qquad \Rightarrow \quad T + R = 1$$

Furthermore $\quad S = 0$ for all x

The Potential Barrier



$$V(x) = \begin{cases} V_0 & 0 \le x \le a \\ 0 & x < 0 \ , \ x > a \end{cases}$$

$E < V_0$

Region I

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_1}{dx^2} = E\psi_1$$

$$\psi_1(x) = Ae^{ik_1x} + Be^{-ik_1x}$$

$$k_1 = \frac{\sqrt{2mE}}{\hbar}$$

Region II

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_2}{dx^2} + V_0\psi_2 = E\psi_2$$

$$\psi_2(x) = Fe^{-k_2x} + Ge^{k_2x}$$

$$k_2 = \frac{\sqrt{2m(V_0-E)}}{\hbar}$$

Region III

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_3}{dx^2} = E\psi_3$$

$$\psi_3(x) = Ce^{ik_3x} + De^{-ik_3x}$$

$$k_3 = \frac{\sqrt{2mE}}{\hbar} = k_1$$

Tunneling problem
↓
Incident wave is partially reflected and partially transmitted.

[Note, only the origin is shifted between the two figures]

In classical mechanics, the particle cannot be transmitted.

A particle may transmit through a potential barrier is due to the wave property of particle
↓
quantum effect

[Furthermore, a "whole" particle (electron) is transmitted with probability, related to T

This quantum effect is known as tunneling phenomena.

Matching the boundary condition at $x=0$ and $x=a$.

$\psi_1(x=0) = \psi_2(x=0)$ $\qquad A+B=F+G$

$\left.\frac{d\psi_1}{dx}\right|_{x=0} = \left(\frac{d\psi_2}{dx}\right)_{x=0}$ $\qquad ik_1(A-B) = k_2(G-F)$

$\psi_2(x=a) = \psi_3(x=a)$ $\qquad Ge^{k_2 a} + Fe^{-k_2 a} = Ce^{ik_1 a}$

$\left(\frac{d\psi_2}{dx}\right)_{x=a} = \left(\frac{d\psi_3}{dx}\right)_{x=a}$ $\qquad k_2(Ge^{k_2 a} - Fe^{-k_2 a}) = ik_1 C e^{ik_1 a}$

There are 5 unknowns (A, B, G, F, C) and 4 equations

$\Rightarrow$ A, B, G, F can be solved in terms of C.

$$A = C\left\{\cosh(k_2 a) + i\frac{k_2^2 - k_1^2}{2k_1k_2}\sinh(k_2 a)\right\}e^{ik_1 a}$$

$$B = -i\left(C\frac{k_1^2+k_2^2}{2k_1k_2}\sinh k_2 a\right)e^{ik_1 a}$$

$$F = \frac{C}{2}\left(1 - i\frac{k_1}{k_2}\right)e^{(k_2+k_1)a}$$

$$G = \frac{C}{2}\left(1 + i\frac{k_1}{k_2}\right)e^{(-k_2+ik_1)a}$$

$\psi(x,t)$ is given (up to a constant C)

$$\psi_1(x,t) = \psi_1(x)e^{-i\omega t} = iC\frac{k_1^2+k_2^2}{2k_1k_2}\sinh(k_2 a)\left(e^{i(k_1x+\omega t)} + e^{i(k_1x-\omega t)}\right)e^{ik_1 a} + C\left(\cosh k_2 a + i\frac{k_2}{k_1}\sinh(k_2 a)\right)e^{ik_1 a}\, e^{i(k_1x-\omega t)}$$

$$\psi_2(x,t) = \psi_2(x)e^{-i\omega t}$$
$$= C\left\{\cosh[k_2(x-a)] + i\frac{k_1}{k_2}\sinh[k_2(x-a)]\right\}e^{i(k_1 a-\omega t)}$$

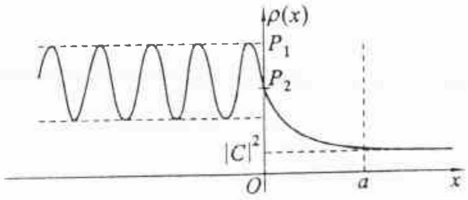
$$\psi_3(x,t) = \psi_3(x)e^{-i\omega t} = Ce^{i(k_1x-\omega t)}$$

Using $\rho(x,t) = \psi^*(x,t)\,\psi(x,t)$, $\rho(x,t)$ can be calculated.

$\downarrow$

$\rho(x,t)$ is positive definite and independent of time

$\rho(x,t) = \rho(x)$



The most interesting quantity for tunneling problem is the transmission coefficent T

$$T = \frac{\text{transmitted probability flux}}{\text{incident probability flux}}$$

$$= \frac{\left|\frac{\hbar}{2im}\left\{e^{-ik_1x}\frac{d}{dx}e^{ik_1x} - e^{ik_1x}\frac{d}{dx}e^{-ik_1x}\right\}\right||C|^2}{\left|\frac{\hbar}{2im}\left\{e^{-ik_1x}\frac{d}{dx}e^{ik_1x} - e^{ik_1x}\frac{d}{dx}e^{-ik_1x}\right\}\right||A|^2}$$

$$= \frac{\frac{\hbar k_1}{m}|C|^2}{\frac{\hbar k_1}{m}|A|^2} = \frac{|C|^2}{|A|^2}$$

$$\Rightarrow \quad T = \left[\cosh^2(k_2 a) + \frac{1}{4}\left(\frac{k_2^2 - k_1^2}{k_1 k_2}\right)^2 \sinh^2(k_2 a)\right]^{-1}$$

$$= \left[1 + (\sinh^2(k_2 a))\left(1 + \frac{1}{4}\frac{(k_2^2-k_1^2)^2}{k_1^2 k_2^2}\right)\right]^{-1}$$

$$= \left[1 + \frac{\sinh^2 k_2 a}{4\frac{E}{V_0}(1-\frac{E}{V_0})}\right]^{-1} = \left[1 + \frac{(e^{k_2 a} - e^{-k_2 a})^2}{16\frac{E}{V_0}(1-\frac{E}{V_0})}\right]^{-1}$$

$$= \left[1 + \frac{e^{2k_2 a}(1 - 2e^{-2k_2 a} + e^{-4k_2 a})}{16\frac{E}{V_0}(1-\frac{E}{V_0})}\right]^{-1}$$

T is a function of E, V_0 and a.

This is the fundamental equation for discussing the tunneling problem.

If $k_2 a \gg 1$, then

$$T \sim \left[\frac{e^{2k_2 a}}{16\frac{E}{V_0}(1-\frac{E}{V_0})}\right]^{-1} = 16\frac{E}{V_0}\left(1-\frac{E}{V_0}\right)e^{-2k_2 a}$$

$$= 16\frac{E}{V_0}\left(1-\frac{E}{V_0}\right)e^{-2\sqrt{2m(V_0-E)}\,a/\hbar}$$

Usually, the exponential is the dominating factor.

Potential barrier with $E > V_0$ can be carried out with the same method. (with appropriate changes in region II

$$R = \frac{\sin^2\left[\frac{\sqrt{2m(E-V_0)}}{\hbar}a\right]}{\sin^2\left[\frac{\sqrt{2m(E-V_0)}}{\hbar}a + 4\frac{E}{V_0}\left(\frac{E}{V_0}-1\right)\right.}$$

$$T = \frac{4\frac{E}{V_0}\left(\frac{E}{V_0}-1\right)}{\sin^2\left[\frac{\sqrt{2m(E-V_0)}}{\hbar} + 4\frac{E}{V_0}\left(\frac{E}{V_0}-1\right)\right.}$$

Although the reflection and transmission probabilities are in general non-zero, the numerator of the reflection probability involve a sine. When the sine is zero, there is no reflection

$\downarrow$

resonant transmission.

The condition is

$$\frac{\sqrt{2m(E-V_0)}}{\hbar}a = n\pi \quad \Rightarrow \quad E = V_0 + \frac{n^2\pi^2\hbar^2}{2ma^2}$$

$\hookrightarrow$ integer

分類:	
編號:	8-14
總號:	

Compare with the formula in the textbook (where the detail has not been worked out)

$k_2 a \gg 1$

$$T \cong \left[\frac{1}{4}\left(\frac{k_2^2+k_1^2}{k_1 k_2}\right)^2 \frac{1}{4} e^{2k_2 a}\right]^{-1}$$

$$= \frac{16 k_1^2 k_2^2}{k_1^2+k_2^2} e^{-2k_2 a}$$

[$\cosh k_2 a \sim \sinh k_2 a \sim \frac{1}{2} e^{k_2 a}$ as $ka \gg 1$]

With the identification

	our notation	notation of the textbook
	k_1	k
	k_2	κ
width	a	$2a$
	T	$\lvert T\rvert^2$

$\Rightarrow$ we recover the equation (8-18)

$$T = \frac{16 k^2 \kappa^2}{k^2+\kappa^2} e^{-4\kappa a}.$$

[Our notation follow that of 林清涼 "近代物理" I 第十章]

In general, the barriers that encounter in physical phenomena are not square

$\Rightarrow$ we want to obtain an approximate expression for the transmission coefficient $|T|^2$ through irregular barrier

Proper way: WKB method will not be discussed here
still an approximate method

The most important factor $e^{-4\kappa a} = e^{-2\kappa(2a)}$
width

Other factors are slowly varying compared with this factor

For a square barrier

$$\ln|T|^2 = -2\kappa(2a) + \underbrace{2\ln\frac{2(ka)(\kappa a)}{(ka)^2+(\kappa a)^2}}_{\text{will neglect this term}}$$

Approximate a smooth barrier by a juxaposition of square potential barrier (See the following figure

$$\ln|T|^2 = \sum_{\substack{\text{partial}\\ \text{barrier}}} \ln|T_{\substack{\text{partial}\\ \text{barrier}}}|^2$$

$$\simeq -2\sum \underbrace{\Delta x}_{\substack{\text{width of}\\ \text{the barrier}}} \underbrace{\langle\kappa\rangle}_{\substack{\text{average } \kappa \text{ in}\\ \text{the inverval}}}$$

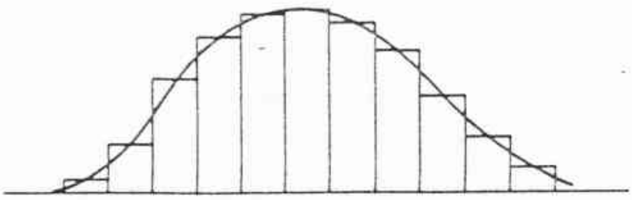
$$\simeq -2\int dx\sqrt{\frac{2m}{\hbar^2}[V(x)-E]}$$

$$\Rightarrow |T|^2 \simeq e^{-2\int dx\sqrt{\frac{2m}{\hbar^2}[V(x)-E]}}$$

The equation requires for each partial barrier $2\Delta x\cdot\kappa \gg 1$

$\Rightarrow$ (i) the above approximation is poor near the turning point (i.e., $V(x)=E \Rightarrow \kappa=0$)

(ii) $V(x)$ must be smooth so that one can approximate a curved barrier by a stack of sufficient large width square barrier

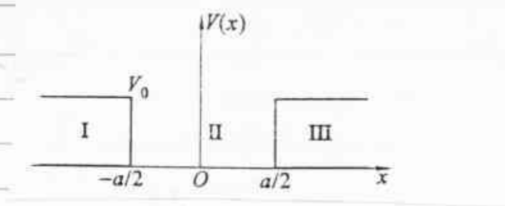


Approximation of smooth barrier by a juxtaposition of square potential barriers.

Potential Well

We have already discussed the problem of infinite potential well.

In this section, we shall discuss the finite potential well problem.



$E < V_0$

Region I

$x < -\frac{a}{2}$

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V_0\right)\psi_1(x) = E\psi_1(x)$$

$$\Rightarrow \psi_1(x) = Ce^{k_1 x} + De^{-k_1 x}$$

$$k_1 = \frac{\sqrt{2m(V_0 - E)}}{\hbar}$$

The wave function is finite at $x = -\infty$

$\Rightarrow D = 0$

Region II

$-\frac{a}{2} < x < \frac{a}{2}$

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi_2(x) = E\psi_2(x)$$

$$\Rightarrow \psi_2(x) = A'e^{ik_2 x} + B'e^{-ik_2 x}$$

$$= A\sin k_2 x + B\cos k_2 x$$

$$k_2 = \frac{\sqrt{2mE}}{\hbar}$$

we use sin and cos because we want to take advantage of the symmetry property

Region III

$\frac{a}{2} < x$

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V_0\right)\psi_3(x) = E\psi_3(x)$$

$$\Rightarrow \psi_3(x) = Fe^{k_1 x} + Ge^{-k_1 x}$$

The wave function must be finite at $x = \infty$

$\Rightarrow F = 0$

$$\psi(x) = \begin{cases} \psi_1(x) = Ce^{k_1 x} & x < -\frac{a}{2} \\ \psi_2(x) = A\sin k_2 x + B\cos k_2 x & -\frac{a}{2} < x < \frac{a}{2} \\ \psi_3(x) = Ge^{-k_1 x} & \frac{a}{2} < x \end{cases}$$

Symmetry of the potential

$$V(x) = V(-x)$$

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

Let $x \rightarrow -x$ (we just rename our variable

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

With $V(x) = V(-x)$, the equation becomes

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

If $\psi(x)$ is eigenfunction of the Schrodinger equation with eigenvalue E, then $\psi(-x)$ is also an eigenfunction of the same Schrodinger equation with the same eigenvalue E.

From superposition principle

$$\psi_{\substack{even \\ odd}}(x) = \frac{1}{\sqrt{2}}\left(\psi(x) \pm \psi(-x)\right)$$

are also eigenfunctions of the Schrodinger equation with eigenvalue E

$$\psi_{even}(x) = \psi_{even}(-x)$$

$$\psi_{odd}(x) = -\psi_{odd}(-x)$$

$\Rightarrow$ With $V(x) = V(-x)$, we can solve the problem by looking for even, odd eigenfunction.

Even solution

$$\psi_1(x) = Ce^{k_1 x} \qquad x < -\frac{a}{2}$$

$$\psi_2(x) = B\cos k_2 x \qquad -\frac{a}{2} < x < \frac{a}{2}$$

$$\psi_3(x) = Ce^{-k_1 x} \qquad x > \frac{a}{2}$$

Matching the boundary condition at $x = -\frac{a}{2}$

$$\psi_1\left(x = -\frac{a}{2}\right) = \psi_2\left(x = -\frac{a}{2}\right)$$

$$B\cos\frac{k_2 a}{2} = Ce^{-k_1\frac{a}{2}}$$

$$\left(\frac{d\psi_1}{dx}\right)_{x=-\frac{a}{2}} = \left(\frac{d\psi_2}{dx}\right)_{x=-\frac{a}{2}}$$

$$-Bk_2\sin\left(k_2\left(\frac{-a}{2}\right)\right) = Ck_1 e^{k_1\left(-\frac{a}{2}\right)}$$

$$\Rightarrow \quad k_2 \tan k_2 a = k_1$$

Compare our notation with that used in the textbook

Our notation	Notation of the textbook
k_2	q
k_1	$\varkappa$

We recover the equation (8-35) of the textbook, i.e.,

$$q \tan qa = \kappa \qquad (A)$$

- With V_0, a given, (A) is an equation for E

$\downarrow$

only certain values of E will satisfy (A)

$\downarrow$

only discrete energies are allowed.

- The boundary conditions at $x = \frac{a}{2}$, can be shown, are satified automatically

- Equation (A) is solved graphically

From Equation (A), we have

$$\sqrt{\frac{2mE}{\hbar}} \tan \sqrt{\frac{mEa^2}{2\hbar^2}} = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$$

Eigenvalue of E can be found by solving above equation.

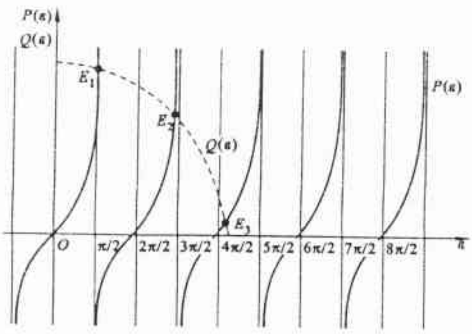
Analytic solutions are difficult to find, we usually solved it using graphic method, i.e., plot LHS, RHS as function of E. The intersection $\Rightarrow$ eigenvalues of E

Define $\epsilon = \sqrt{\frac{mEa^2}{2\hbar^2}}$

Equation (A) becomes $\underbrace{\epsilon \tan\epsilon}_{P(\epsilon)} = \underbrace{\sqrt{\frac{mV_0a^2}{2\hbar^2} - \epsilon^2}}_{Q(\epsilon)}$

$$Q(\epsilon) = \sqrt{\frac{mV_0a^2}{2\hbar^2} - \epsilon^2} \quad \Rightarrow \quad Q^2 + \epsilon^2 = \frac{mV_0a^2}{2\hbar^2}$$

(a circle when Q is plotted against ϵ.)



The energy eigenvalues: $\underset{\overset{\shortparallel}{E_{e0}}}{E_{even,0}}, \underset{\overset{\shortparallel}{E_{e1}}}{E_{even,1}}, \cdots$ can be found.

Odd solution.

$$\psi_1(x) = C e^{k_1 x} \qquad x < -\frac{a}{2}$$

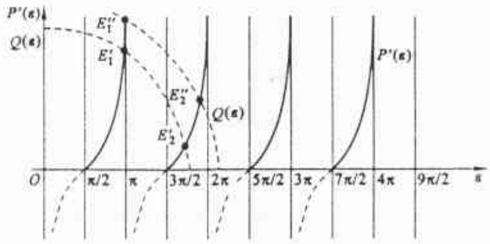
$$\psi_2(x) = A \sin k_2 x \qquad -\frac{a}{2} < x < \frac{a}{2}$$

$$\psi_3(x) = -C e^{-k_1 x} \qquad x > \frac{a}{2}$$

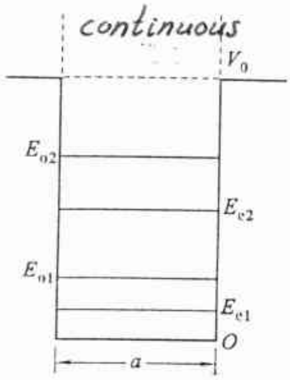
$k_2 \cot \frac{k_2 a}{2} = -k_1$ (from matching the boundary conditions)

$$\Rightarrow \sqrt{\frac{2mE}{\hbar^2}} \cot \sqrt{\frac{mEa^2}{2\hbar^2}} = -\sqrt{\frac{2m(V_0-E)}{\hbar^2}}$$

Again, graphic method can be used to find E_{o1}, E_{o2}, ...



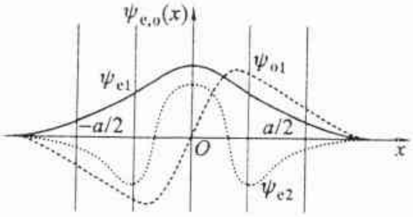
From these calculation, we find the energy spectrum of this finite square well problem.

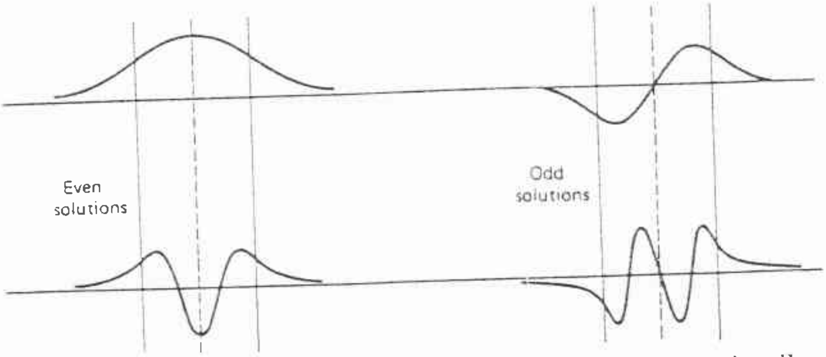


With eigenvalue E given, the wave function is now determined

- k_1, k_2 are known
- the only free parameter is C, can be determined through normalization.

The wave functions (eigenfunctions) corresponding to the first few lowest eigenvalues (energy) E_{e1}, E_{e2}, E_{o1}, E_{o2} are given in the following figure.





Solutions for discrete spectrum in attractive potential well.

The more nodes, the higher are the energies of the bound states.

This can be understood as follows

- $p \propto \frac{d\psi}{dx}$

  $\downarrow$

  roughly speaking, the more a wave function wiggles, the higher is the average value of the slope, and accordingly the higher is the average kinetic energy

- The sign of the slope is not important, since the kinetic energy involves the square of the momentum.

Single and Double δ-Function Potential

Single δ-Function Potential

$V(x) = -V_0\,\delta(x)$ $\qquad V_0 > 0$ → attractive potential

The Schrodinger equation is

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}u(x) - V_0\,\delta(x)\,u(x) = E\,u(x)$$

$$\Rightarrow \frac{d^2}{dx^2}u(x) + \frac{2mE}{\hbar^2}u(x) = -\frac{2mV_0}{\hbar^2}\delta(x) = -\lambda\,\delta(x)$$

$$\lambda \equiv \frac{2mV_0}{\hbar^2}$$

$E<0$ $\qquad \frac{d^2u}{dx^2} - \kappa^2 u(x) = 0$ for $x \neq 0$

$$\kappa^2 = \frac{2m|E|}{\hbar^2}$$

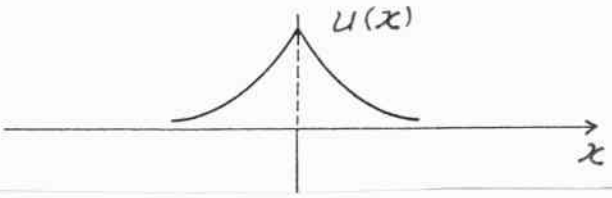
$u(x) = A e^{-\kappa x} + A' e^{\kappa x}$ $\qquad$ for $x>0$

$A' = 0$ required by normalization condition

$u(x) = B e^{\kappa x} + B' e^{-\kappa x}$ $\qquad$ for $x<0$

$B' = 0$ required by normalization condition

The wave function must be continuous at $x=0 \Rightarrow A = B$



The derivative of the wave function has a discontinuity at $x=0$

$$\left(\frac{du}{dx}\right)_{x=0^+} - \left(\frac{du}{dx}\right)_{x=0^-} = -\lambda u(0)$$

$$-\kappa A - \kappa a = -\lambda A$$

$$\Rightarrow \kappa = \frac{\lambda}{2} \Rightarrow \frac{\lambda^2}{4} = \frac{2m|E|}{\hbar^2}$$

$\Rightarrow$ only at $|E| = \dfrac{\hbar^2\lambda^2}{8m}$ there exists solution

Normalization $|A|^2 \left[\int_0^\infty e^{-2\kappa x} dx + \int_{-\infty}^0 e^{2\kappa x} dx \right] = 1$

$\Rightarrow |A|^2 \frac{1}{2\kappa} \cdot 2 = 1 \Rightarrow |A|^2 = \kappa$

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

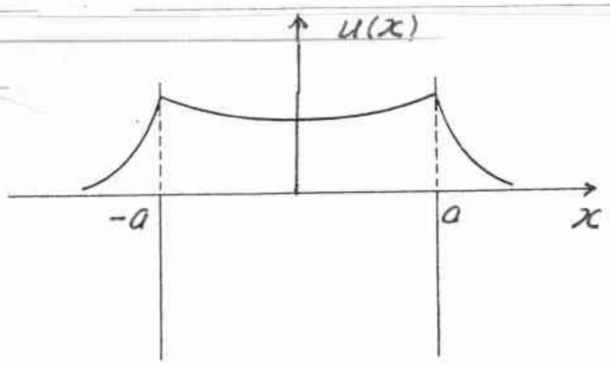
Double δ - Function Potential

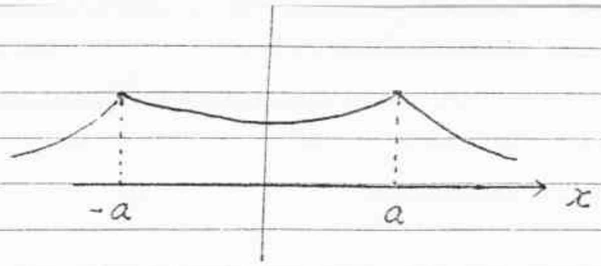
$$V(x) = -V_0\,\delta(x+a) - V_0\,\delta(x-a)$$

$V(-x) = V(x)$, the potential is symmetric under $x \to -x$.
The solution should be either even or odd
We shall discuss the case. $E < 0$

Even solution.
We are looking for the eigenvalue of the problem, we may leave the overall normalization to be open.

$u(x) = e^{-\kappa x}$ for $x > a$ ($e^{\kappa x}$ term is absent due to normalization requirement)
$u(x) = A\cosh \kappa x$ for $a > x > -a$ (originally, it is a linear combination of $e^{\kappa x}$ and $e^{-\kappa x}$, even solution requirement makes it possible to write it as $\cosh \kappa x$)
$u(x) = e^{\kappa x}$ for $x < -a$ (from even solution requirement)





Wave function is continuous at $x=a$

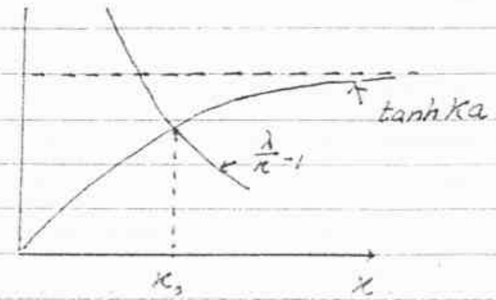
$$e^{-\kappa a} = A\cosh \kappa a$$

Derivative of the wave function has a discontinuity at $x=a$

$$-\kappa e^{-\kappa a} - \kappa A \sinh \kappa a = -\lambda \underbrace{e^{-\kappa a}}_{u(a)} \qquad \lambda = \frac{2mV_0}{\hbar^2}$$

Due to symmetry requirement, the boundary condition at $x=-a$ will give no new result.

$\Rightarrow \quad \tanh \kappa a = \frac{\lambda}{\kappa} - 1$ eigenvalue equation



$\kappa = \sqrt{\frac{2m|E|}{\hbar^2}}$

$\kappa_0 \rightarrow$ eigenvalue of energy

Discussion

$\tanh \kappa a > 0 \qquad \frac{\lambda}{\kappa_0} - 1 > 0 \Rightarrow \lambda > \kappa_0$

$\tanh \kappa a < 1 \qquad \frac{\lambda}{\kappa_0} - 1 < 1 \Rightarrow \frac{\lambda}{2} < \kappa_0$

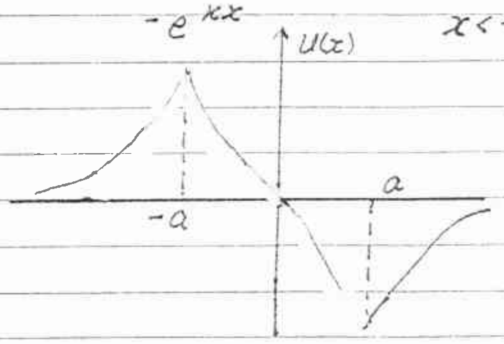
$\Rightarrow \quad \lambda > \kappa_0 > \frac{\lambda}{2} \qquad \kappa = \frac{\lambda}{2}$ for single δ function

Energy of the double well is a larger negative number than that of a single δ function potential with the same strength

In real world, an electron bound to two nuclei seperated by a small distance (similar to a double δ-function potential) will have lower energy than bound to a single nuclei (similar to a single δ-function potential)

Odd solution

$$u(x) = \begin{cases} e^{-\kappa x} & x > a \\ A\sinh\kappa x & a > x > -a \\ -e^{\kappa x} & x < -a \end{cases}$$



Boundary condition at $x = a$

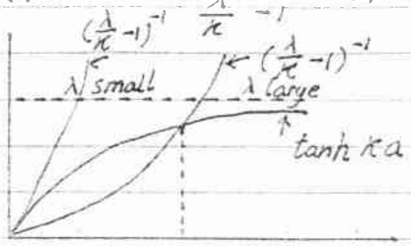
$$A\sinh\kappa a = e^{-\kappa a}$$

$$-\kappa e^{-\kappa a} - \kappa a\cosh\kappa a = -\lambda e^{-\kappa a}$$

$$\Rightarrow \quad \coth\kappa a = \frac{\lambda}{\kappa} - 1 \qquad \Rightarrow \quad \tanh\kappa a = \frac{1}{(\frac{\lambda}{\kappa} - 1)}$$

$$\tanh\kappa a > 0 \quad \Rightarrow \quad \frac{\lambda}{\kappa} - 1 > 0 \quad \Rightarrow \quad \frac{\lambda}{\kappa} > 1 \quad \Rightarrow \quad \lambda > \kappa$$

$$\tanh\kappa a < 1 \quad \Rightarrow \quad \frac{1}{\frac{\lambda}{\kappa} - 1} < 1 \quad \Rightarrow \quad 1 < \frac{\lambda}{\kappa} - 1 \quad \Rightarrow \quad \kappa < \frac{\lambda}{2}$$



⇒ The odd solution, if there is a bound state, is less strongly bound than the even solution.
The wave function, which has to go through zero, is forced to be steep because the wells, and thus can only accommodate to a less rapidly falling exponential.
Depending on the size of λ, there may or may not exist an odd bound state.