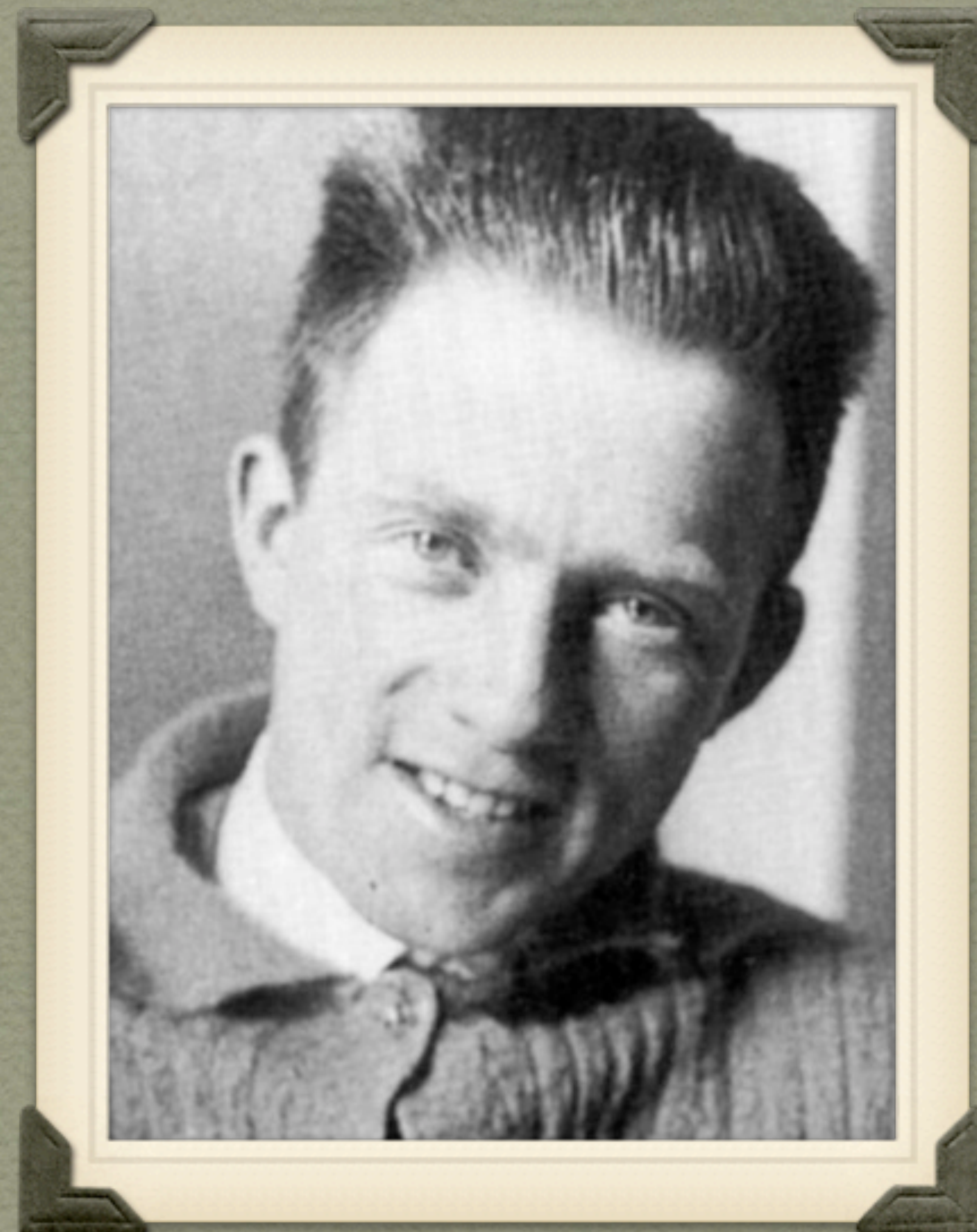
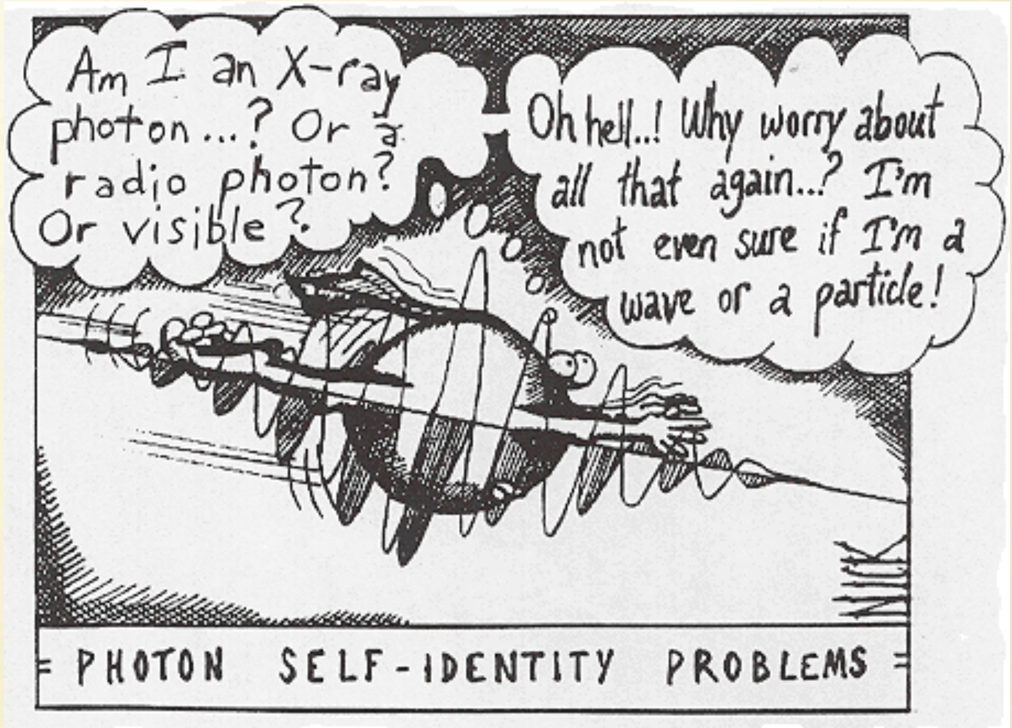
UNCERTAINTY PRINCIPLES

BY W. HEISENBERG



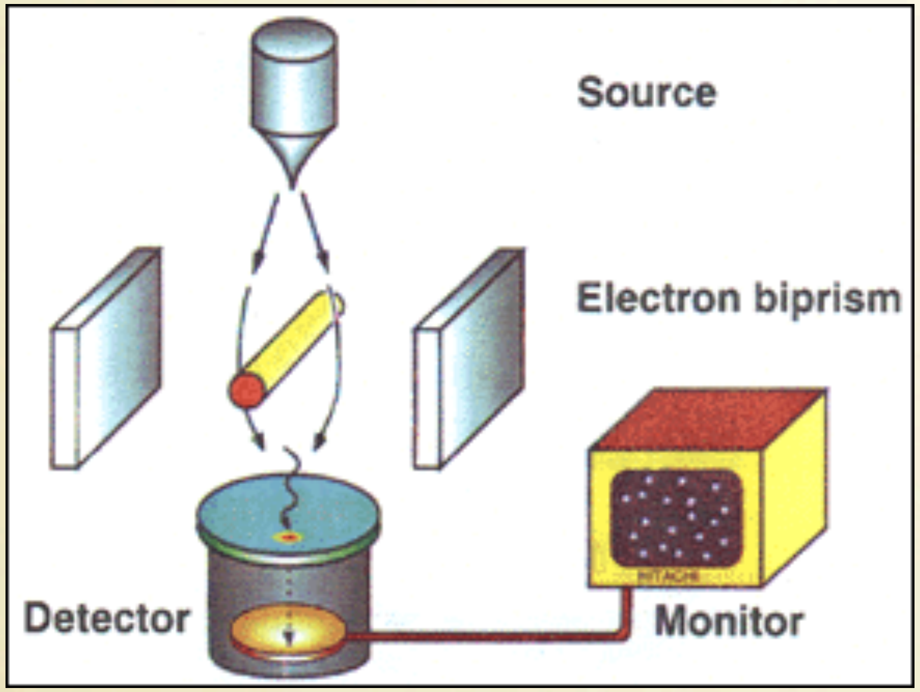
PARTICLE V.S. WAVE

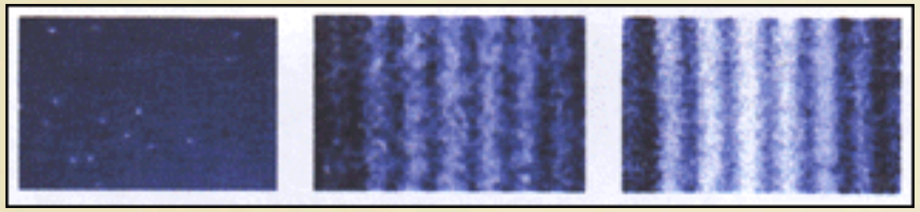
光波在高能量時看起來像粒子



原子在低能量時看起來像波動

SELF INTERFERENCE?

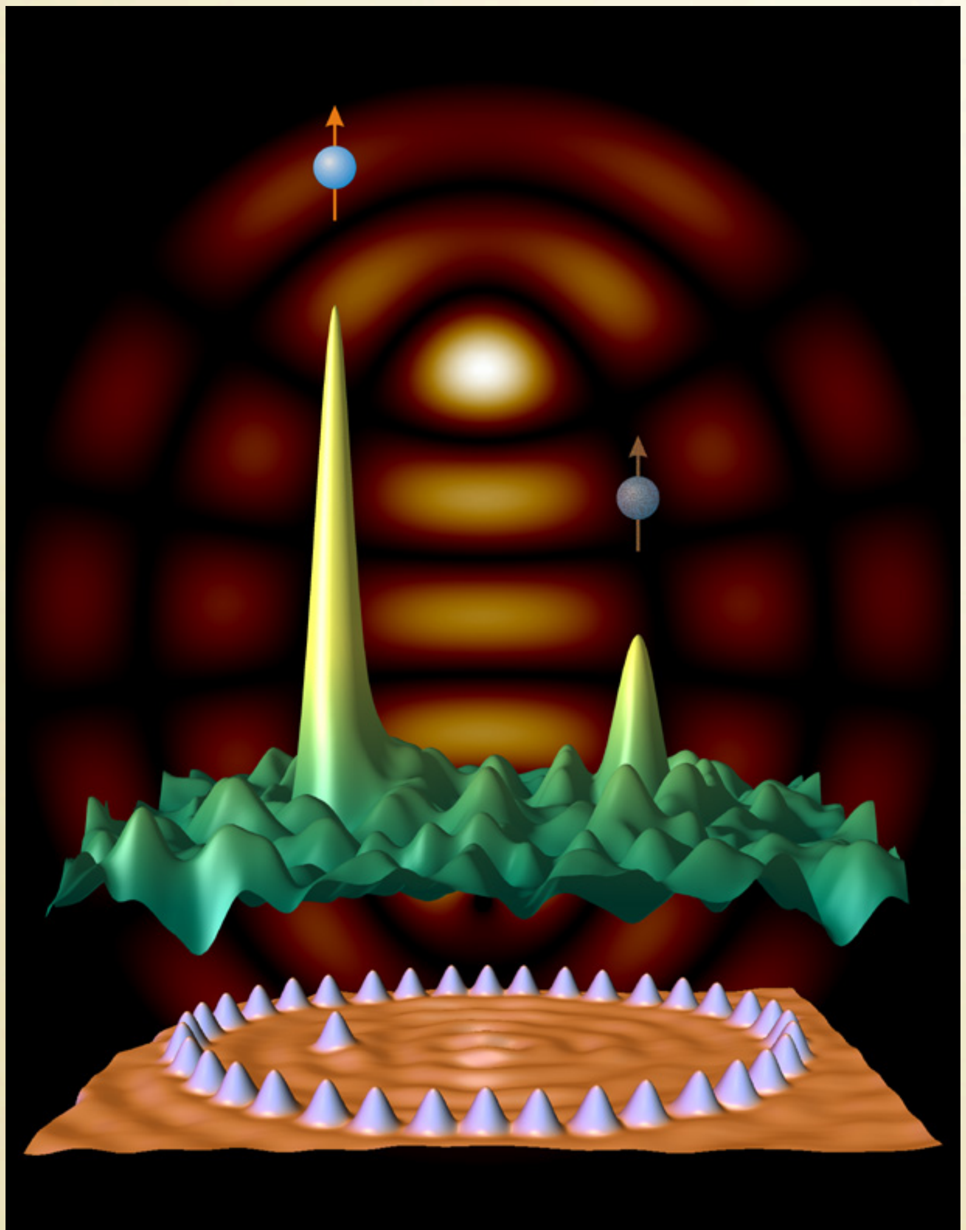




結果電子們也會有干涉條紋！

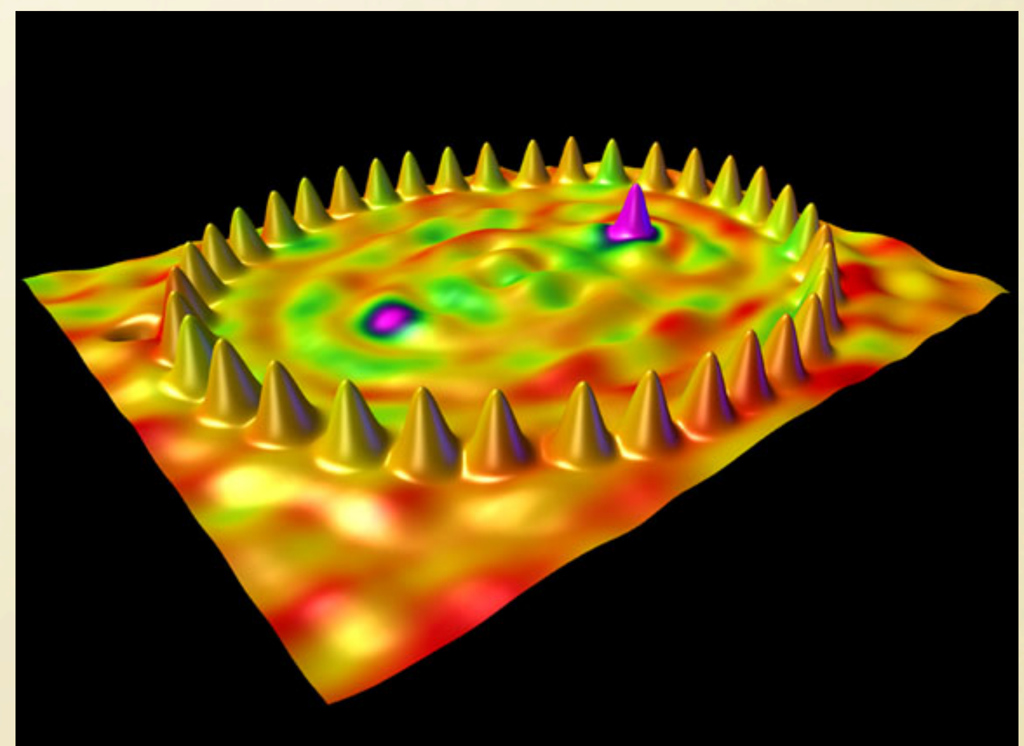
神奇的是…
一隻電子
就可以和自己干涉！

QUANTUM MIRAGE



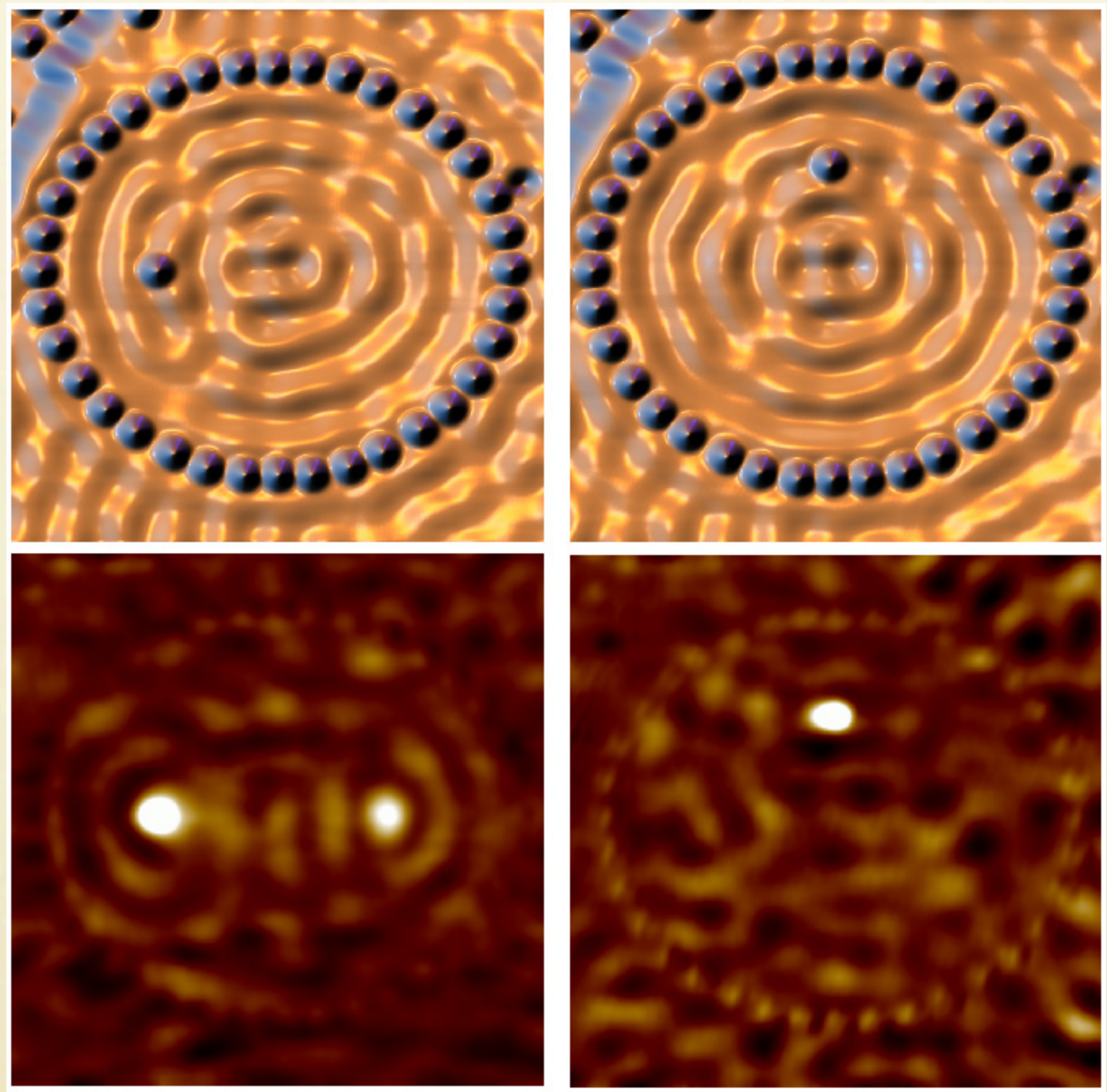
量子力學教會電子如何分身！

在橢圓形的奈米巨蛋球場中，
在焦點上的電子會有分身。



MATTER WAVE!

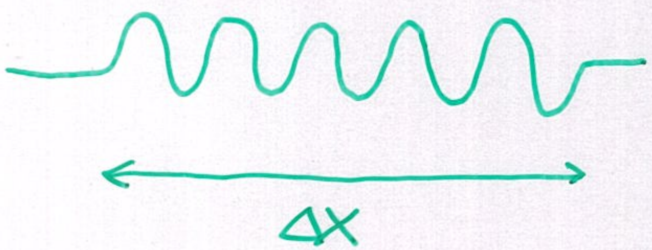
忽焉在前



忽焉在後

Uncertainty Principle.

Consider the following wave packet (e^- can be viewed as wave !!) with finite width Δx.



Count the number of wave front to determine k.

$$k \cdot \Delta x \cong 2\pi\,(N,\ N+1)$$

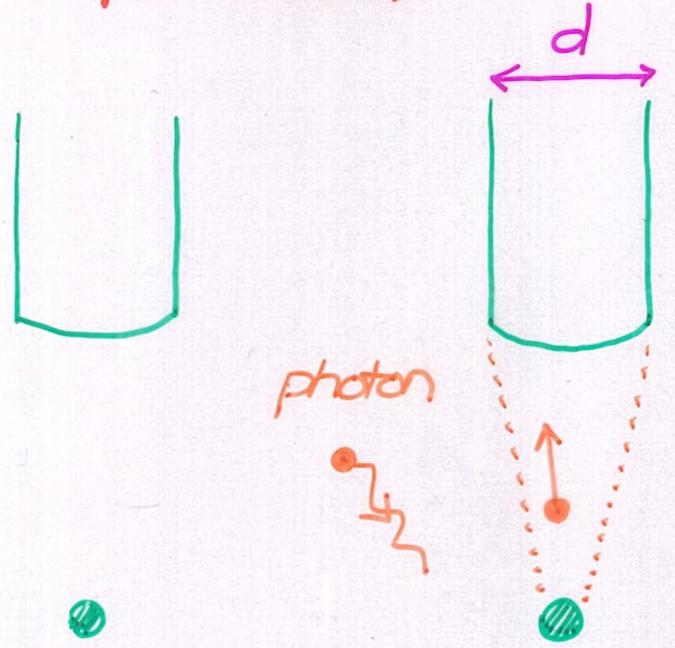
uncertain

The uncertainty in k is $\Rightarrow$ $\Delta k \cong \dfrac{2\pi}{\Delta x}$

Thus, we arrive at the conclusion:

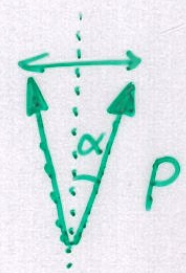
$$\boxed{\Delta x\,\Delta k \cong 2\pi} \xrightarrow{p=\hbar k} \boxed{\Delta x\,\Delta p \cong h}$$

A simple example



$t=0$	$t>0$
know p but not x	$\Delta p \neq 0$ $\Delta x \neq 0$

The momentum uncertainty comes from interaction with photons.



$$\Delta P_e = \Delta P_{photon}$$

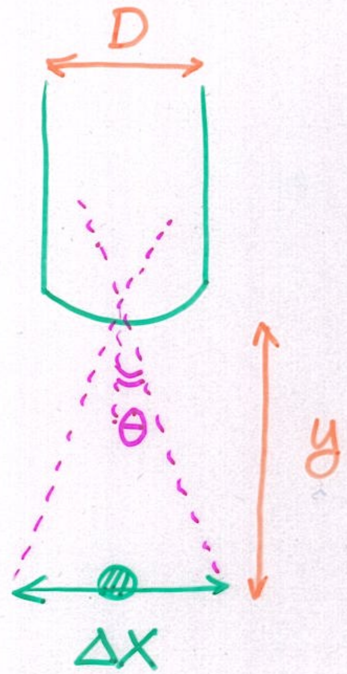
$$\Rightarrow \Delta P_{photon} = P_{photon} \cdot \sin\alpha$$

$$\approx \left(\frac{h}{\lambda}\right)\left(\frac{d}{2y}\right) = \frac{hd}{2\lambda y}$$

Finally,

$$\boxed{\Delta P_e \approx \frac{hd}{2\lambda y}}$$

To reduce error, we want small $\underline{\underline{d}}$ and long $\underline{\underline{\lambda}}$!!



Since the microscope has limited resolution, one can not know the position precisely.

$$\Delta x \approx 2y \sin\theta \approx 2y \cdot \theta$$

Note that the minimum angle $\theta \approx \frac{\lambda}{d}$

$$\boxed{\Delta x \approx \frac{2y\lambda}{d}}$$

Collect results:

$$\Delta p \approx \frac{hd}{2\lambda y}$$

$$\Delta x \approx \frac{2\lambda y}{d}$$

$$\Longrightarrow \quad \Delta x \, \Delta p \approx h \quad !!$$

uncertainty principle ☺

More rigorous results for nuts

Previous arguments are nice. The crucial point for Heisenberg Uncertainty Principle to exist is the <u>wave nature of matters.</u>

$$\Delta P_x \, \Delta x \geq \frac{1}{2}\hbar$$

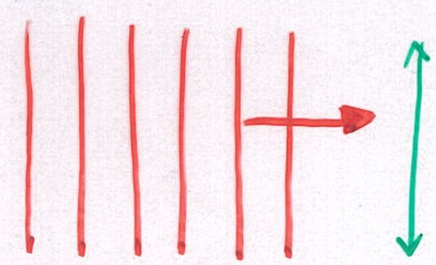
$$\Delta P_y \, \Delta y \geq \frac{1}{2}\hbar$$

$$\Delta P_z \, \Delta z \geq \frac{1}{2}\hbar$$

conjugate variables

☆ Note that only "conjugate variables" have uncertainty relations !!

i.e.



$\Delta y \to 0$ is possible.

definite P_x

$\Delta P_x = 0$

Another point of view: $\quad x P_x - P_x x = i\hbar$

Size of H atom.

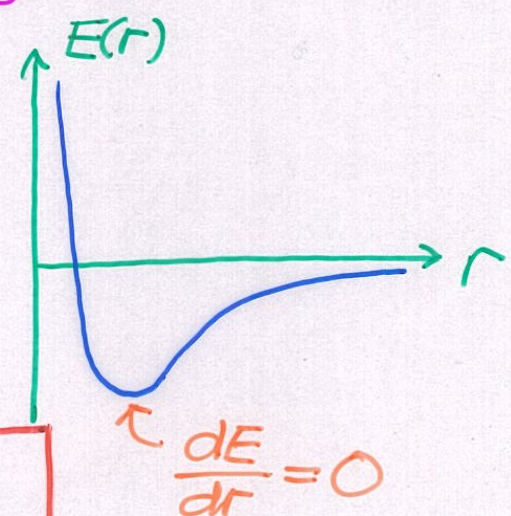
$\Delta x \approx r$

Use uncertainty principle to estimate the size of H atom. Assume $\Delta x \approx r$.

$$\Rightarrow \qquad \Delta p \approx p \approx \frac{\hbar}{r}$$

The total energy of electron is

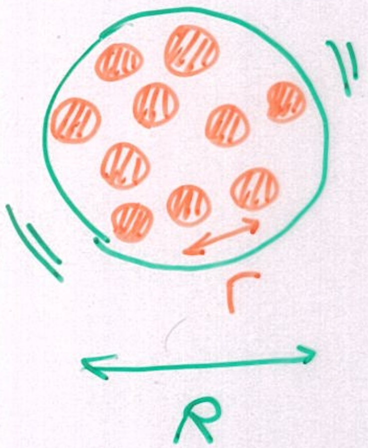
$$E = \frac{p^2}{2m_e} - \frac{Ze^2}{4\pi\epsilon_0 r} \approx \frac{\hbar^2}{2m_e r^2} - \frac{Ze^2}{4\pi\epsilon_0 r}$$



Set $\frac{dE}{dr} = 0$ to determine r.

$$-\frac{\hbar^2}{m_e r^3} + \frac{Ze^2}{4\pi\epsilon_0 r^2} = 0 \quad \Rightarrow \quad \boxed{r = \frac{4\pi\epsilon_0 \hbar^2}{m_e Z e^2}}$$

The mass of star (I)



Consider a star with N particles, each of mass m.

$$E = \sqrt{m^2c^4 + p^2c^2} \approx pc$$ ← relativistic limit.

Making use of uncertainty relation $p \sim \frac{\hbar}{r}$

The kinetic energy K is roughly,

$$K \approx pc \approx \frac{\hbar c}{r}$$

On the other hand, $V \sim -\frac{GMm}{R} = -\frac{GNm^2}{R} \longrightarrow -\frac{GN^{2/3}m^2}{r}$

Note that $\frac{4}{3}\pi R^3 \approx N\,\frac{4}{3}\pi r^3 \longrightarrow R = \sqrt[3]{N}\,r$

The total energy of the star is

$$E = \frac{\hbar c}{r} - \frac{GN^{2/3}m^2}{r}$$

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The mass of star (II)

The total energy is $E = \frac{1}{r}\left(\hbar c - G N^{2/3} m^2\right)$

$$N_c = \left(\frac{\hbar c}{G m^2}\right)^{3/2} \approx 2 \times 10^{57} \sim 1.4\,\odot$$

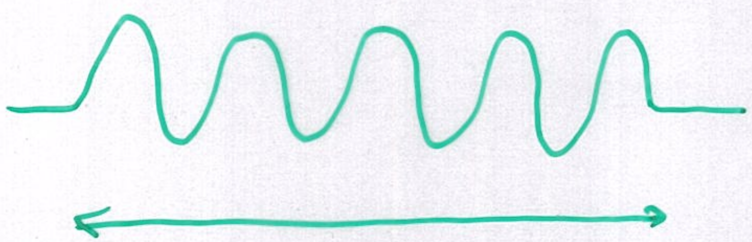
For $N > N_c$, the total energy is always negative $\Rightarrow$ $r \downarrow$ indefinitely..... the so-called gravitational collapse ☹

the quantum uncertainty gives rise to some pressure to resist gravitational contraction !!

Thursday, May 19, 2011

Life time and energy width.

Again, consider a train of signal with duration Δt. Now try to determine the angular frequency ω



$$\omega \Delta t \approx 2\pi \, (N, N+1)$$

Thus, the uncertainty in ω is $\boxed{\Delta\omega = \frac{2\pi}{\Delta t}}$

$$\Delta\omega \, \Delta t \approx 2\pi \quad \Longrightarrow \quad (\hbar \Delta\omega)\, \Delta t \approx \hbar \cdot 2\pi$$

$$\Rightarrow \quad \boxed{\Delta E \, \Delta t \approx h}$$

Δt : life time

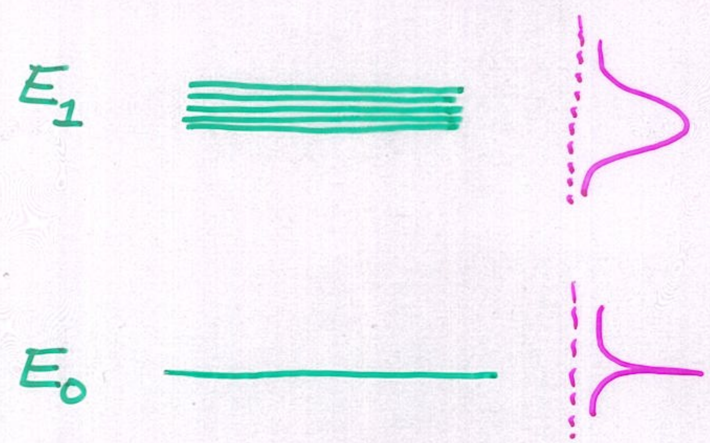
ΔE : energy width

Consider excited state in H atom

Since its life time Δt is finite, its energy can not be determined without uncertainty ΔE,

$$\Delta E \approx \frac{\hbar}{\Delta t} \approx 10^{-7}\ eV$$

Quite small ☺



$\Delta E_1 \cdot \Delta t \approx \hbar$ finite life time.

$\Delta E_0 \approx 0$ life time $\rightarrow \infty$

WAVE FUNCTION

by E. Schrodinger

Quantum Mechanics

To describe a quantum particle, one needs to know its Wave Function $\Psi(x,y,z,t)$.

$|\Psi(x,y,z,t)|^2\,dx\,dy\,dz$ = probability in 

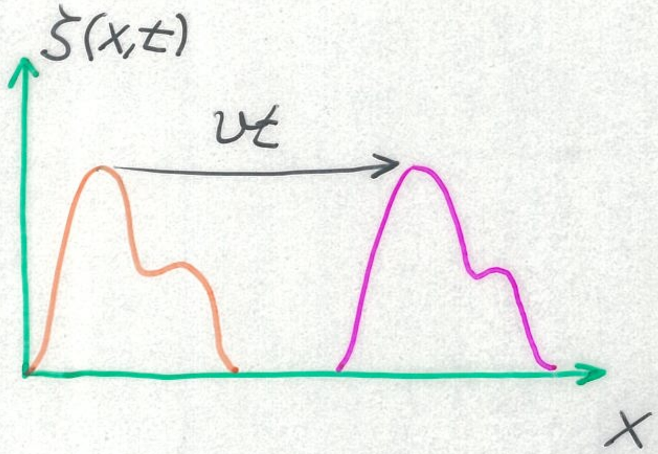
at (x,y,z)

To solve for the wave function $\Psi(x,y,z,t)$, one needs to understand Schrödinger Equation.

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\left[\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}+\frac{\partial^2\psi}{\partial z^2}\right]+V\psi$$

For simplicity, we would mainly concentrate on the 1D case. Note that it is NOT the same as wave equation....

Compare with Wave Equation



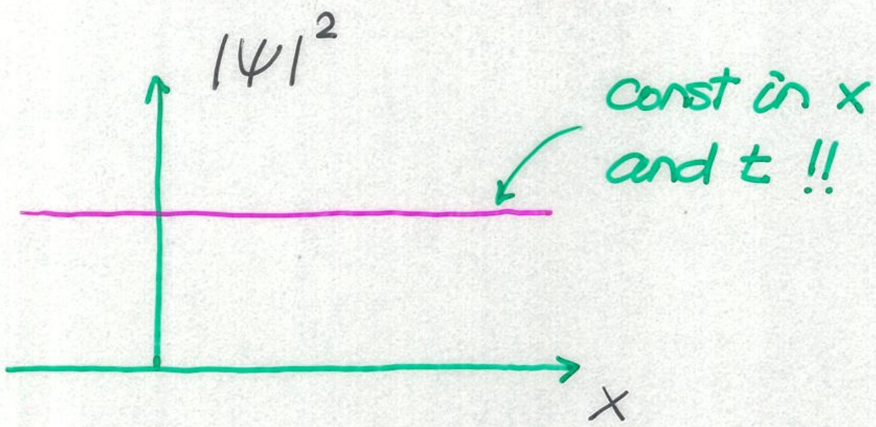
A conventional wave obeys the following equation.

$$\frac{\partial^2 \xi}{\partial t^2} = v^2 \frac{\partial^2 \xi}{\partial x^2}$$

v : wave velocity.

On the other hand, the free particle satisfies the Schrödinger equation

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} \Longrightarrow \psi(x,t) = \frac{1}{\sqrt{L}} e^{i(kx - \omega t)}$$

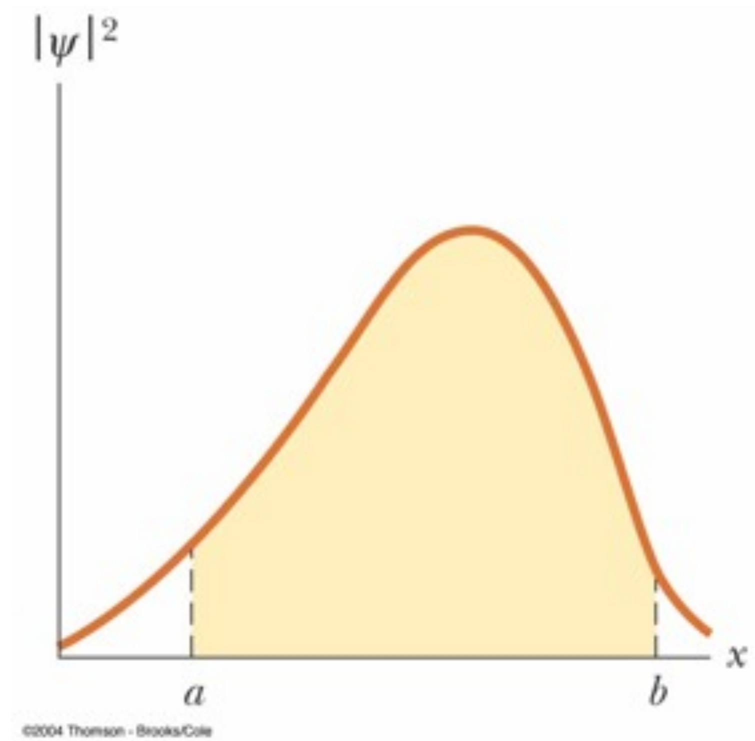


The wave seems static if only $\rho(x,t)$ is measured.....

Wave function

To describe a quantum particle, we need the new concept of wave function:

$$\psi(x,t)$$



The interpretation of the wave function is the following: the square of the wave function is the probability density to find the particle at the location x and at the time t,

$$P(x,t) = |\psi(x,t)|^2 .$$

For instance, the probability to find the particle at the interval between a and b is the spatial integral of $|\psi(x,t)|^2$ in this regime.

Schrodinger equation

The dynamics of the wave function is described by the Schrodinger equation. Note that the time derivative is only first-order.

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

Solving time dependence

The time dependence of the wave function can be solved rather easily. Make an educated guess of the following form:

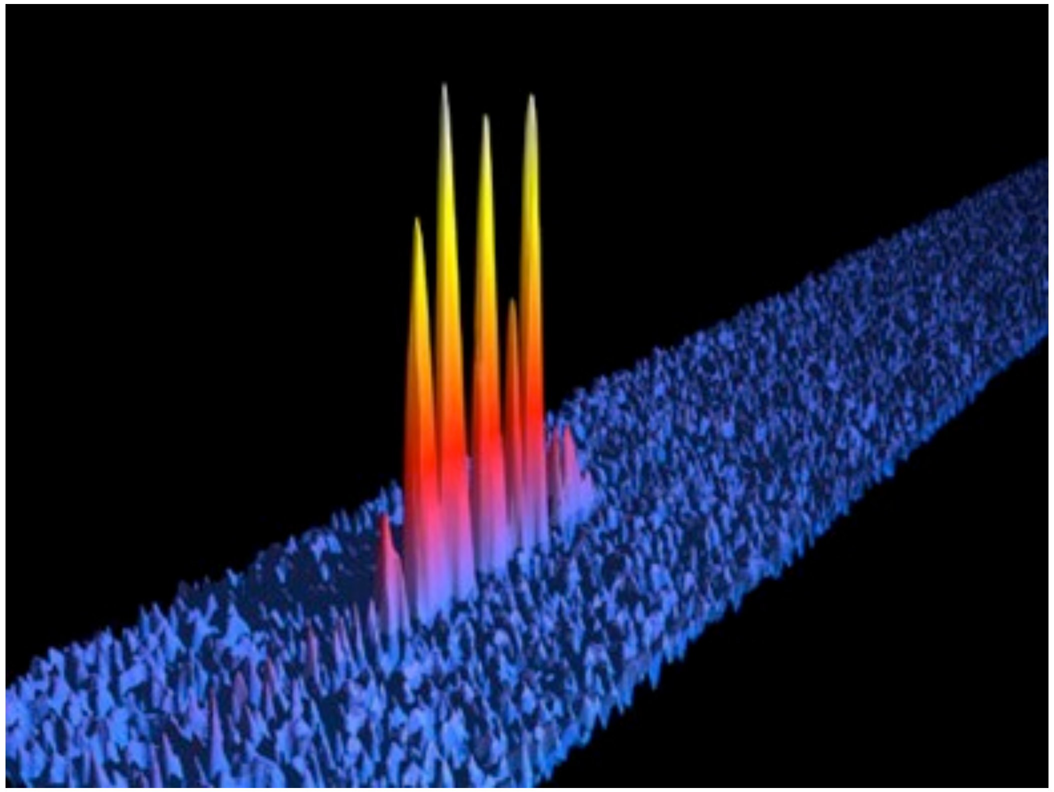
$$\psi(x,t) = \phi(x)e^{-iEt/\hbar}$$

The time dependence of the Schrodinger equation drops out. This is the so-called time-independent Schrodinger equation:

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\phi(x) + V(x)\phi(x) = E\phi(x)$$

Frequency of matter wave

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



There is some physics in the time-varying phase we just solved. Note that when the phase winds by

$$Et/\hbar = 2\pi$$

the wave function comes back to itself. That is to say,

$$E = \hbar\omega$$

Schrodinger equation

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\phi(x) = E\phi(x)$$

We can solve the spatial part of the wave function:

$$\phi(x) = e^{ikx}$$

Combined with the time varying phase, we obtain the solution for a free particle:

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

Wavelength of matter wave

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\phi(x) = E\phi(x)$$

Substitute the solution into the Schrodinger eq.

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

It is easy to verify the other relation postulated by de Broglie:

$$E = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}$$

$$p = \hbar k = \frac{h}{\lambda}$$

Time-Independent Schrödinger equation

Since the Schrödinger equation is first-order in time, its time dependence can be solved easily

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

educated guess !!

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

$$i\hbar(-i\omega)\,\Phi\, e^{-i\omega t}$$

$$= \left[-\frac{\hbar^2}{2m}\frac{\partial^2 \Phi}{\partial x^2} + V\Phi\right] e^{-i\omega t}$$

, note that $E = \hbar\omega$

$$\Rightarrow \quad -\frac{\hbar^2}{2m}\frac{d^2\Phi}{dx^2} + V\Phi = E\Phi$$

should always keep in mind the t dependence !!

Or, sometimes in the form of

$$\frac{d^2\Phi}{dx^2} + \frac{2m}{\hbar^2}(E-V)\Phi = 0$$

Q: Is E arbitrary?
Or.... NOT....

Revisit Free Particle.

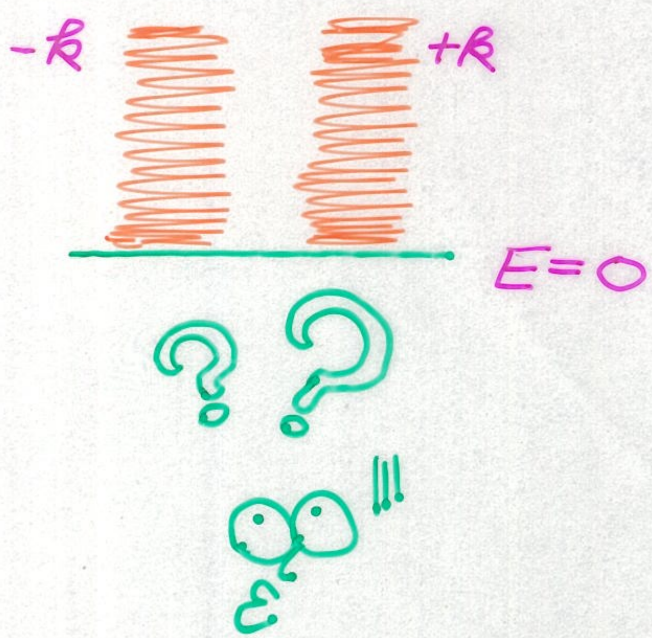
Since $V=0$, the equation is rather trivial.

$$\frac{d^2\psi}{dx^2} + \frac{2mE}{\hbar^2}\psi = 0 \qquad \psi(x) = e^{ikx} \quad \text{with} \quad k^2 = \frac{2mE}{\hbar^2}$$

Or, in more familiar format $\frac{\hbar^2 k^2}{2m} = E \Rightarrow k = \pm\sqrt{\frac{2mE}{\hbar^2}}$

For convenience, $k = \sqrt{\frac{2mE}{\hbar^2}}$ and the two degenerate solutions are

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



As long as $E>0$, there are pairs of solutions with the same energy.

Q: (1) Why the 2-fold degeneracy?

(2) What happens if $E<0$?

Kramers Degeneracy

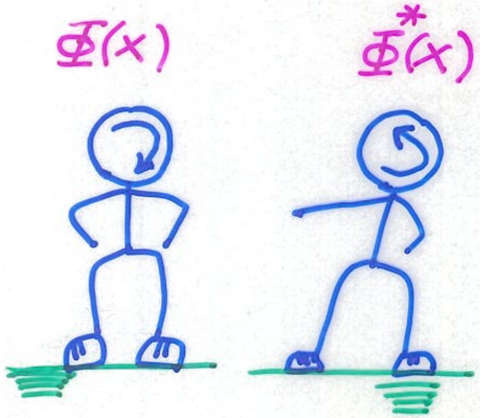
Suppose the wave function describes a stationary state with definite energy E :

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

Its twin brother state under time reversal transformation is

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

One notices that they share the same energy E !!



degenerate in energy !!

Example: plane-wave solution

$$\psi(x,t) = e^{ikx}\, e^{-i\omega t} \qquad \text{R-moving}$$

$$\psi^*(x,-t) = e^{-ikx}\, e^{-i\omega t} \qquad \text{L-moving}$$

☆ By switching the direction of time, the $R \leftrightarrow L$ moving states also switch.

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E<0 Solution

Consider the E<0 solution for a free particle.

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = -|E|\,\psi \quad \Rightarrow \quad \frac{d^2\psi}{dx^2} = \alpha^2\psi \qquad \alpha^2 = \frac{2m|E|}{\hbar^2}$$

The general solution can be written down rather easily,

$$\psi(x) = A\,e^{\alpha x} + B\,e^{-\alpha x}$$

← something wrong with this solution ??

Consider the special case where $B=0$

$$\psi(x) = A\,e^{\alpha x} \;\rightarrow\; \rho(x) = |\psi(x)|^2 = A^2 e^{2\alpha x}$$

to infinity and beyond....

The wave function diverges at $x \rightarrow +\infty$. Thus, the solution can not be used to generate a sensible probability density !!

$$\int dx\,|\psi(x)|^2 \rightarrow \infty \;!!$$

linear superposition at work again....

$$\Psi(x,t) = \frac{1}{\sqrt{2}}\,\psi_1(x,t) + \frac{1}{\sqrt{2}}\,\psi_2(x,t) = \frac{1}{\sqrt{2}}\,\Phi_1(x)\,e^{-i\omega_1 t} + \frac{1}{\sqrt{2}}\,\Phi_2(x)\,e^{-i\omega_2 t}$$

Let's compute the probability density

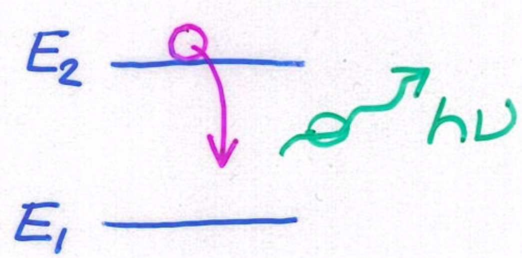
$$\rho(x,t) = |\Psi(x,t)|^2 = \frac{1}{\sqrt{2}}\left[\Phi_1^* e^{i\omega_1 t} + \Phi_2^* e^{i\omega_2 t}\right]\frac{1}{\sqrt{2}}\left[\Phi_1 e^{-i\omega_1 t} + \Phi_2 e^{-i\omega_2 t}\right]$$

$$= \frac{1}{2}\left(\Phi_1^*\Phi_1 + \Phi_2^*\Phi_2\right) \quad \leftarrow \text{stationary part}$$

$$+ \frac{1}{2}\left[\Phi_2^*\Phi_1\, e^{i(\omega_2-\omega_1)t} + \Phi_1^*\Phi_2\, e^{i(\omega_1-\omega_2)t}\right] \quad \leftarrow \text{oscillatory part.}$$

$$\Phi_2^*\Phi_1 = |\Phi_1||\Phi_2|\,e^{-i\delta} \qquad \Phi_1^*\Phi_2 = |\Phi_1||\Phi_2|\,e^{i\delta}$$

$$\Rightarrow \boxed{|\Phi_1||\Phi_2|\cos(\omega_1 t - \omega_2 t + \delta)}$$



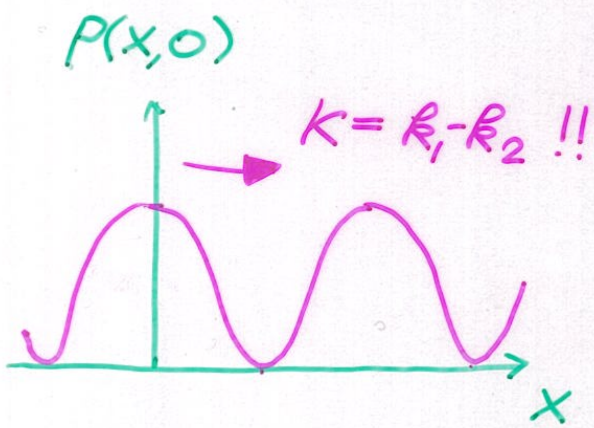
Choose $\psi_1(x,t) = \frac{1}{\sqrt{L}} e^{i(k_1 x - \omega_1 t)}$

$\psi_2(x,t) = \frac{1}{\sqrt{L}} e^{i(k_2 x - \omega_2 t)}$ $\quad k_1 \neq k_2, \quad \omega_1 \neq \omega_2$

The probability density is $\rho(x,t) = \left| \frac{1}{\sqrt{2}} \psi_1 + \frac{1}{\sqrt{2}} \psi_2 \right|^2$

$$\rho(x,t) = \frac{1}{2}\left(|\Phi_1|^2 + |\Phi_2|^2\right) + |\Phi_1||\Phi_2| \cos(\Omega t + \delta) \qquad \Omega = \omega_1 - \omega_2$$

$$= \frac{1}{L} + \frac{1}{L} \cos(\Omega t - kx) \qquad \delta = (k_2 - k_1)x$$



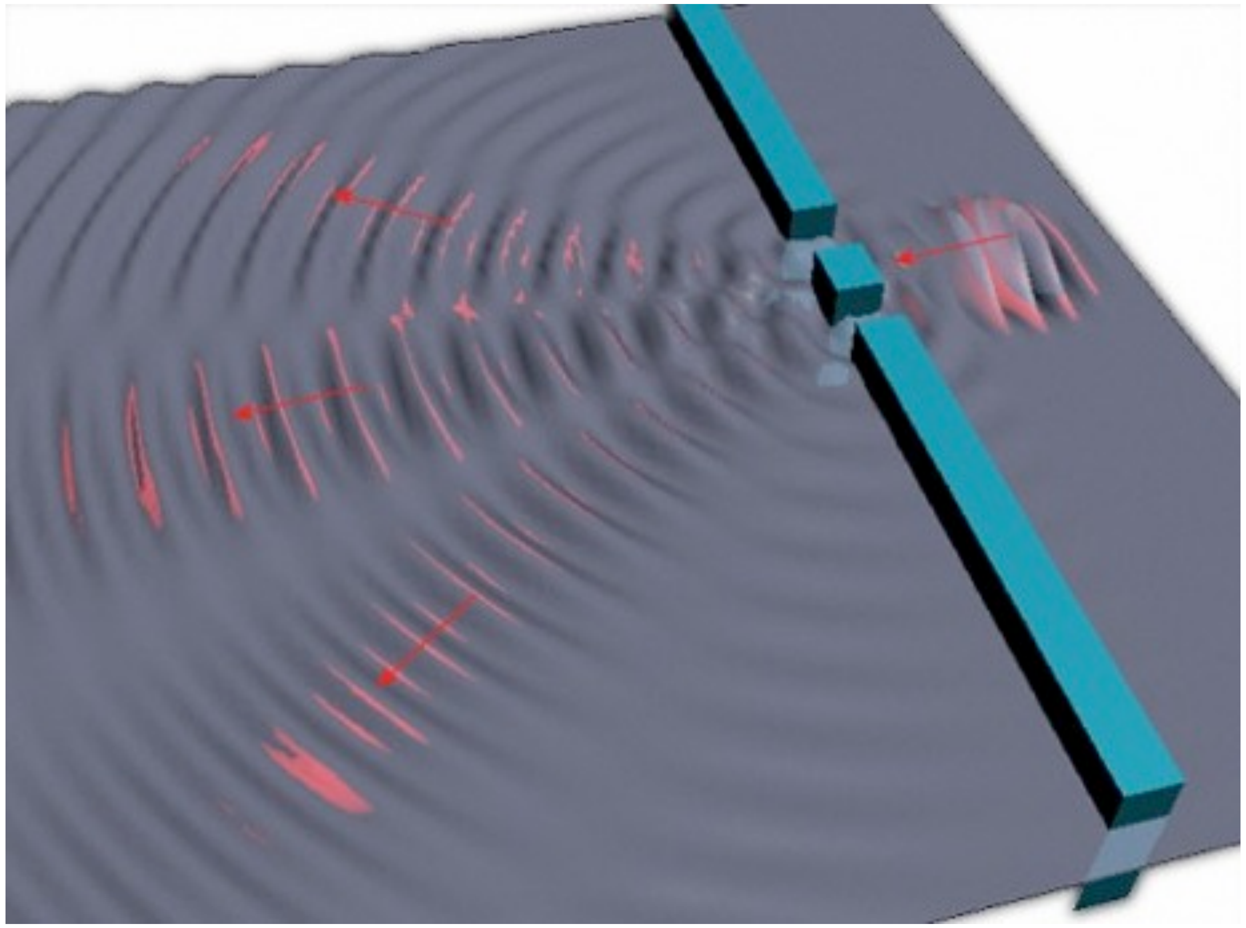
The oscillating frequency is $\Omega = \omega_1 - \omega_2$ and the wave number is $k = k_1 - k_2$

Q: What happens when $\omega_1 = \omega_2$ but $k_1 \neq k_2$?

PARTICLE IN BOX

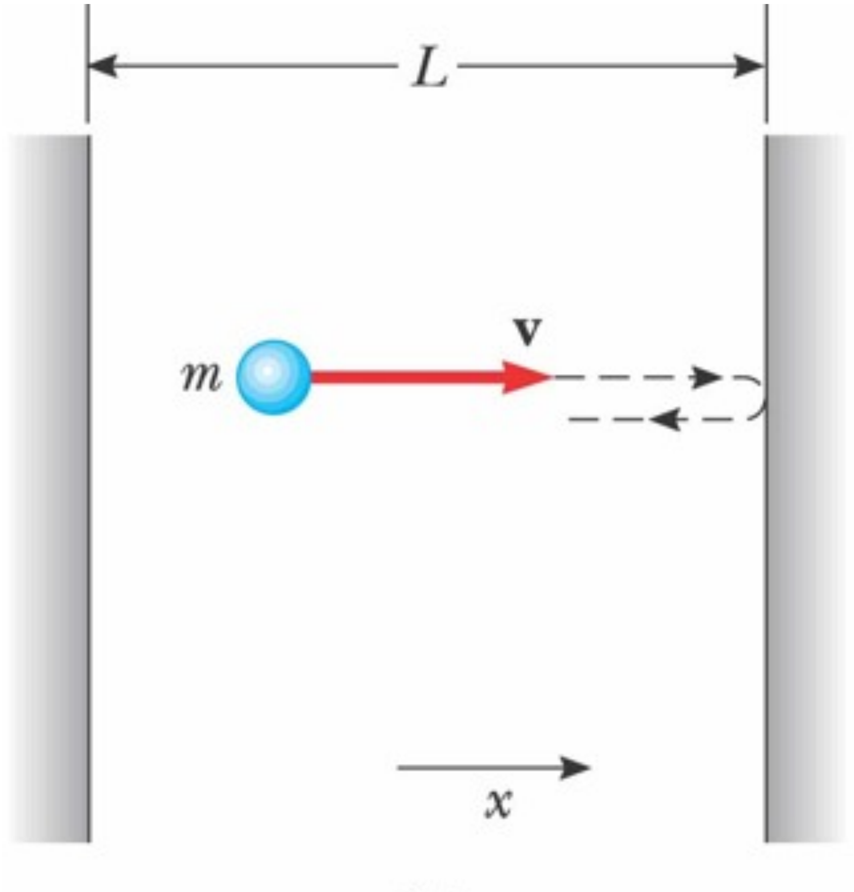
Free quantum particle

How does a free particle propagate according to quantum mechanics?



Particle in a box

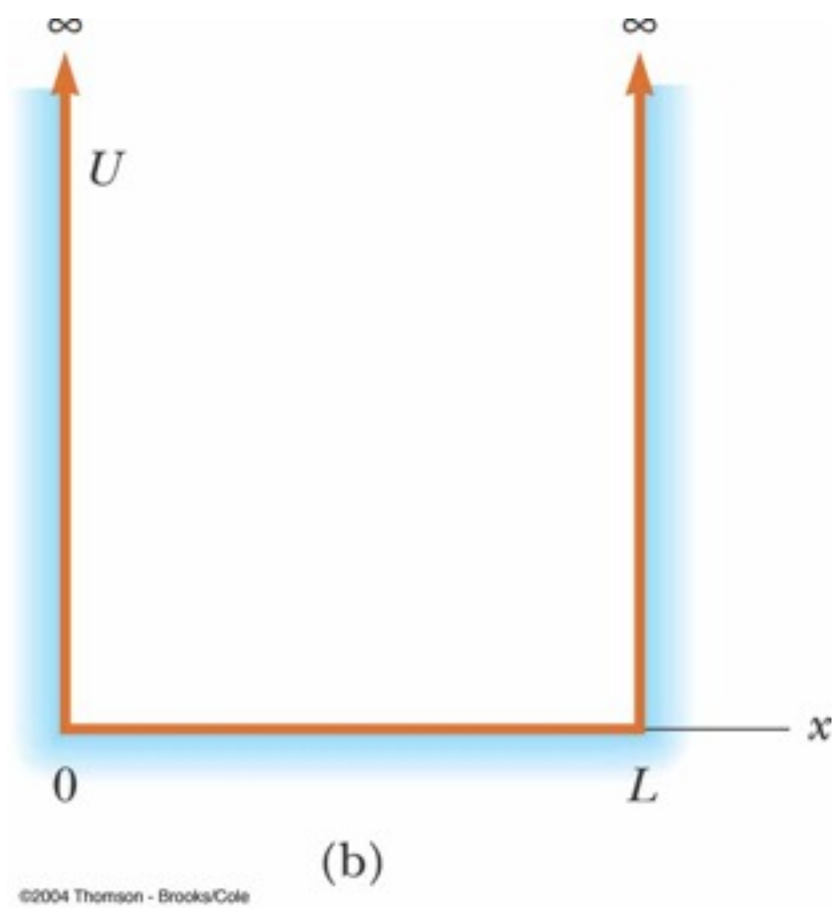
For a classical particle, since the speed is constant, the probability density to detect the particle anywhere inside the box is also a constant.



Boundary conditions

Since the potential energy is infinite outside the well, the wave function is also zero.

But the wave function should be continuous, thus we expect it also vanishes at the boundaries.



$$\phi(0) = 0 = \phi(L)$$

Finding solutions...

Inside the potential well, the particle is free. Thus, the Schrodinger equation is identically the same.

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\phi(x) = E\phi(x)$$

With a given energy, the general solution is a linear superposition of the right-going and left-going solutions,

$$\phi(x) = Ae^{ikx} + Be^{ikx}$$

where A and B are constants determined by the boundary conditions.

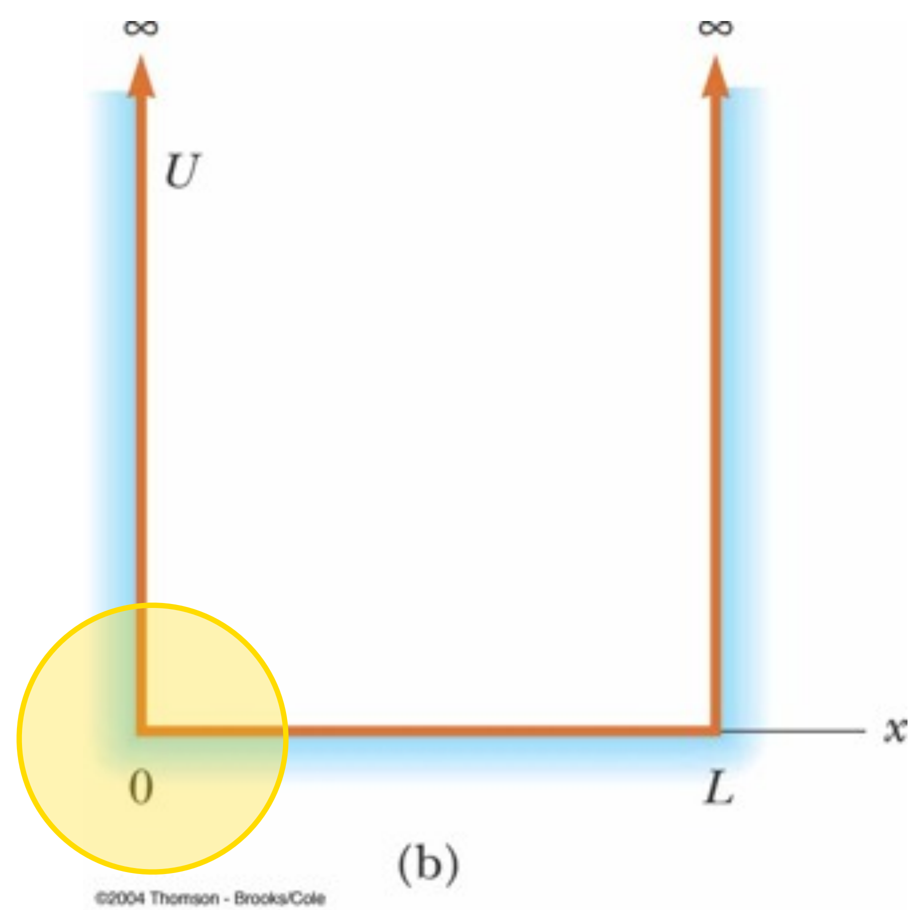
B.C. at x=0

The boundary condition of the wave function at x=0 leads to

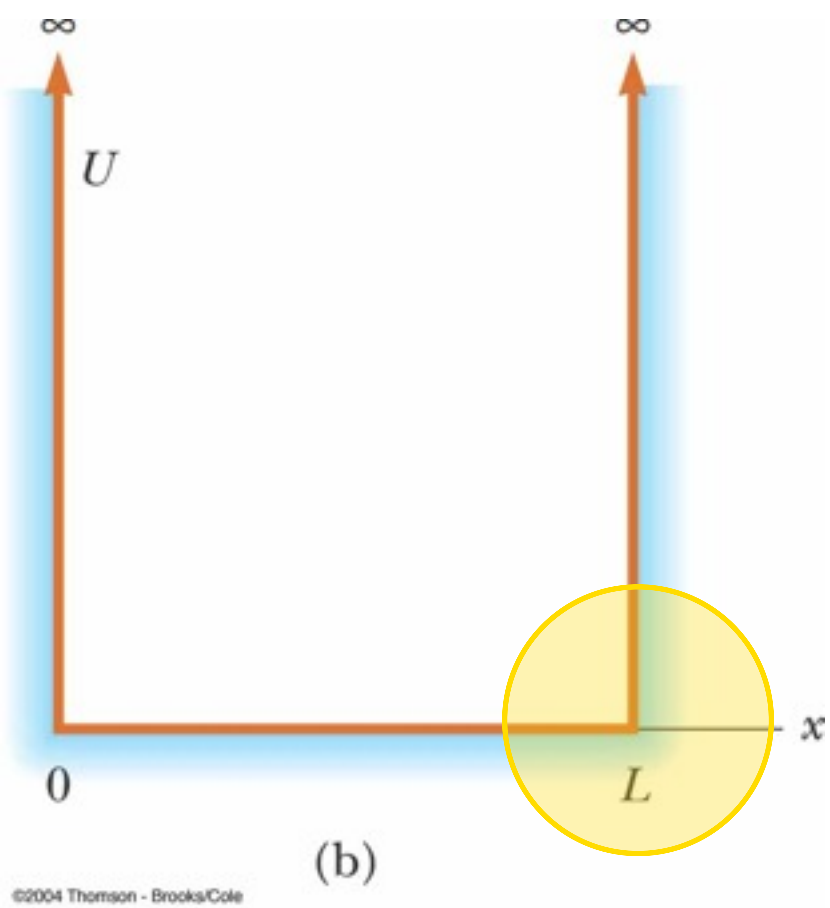
$$A + B = 0 \rightarrow A = -B$$

The solution takes the form of sine,

$$\phi(x) = C\sin(kx)$$



B.C. at x=L



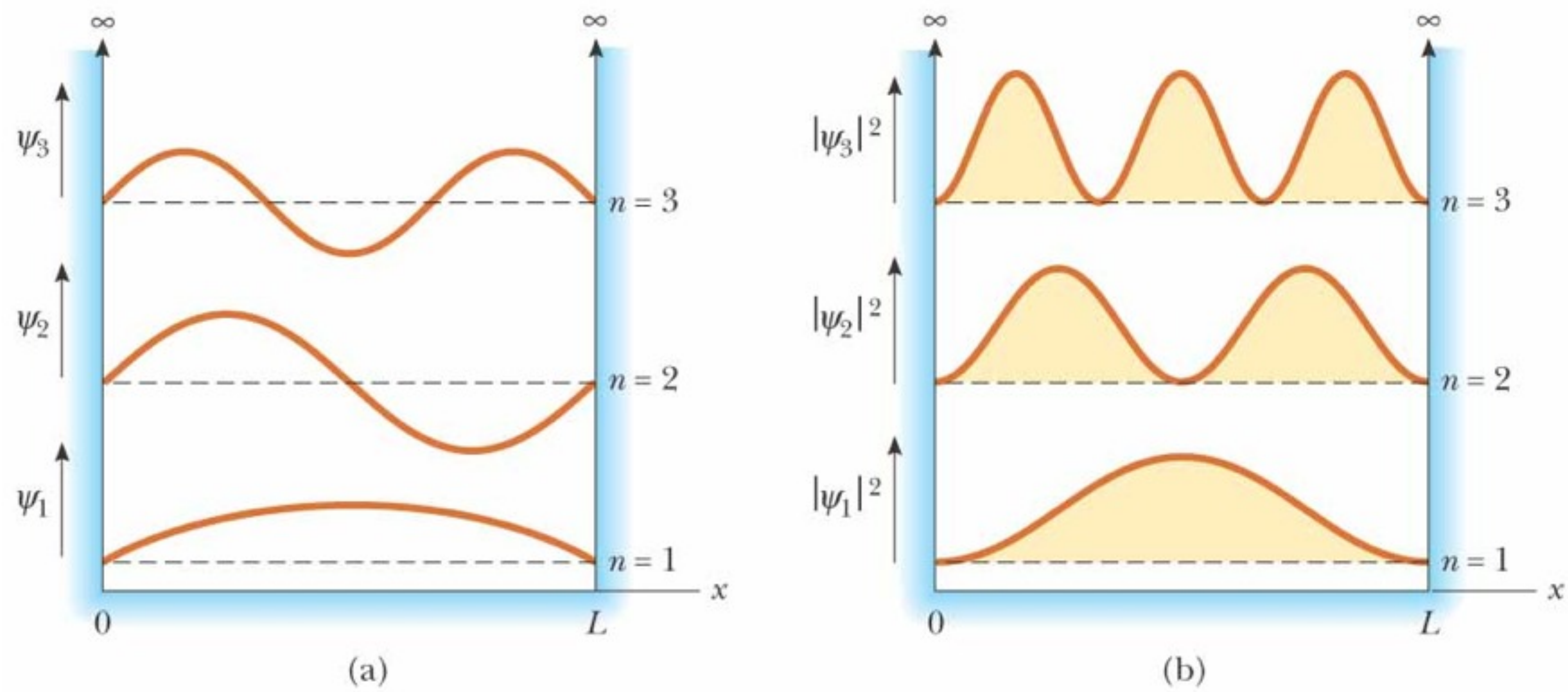
The boundary condition at x=L gives rise to the constraint on the momentum

$$\sin kL = 0 \rightarrow kL = n\pi$$

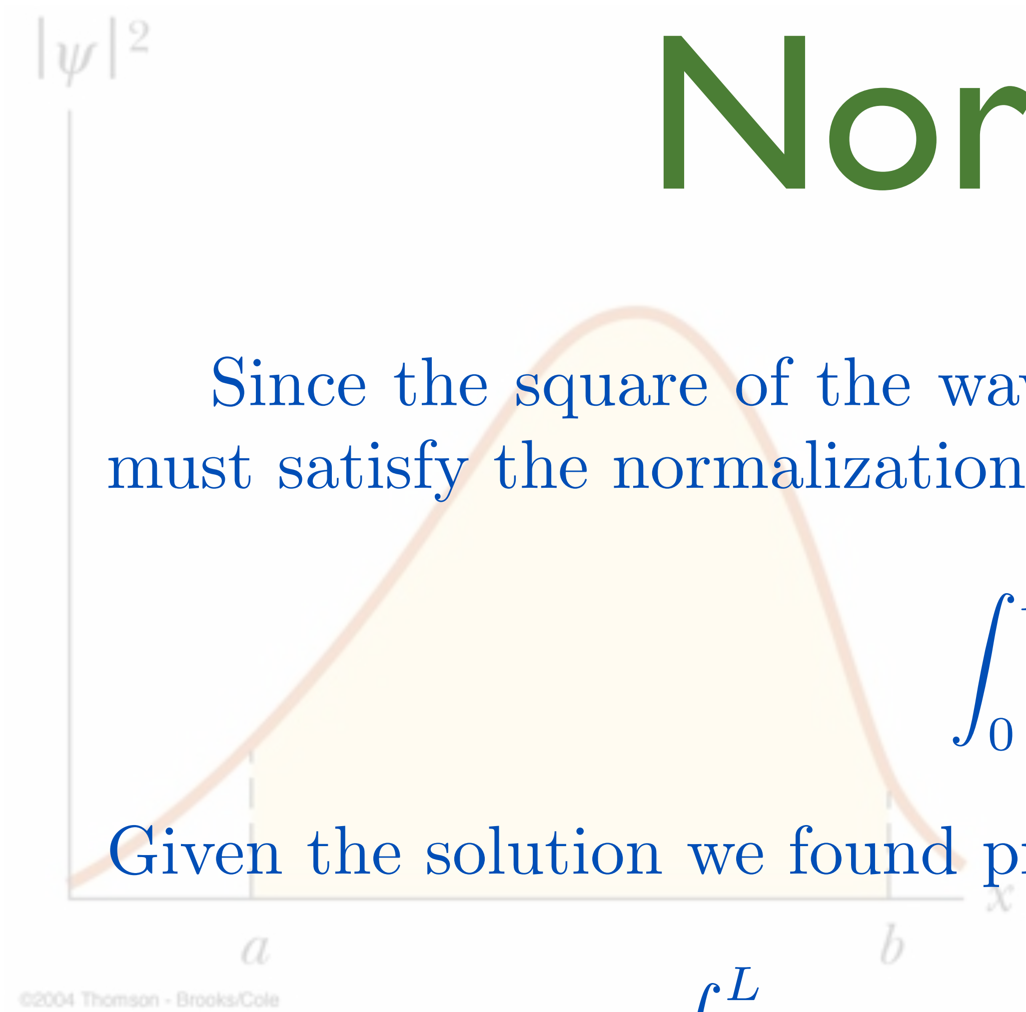
The momentum is quantized!!

$$k = \frac{n\pi}{L} = \frac{\pi}{L}, \frac{2\pi}{L}, \frac{3\pi}{L}, \ldots$$

Nodal structure



Normailzation



Since the square of the wave function represents the probability denisty, it must satisfy the normalization condition

$$\int_0^L dx\, |\phi(x)|^2 = 1.$$

Given the solution we found previously, the normalization condition leads to

$$C^2 \int_0^L dx\, \sin^2\left(\frac{n\pi x}{L}\right) = 1 \quad \rightarrow \quad C = \sqrt{\frac{2}{L}}.$$

Finally, the properly normalized wave function for the particle inside the infinite potential well is

$$\phi(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)$$

Energy quantization

Because the momentum is quantized, the energy is also quantized,

$$E = \frac{\hbar^2 k^2}{2m} = \frac{n^2 \hbar^2 \pi^2}{2mL^2}$$

Compare with photons!