HH0133 - Schrodinger Equation

Schrodinger equation

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

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

Quantum Mechanics

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

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

at (x,y,z)

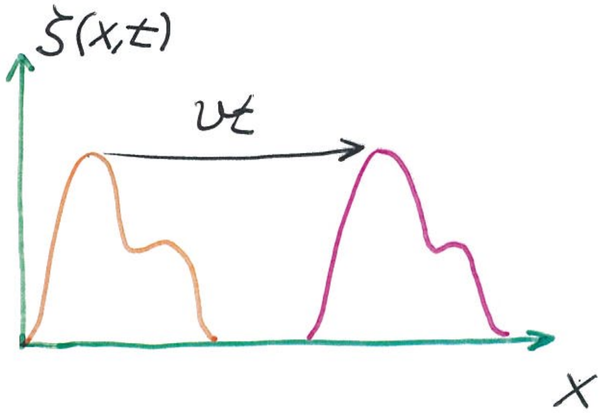
To solve for the wave function $\Psi(x,y,z,t)$, one needs to understand Schrödinger Equation.

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

For simplicity, we would mainly concentrate on the 1D case.

Note that it is NOT the same as wave equation ....

Compare with Wave Equation



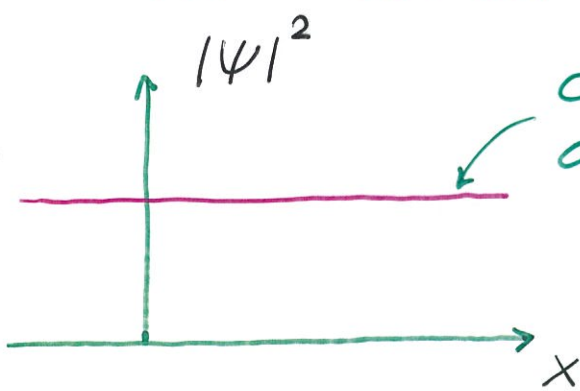
A conventional wave obeys the following equation.

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

v : wave velocity.

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

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



const in x and t !!

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

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 !!

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

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

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

, 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.

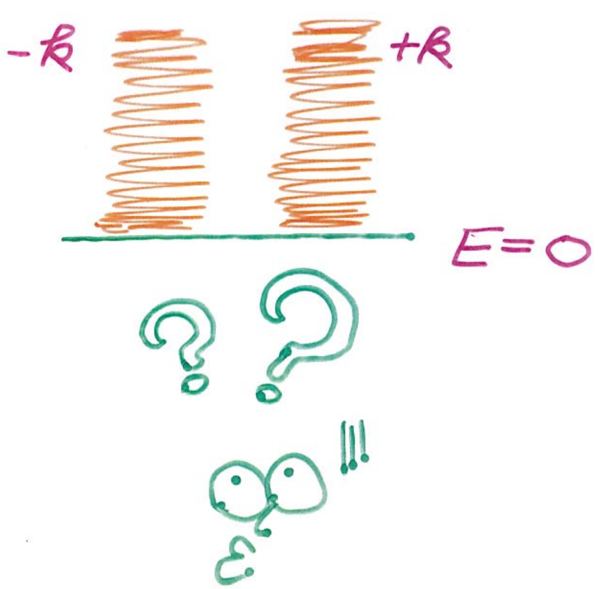
Since $V=0$, the equation is rather trivial.

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

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 $E<0$?

Time-Reversal Symmetry

Suppose a wave function $\psi(x,t)$ satisfies the Schrödinger equation:

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

Now we want to show $\psi^*(x,-t)$ is a solution as well.

PROOF:  (1) take complex conjugate

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

[assuming the potential is time-independent $V(x,t) = V(x)$ here]

(2) change variable $t \to -t$

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

It's clear that $\psi^*(x,-t)$ also satisfies the Schrödinger equation.

Kramers Degeneracy

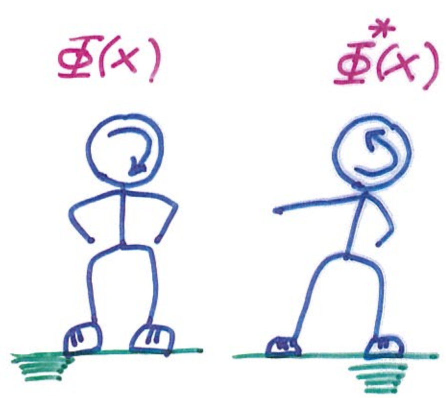
Suppose the wave function describes a stationary state with definite energy E :

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

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

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

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

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

E<0 Solution

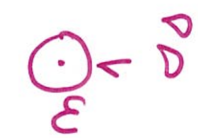
Consider the E<0 solution for a free particle.

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

The general solution can be written down rather easily.

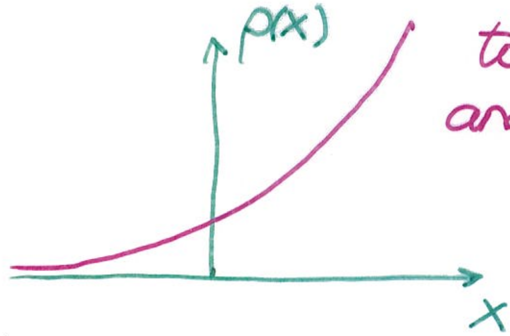
$$\psi(x) = A\,e^{\alpha x} + B\,e^{-\alpha x}$$

something wrong with this solution ??



Consider the special case where $B=0$

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



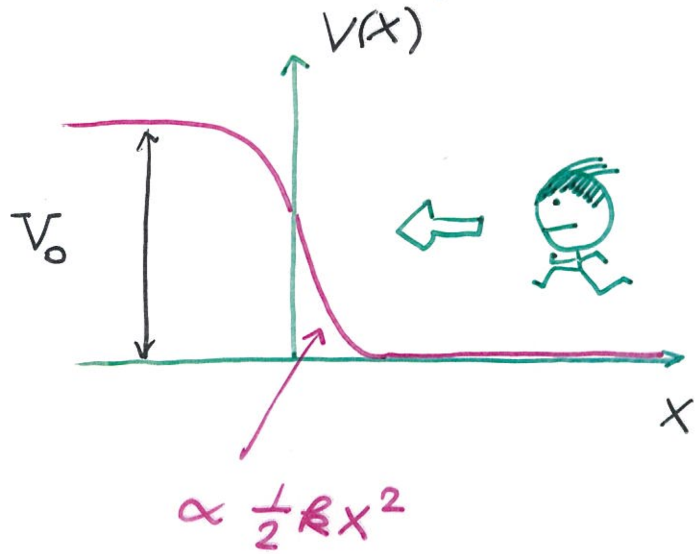
to infinity and beyond....

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

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

Potential Wall.

Consider a particle and a wall at $x=0$. However, to



simplify the problem, it is often approximated by the so-called hard-wall condition.

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

From linear superposition, the general solution with energy $E = \frac{(\hbar k)^2}{2m}$ takes the form:

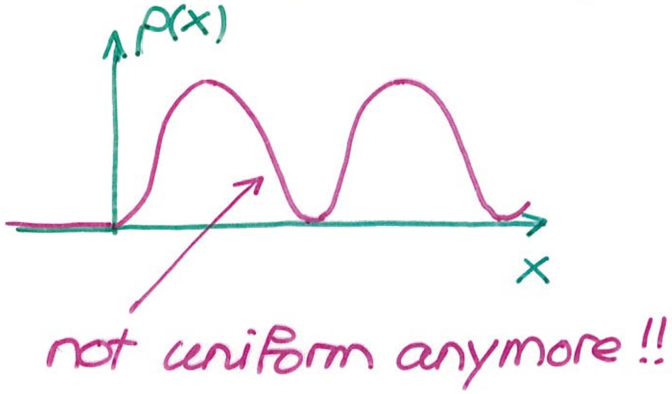
$$\psi(x) = A\, e^{ikx} + B\, e^{-ikx}$$

Since the wave function vanishes at $x=0$, we need to enforce to boundary condition $\psi(0)=0$.

$\psi(0) = 0 \quad \Rightarrow \quad A + B = 0 \quad B = -A.$

Thus, $\psi(x) = A e^{ikx} - A e^{-ikx} = 2iA \sin kx = \underline{\underline{C \sin kx}}$

We can plot the probability density $\rho(x,t)$.



(1) $\rho(x,t)$ is not uniform anymore.

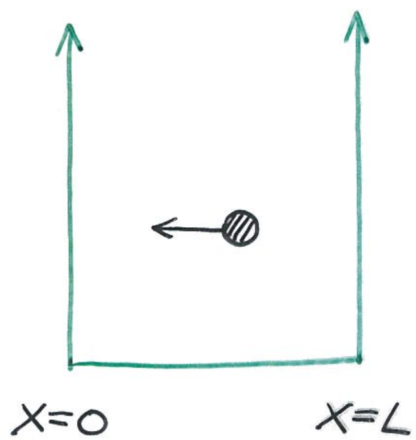
(2) $\rho(x,t)$ is static (not like the usual standing wave).

Furthermore, we can compute the probability current

$$j(x) = \frac{\hbar}{2mi}\left(\psi^* \frac{\partial \psi}{\partial x} - \frac{\partial \psi^*}{\partial x}\psi\right) = \frac{\hbar}{2mi}\left(\psi \frac{\partial \psi}{\partial x} - \frac{\partial \psi}{\partial x}\psi\right) = 0$$

- The probability current is zero as we expected.
- Hard wall gives rise to $k \rightarrow -k$ plus π shift !!

Potential Box



The Schrödinger eq reads $\frac{d^2\psi}{dx^2} + k^2\psi = 0$

where $k^2 = \frac{2mE}{\hbar^2}$. The general solution is

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

Now, needs to satisfy two boundary conditions

(1) $\psi(0) = 0$ (2) $\psi(L) = 0$ From the first B.C.

$$A + B = 0 \Rightarrow \psi(x) = A e^{ikx} - A e^{-ikx} = 2iA \sin kx$$
$$= C \sin kx$$

Now, ready to apply the 2nd B.C. $\psi(L) = 0$

$$\sin kL = 0 \Rightarrow k_n = \frac{n\pi}{L}$$

momentum is quantized!!

Energy Quantization

From the quantized momentum $P_n = \hbar k_n = \frac{n\pi\hbar}{L}$, it's easy to show that energy is also quantized.

$$E_n = \frac{P_n^2}{2m} = \frac{n^2\pi^2\hbar^2}{2mL^2} \qquad E_n \propto n^2 \quad \text{quantized !!}$$

We are NOT done yet.... $\psi_n(x) = C \sin(k_n x)$

Still need to figure out the const C ☹

$$\int dx\, |\psi(x)|^2 = 1 \quad \Rightarrow \quad \int_0^L dx\; C^2 \sin^2(k_n x) = 1$$

Recall that $\sin^2(k_n x) = \frac{1}{2}(1 + \cos 2k_n x)$

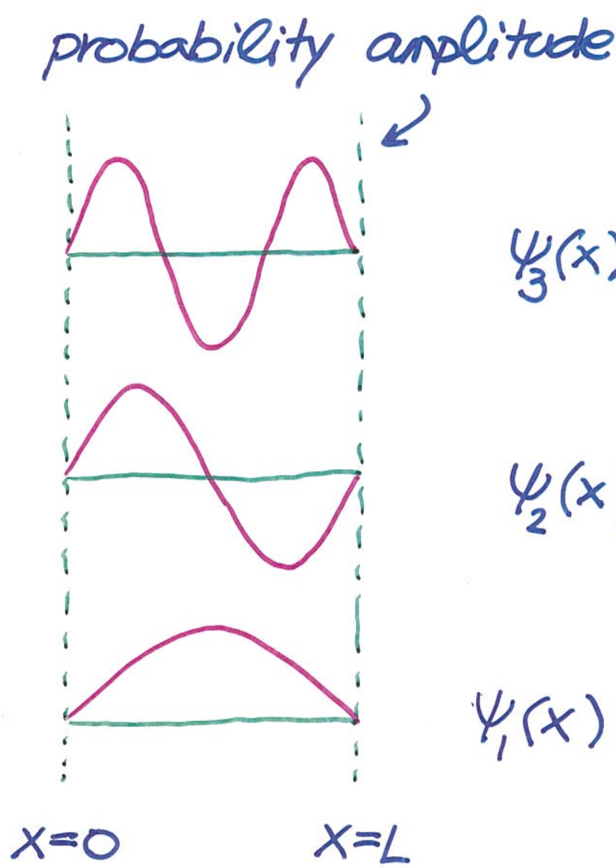
$$\int_0^L \sin^2(k_n x)\, dx = \int_0^L \frac{1}{2} + \frac{1}{2}\cos(2k_n x)\, dx = \frac{L}{2}$$

Thus, the wave function is $\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)$

Wave Function

Just as in conventional standing waves, we see nodal structure in wave functions. Note that, except the ground state, all excited states have nodes.

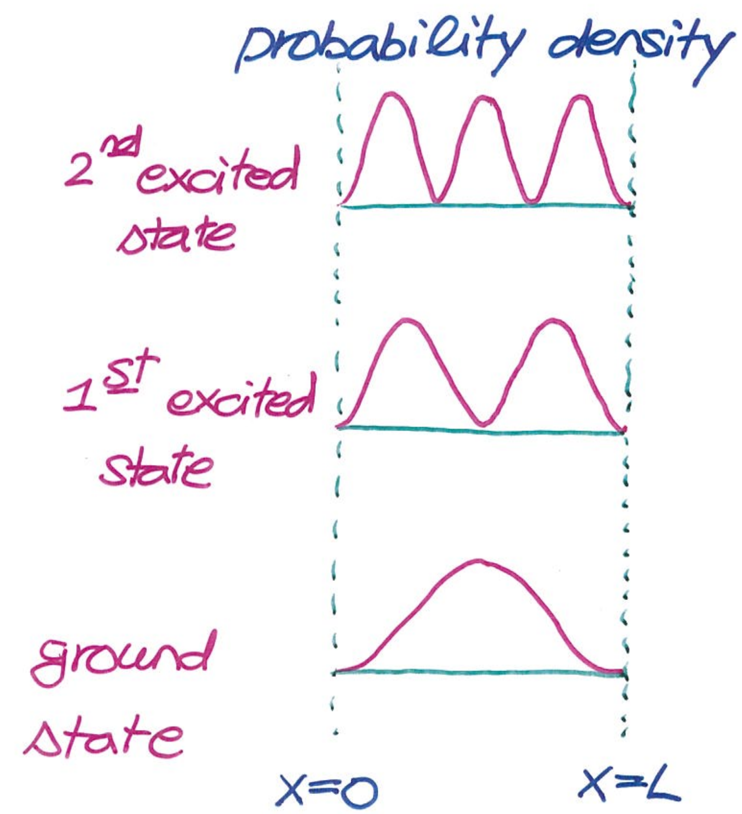
$$\boxed{\#\text{ of nodes} = n-1}$$



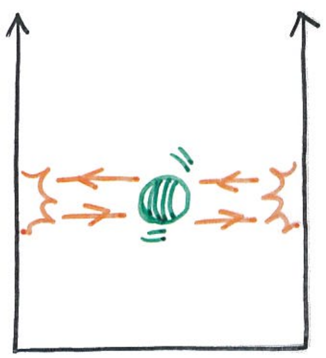
$$\psi_3(x) = \sqrt{\frac{2}{L}}\,\sin\left(\frac{3\pi x}{L}\right)$$

$$\psi_2(x) = \sqrt{\frac{2}{L}}\,\sin\left(\frac{2\pi x}{L}\right)$$

$$\psi_1(x) = \sqrt{\frac{2}{L}}\,\sin\left(\frac{\pi x}{L}\right)$$



Bohr Quantization



View the stationary solution as multiple self constructive interference. The phase difference is

$$\delta = 2\pi\left(\frac{2L}{\lambda}\right) - \varphi_s \qquad \varphi_s = \pi + \pi$$

The constructive interference requires $\delta = 2n\pi$

$$2n\pi = 2\pi\left(\frac{2L}{\lambda}\right) - 2\pi \quad \Rightarrow \quad \frac{2L}{\lambda} = (n+1)$$

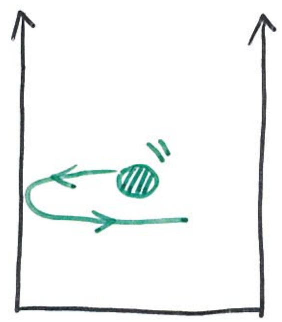
Using the relation $p = \frac{h}{\lambda}$ $\Rightarrow$ $2L\frac{h}{\lambda} = (n+1)h$

Finally, we arrive at $2pL = n'h$. OR, in more formal format

$$\oint p\,dx = \hbar\,(2n\pi + \varphi_s)$$

scattering phase.

Simple Applications.



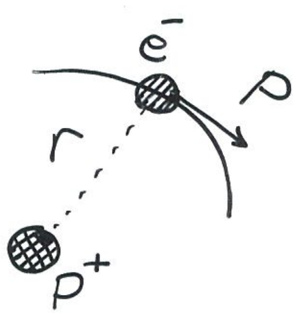
$$\oint p\,dx = \hbar\,(2n\pi + \varphi_s) \Rightarrow p\cdot 2L = \hbar\, 2n'\pi$$

$$p_n = \frac{2n'\pi\hbar}{2L} = \frac{n'\pi\hbar}{L}$$

Another example is Bohr's model for H atom. Somehow, the angular momentum is quantized ....

$$\oint p\,dx = \hbar\,(2n\pi + \varphi_s)$$

$\varphi_s = 0$ in this case !!



$$p\cdot \cancel{2\pi} r = \cancel{2} n \cancel{\pi} \hbar$$

$$\Rightarrow \quad L = n\hbar$$

the angular momentum is quantized in unit of $\hbar$.

Uncertainty Principle.

The wave function $\psi_n(x) = \sqrt{\frac{2}{L}} \sin(k_n x)$. We can calculate the uncertainty in position.

$$\langle x \rangle \equiv \int_0^L dx\, \rho(x) \cdot x = \frac{L}{2} \quad \text{by symmetry.}$$

$$(\Delta x)^2 \equiv \left\langle (x - \langle x \rangle)^2 \right\rangle = \langle x^2 - 2x\langle x \rangle + \langle x \rangle^2 \rangle$$

$$= \langle x^2 \rangle - 2\langle x \rangle \langle x \rangle + \langle x \rangle^2 = \langle x^2 \rangle - \langle x \rangle^2$$

Only need to compute $\langle x^2 \rangle$ now.

$$\langle x^2 \rangle = \int_0^L dx\, \rho(x)\, x^2 = \frac{2}{L} \int_0^L dx\, x^2 \sin^2(k_n x)$$

The integral is elementary:

$$\int x^2 \sin^2 kx \, dx = \frac{x^3}{6} - \frac{x \cos(2kx)}{4k^2} - \frac{2k^2x^2 - 1}{8k^3} \sin(2kx)$$

$$\langle x^2\rangle = \int_0^L dx\ \frac{2}{L}\sin^2 k_n x \cdot x^2 = \frac{2}{L}\cdot\left[\frac{L^3}{6} - \frac{L}{4k_n^2}\right]$$

$$= \frac{1}{3}L^2 - \frac{1}{2k_n^2} \approx \frac{1}{3}L^2$$

Finally, the uncertainty in x is

$$(\Delta x)^2 = \langle x^2\rangle - \langle x\rangle^2 \approx \frac{1}{3}L^2 - \frac{1}{4}L^2$$

$$= \frac{1}{12}L^2$$

$$\Rightarrow \quad \Delta x \approx \frac{1}{2\sqrt{3}}L$$

On the other hand, the uncertainty in momentum is

$$\langle p^2\rangle = p_n^2$$

$$\langle p\rangle^2 = 0$$

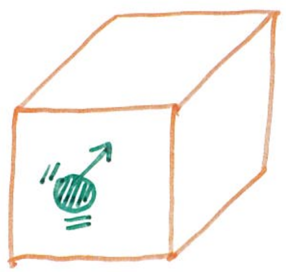
$$\Rightarrow \quad \Delta p = \sqrt{\langle p^2\rangle - \langle p\rangle^2} = p_n = \frac{n\hbar\pi}{L}$$

One can easily see that $\Delta x\, \Delta p \approx \frac{1}{2\sqrt{3}}L \cdot \frac{n\hbar\pi}{L}$

$$\rightarrow \quad \Delta x\, \Delta p \approx n h \quad !!$$

Degeneracy and Symmetry

Now consider a particle in 3D box of length L. The wave function can be solved in a similar fashion.



$$\psi(x,y,z) = \left(\frac{2}{L}\right)^{3/2} \sin\frac{n_x \pi x}{L} \sin\frac{n_y \pi y}{L} \sin\frac{n_z \pi z}{L}$$

The total energy $E = \frac{1}{2m}\left(P_x^2 + P_y^2 + P_z^2\right)$, plug in the quantized momenta P_x, P_y, P_z.

$$E = \frac{\hbar^2}{2m}\left(k_x^2 + k_y^2 + k_z^2\right) = \frac{\hbar^2 \pi^2}{2mL^2}\left(n_x^2 + n_y^2 + n_z^2\right)$$

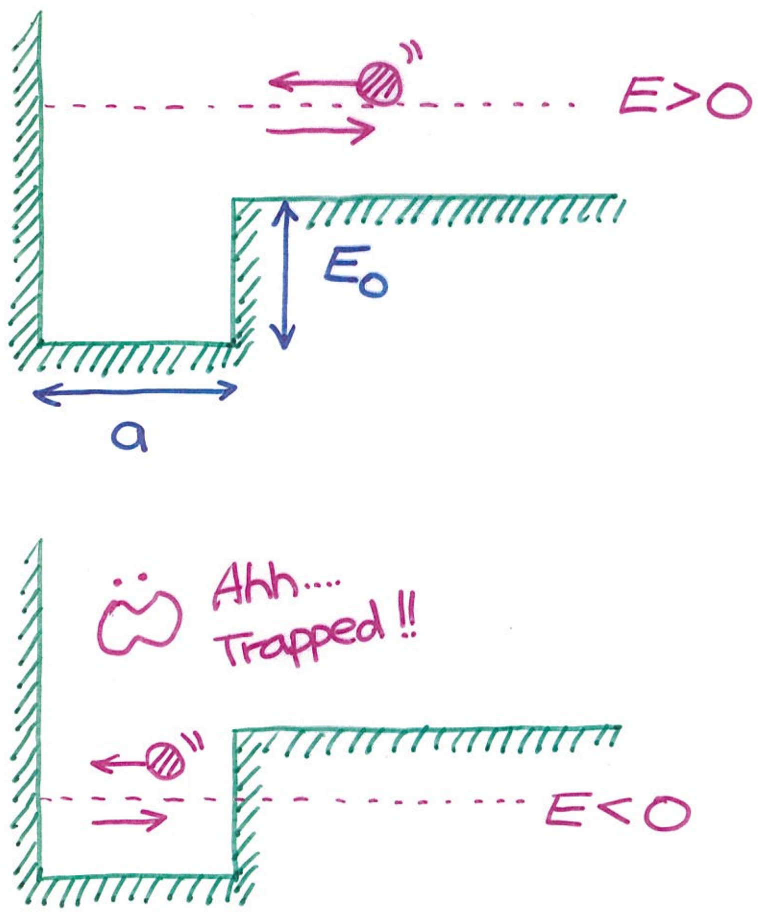
The total energy depends on the quantum numbers (n_x, n_y, n_z)

$3E_1$	$(1,1,1)$	$D = 1$
$6E_1$	$(2,1,1), (1,2,1), (1,1,2)$	$D = 3$
$9E_1$	$(2,2,1), (2,1,2), (1,2,2)$	$D = 3$
$\vdots$	$\vdots$	

related to symmetry.

Finite Potential Well

Consider a finite potential well as shown below. The Schrödinger equation can be solved in two separated regimes easily. Then, we glue the solutions together.



In region I :

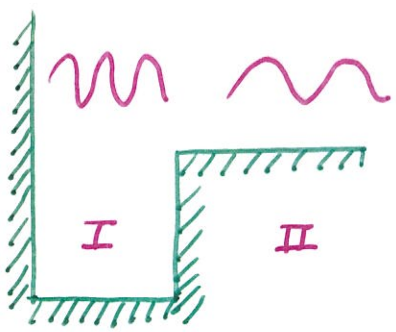
$$-\frac{\hbar^2}{2m}\frac{d^2\psi_I}{dx^2} - E_0\psi_I = E\psi_I$$

In region II :

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

Both ψ_I and ψ_{II} can be solved easily. To glue them together smoothly, $\psi_I(a) = \psi_{II}(a)$, $\frac{d\psi_I}{dx}(a) = \frac{d\psi_{II}}{dx}(a)$

$E>0$ Scattering State



Consider the positive energy solution. In both regimes, the solution is plane wave except the momentum is different.

In regime I : $-\dfrac{\hbar^2}{2m}\dfrac{d^2\psi}{dx^2} - E_0\psi = E\psi$

The general solution is $\psi_I(x) = A\,e^{ik_I x} + B\,e^{-ik_I x}$

where the momentum k_I is $\dfrac{\hbar^2 k_I^2}{2m} - E_0 = E$ $\quad k_I = \sqrt{\dfrac{2m(E+E_0)}{\hbar^2}}$

Due to the hard wall at $x=0$ $\Rightarrow$ $\psi_I(x=0) = 0$

Thus, it requires $A+B=0$.

$$\psi_I(x) = A\,e^{ik_I x} - A\,e^{-ik_I x} = 2Ai\sin k_I x = C\sin k_I x$$

We can now go ahead and compute $\psi_{II}(x)$ in regime II ....

In regime II : $-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi \Rightarrow \psi_{II}(x) = A' e^{ik_{II}x} + B' e^{-ik_{II}x}$

It is equivalent to write the general solution in terms of sin, cos. $k_{II} = \sqrt{\frac{2mE}{\hbar^2}}$

$$\psi_{II}(x) = D' \sin k_{II}x + E' \cos k_{II}x = C' \sin(k_{II}x + \delta)$$

Glue $\psi_I(x)$ and $\psi_{II}(x)$ together at $x=a$.

$$\psi_I(a) = \psi_{II}(a) \Rightarrow C \sin(k_I a) = C' \sin(k_{II}a + \delta)$$

$$\frac{d\psi_I}{dx}(a) = \frac{d\psi_{II}}{dx}(a) \Rightarrow C k_I \cos(k_I a) = C' k_{II} \cos(k_{II}a + \delta)$$

divide both eq's:

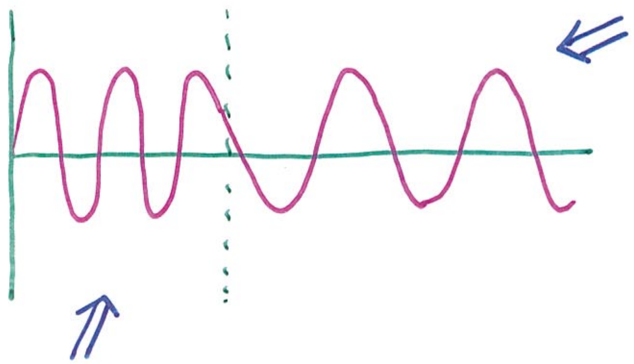
$$\frac{C \sin(k_I a)}{C k_I \cos(k_I a)} = \frac{C' \sin(k_{II}a+\delta)}{C' k_{II} \cos(k_{II}a+\delta)} \Rightarrow \frac{1}{k_I}\tan(k_I a) = \frac{1}{k_{II}}\tan(k_{II}a+\delta)$$

☆ δ can be solved !!

Once the phase shift δ is known, the ratio between C and C' is

$$\frac{C'}{C} = \frac{\sin(k_{I} a)}{\sin(k_{II} a + \delta)}$$

Q: any missing equation ??

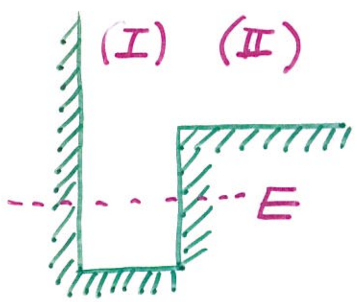


$\psi_{II}(x) = C' \sin(k_{II} x + \delta)$

$\psi_{I}(x) = C \sin(k_{I} x)$

This result is NOT too surprising when comparing with classical one, Except ..... the probability density modulation in space

$E < 0$ Bound State.



For $E<0$ bound state, the solution inside the well is still plane wave. BUT! What about the solution in regime II ? Let's take a closer look.

Following similar algebra, it is easy to show that

$$\psi_I(x) = C \sin(k_I x) \quad \text{where} \quad \frac{\hbar^2 k_I^2}{2m} - E_0 = -|E|$$

The momentum inside the well is $\hbar k_I = \sqrt{2m(E_0 - |E|)}$

Ok. Now turn our attention to regime II. The Schrödinger equation reads:

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

$$\psi_{II}(x) = \cancel{D e^{\alpha x}} + E e^{-\alpha x} \quad \text{with} \quad \hbar\alpha = \sqrt{2m|E|}$$

drop!! Why?

Collect the solution together:

$$\psi(x) = \begin{cases} C \sin k_I x & x \le a \\ D e^{-\alpha x} & x \ge a \end{cases}$$

Try to glue them together smooth and tight !!

We want (1) $\psi_I(a) = \psi_{II}(a)$

(2) $\psi_I'(a) = \psi_{II}'(a)$

Need to do some math in the following ˃˂

From (1), $C \sin k_I a = D e^{-\alpha a}$

From (2), $C k_I \cos k_I a = -D \alpha e^{-\alpha a}$

$\Rightarrow$ $k_I \cot k_I a = -\alpha$

Writing the absolute value of energy $|E| = \mathcal{E}$

$\hbar k_I = \sqrt{2m(E_0 - \mathcal{E})}$

$\hbar \alpha = \sqrt{2m\mathcal{E}}$

$\Rightarrow$ $\hbar^2 k_I^2 = 2mE_0 - 2m\mathcal{E}$

$\hbar^2 \alpha^2 = 2m\mathcal{E}$

$$\alpha = \sqrt{\frac{2mE_0}{\hbar^2} - k_I^2}$$

The matching B.C. gives $k_I \cot(k_I a) = -\alpha$

$$-\cot(k_I a) = \frac{\alpha}{k_I} \quad \Rightarrow \quad -\cot(k_I a) = \frac{\sqrt{\frac{2mE_0}{\hbar} - k_I^2}}{k_I}$$

The bound state energy can be solved by plotting both sides and looking for intersections. Easier if we make everything dimensionless.

$$y = k_I a$$

$$\lambda = \frac{2mV_0 a^2}{\hbar^2}$$

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

energy is quantized !!

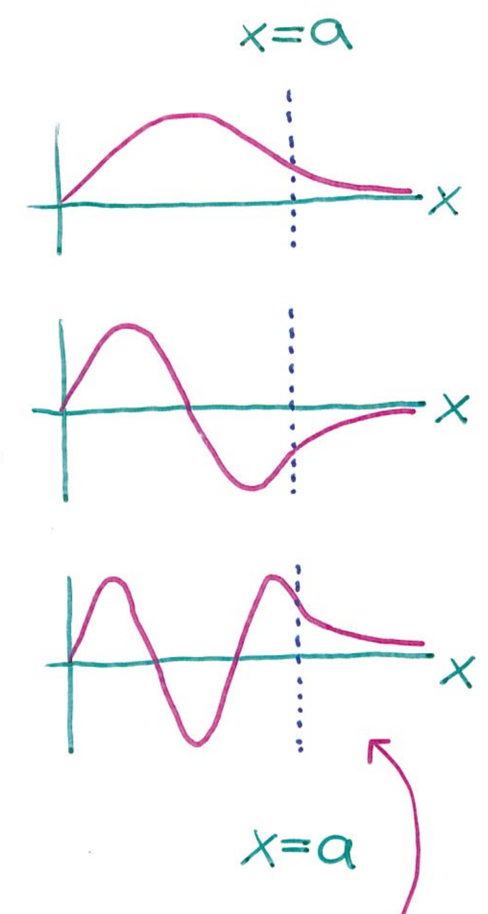
One can read off the minimum λ for the bound state to exist.

$$\lambda - \left(\frac{\pi}{2}\right)^2 \geq 0 \qquad \lambda \geq \frac{\pi^2}{4}$$

Quantum Leakage.

From the matching B.C.

$$-\cot(k_I a) = \frac{\alpha}{k_I} \qquad \alpha = \sqrt{\frac{2mE_0}{\hbar^2} - k_I^2}$$



forbidden regime by classical mechanics.

For steeper potential well, the number of bound states increase. Several important key features:

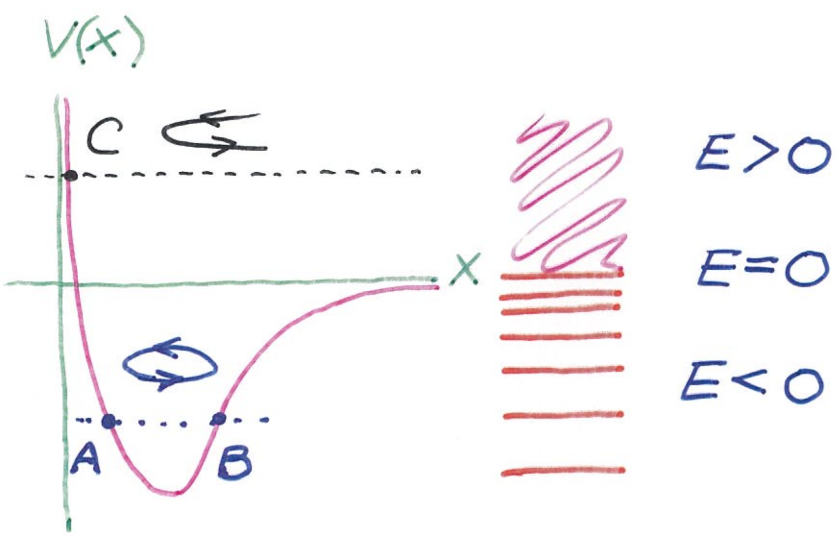
(1) Nodal Structure

(2) Quantum Leakage: it is possible to find the particle in the classically forbidden regime !!

(3) The decaying solution does exist !!

Particle in General Potential

Consider a particle moving in the potential (shown in the left).



Classically

(1) Bounded motion for $E<0$.
The particle moving between two turning points.

(2) Unbounded motion for $E \geqslant 0$
The particle moves inward until the turning point. Then, it changes direction and moves out to infinity.

Turning Point:

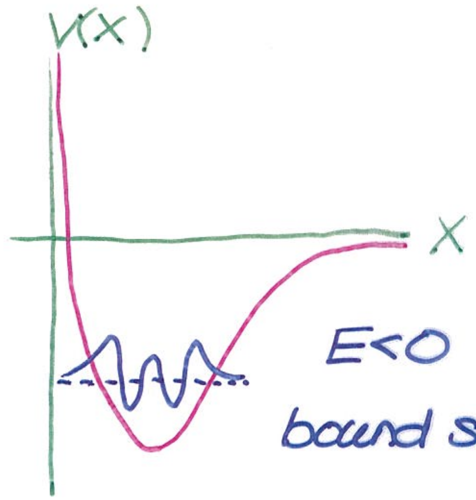
$$\cancel{\frac{p^2}{2m}}^{\,0} + V(x) = E$$

momentum is zero

$$\Rightarrow \quad V(x_c) = E$$

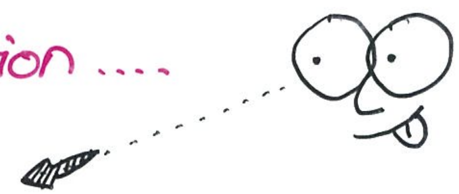
1 turning point for open orbits.
2 turning points for closed orbits.

What's new is quantum physics ??

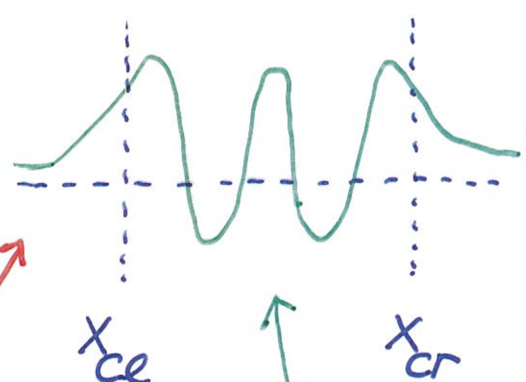


(1) For $E<0$, bound state with discrete energy levels. The typical wave fn is shown on the left.

Look closer into the details of the wave function ....



Solving for the exact wave function can be a true challenge... BUT !! It's quite easy to get a rough idea about the shape of wave function.



decay w.f.

$\psi(x) \sim e^{-\alpha x}$

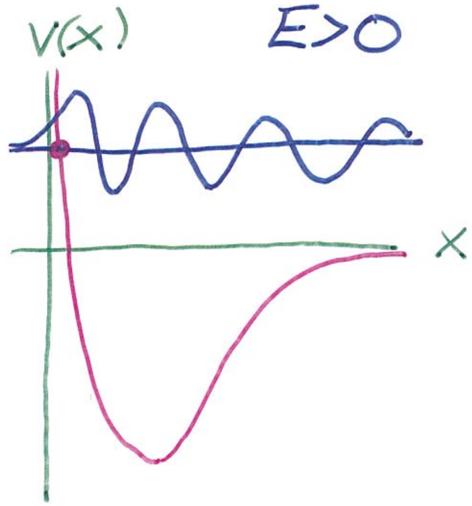
decay w.f.

$\psi(x) \sim e^{\alpha x}$

oscillatory w.f.

$\psi(x) \sim e^{ikx} + e^{-ikx}$

Continuum ....



3.

(2) For $E>0$, continuum with continuous energy levels. Again, one can get a rough idea about wave function easily.

Observation:

$$\frac{p^2}{2m} + V(x) = E \Rightarrow \text{position-dependent momentum}$$

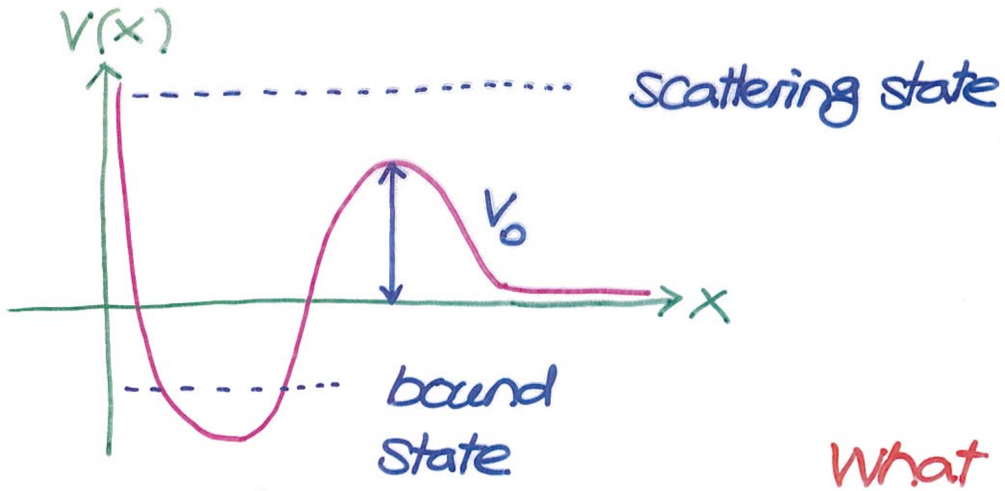
$$p(x) = \pm\sqrt{2m[E-V(x)]}$$

Thus, we can construct the wave function:

$$\psi(x) \sim A\, e^{ik(x)x} + B\, e^{-ik(x)x} = A' \sin[k(x)x + \delta]$$

where the position-dep $p(x) = \hbar k(x)$ and δ is the phase shift.

Quantum Tunneling



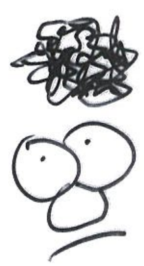
Consider the potential profile.

It's clear that ....

(1) $E<0$ bound state

(2) $E>V_0$ Scattering state

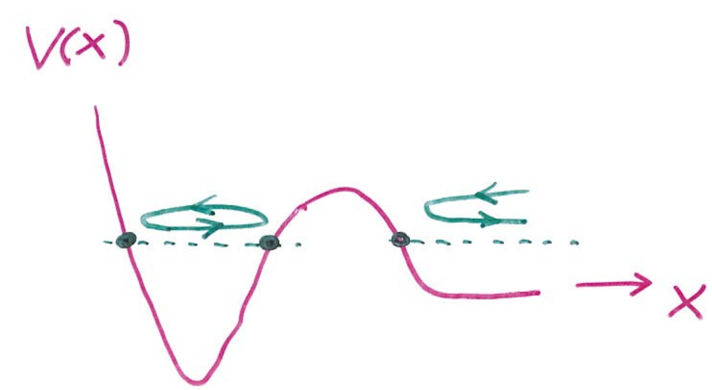
What about the range $0<E<V_0$?



Think, think, think.... Classically, we still find either

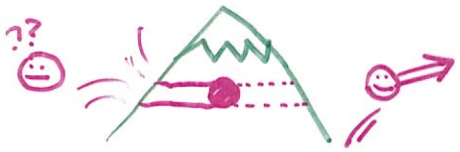
(1) 2 turning points, OR, (2) 1 t.p.

Depending on the initial condition, the particle can be inside the trap with closed orbit, or outside the trap with open orbit !!



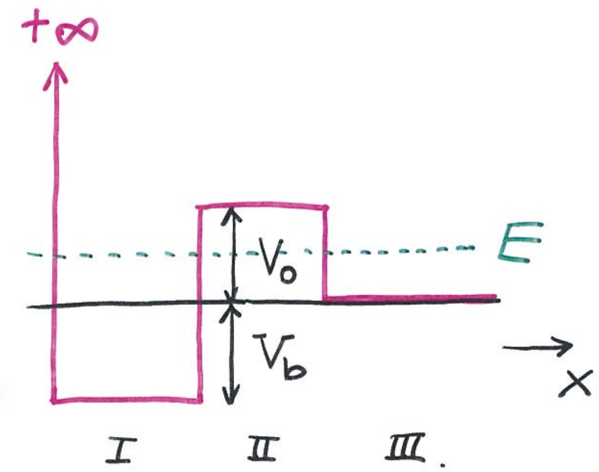
5.

Again, what about quantum mechanics?



Let's simplify the question a bit ☺

We can write down the wave function easily.



$$\psi_{I}(x) = A\,e^{ikx} + B\,e^{-ikx}$$

$$\psi_{II}(x) = C\,e^{-\alpha x} + D\,e^{\alpha x}$$ ← quantum surprise!!

$$\psi_{III}(x) = E\,e^{ik'x} + F\,e^{-ik'x}$$

The momentum in regimes I & III is

$$\frac{p^2}{2m} + (-V_b) = E \qquad p = \sqrt{2m(E+V_b)} \qquad \text{regime I.}$$

$$\frac{p^2}{2m} + 0 = E \qquad p' = \sqrt{2mE} \qquad \text{regime III.}$$

6.

In regime II, the "negative energy" state is

$$\frac{p^2}{2m} + V_0 = E \quad \Rightarrow \quad \frac{p^2}{2m} = E - V_0 < 0 \quad !!$$

$$\frac{p^2}{2m} = -(V_0 - E), \qquad p = \pm i\sqrt{2m(V_0 - E)}$$

Thus, the decaying parameter $\alpha = ip = \pm\sqrt{2m(V_0 - E)}$

$$\psi_{II}(x) = C e^{ipx} + D e^{-ipx} = C e^{-\alpha x} + D e^{\alpha x}$$

☆ Note that, it is impossible to find the particle in regime II in classical limit. However, in quantum mechanics, an imaginary momentum is meaningful and gives rise to the spatially decaying solutions !!

☆ The presence of these decaying states give quantum tunneling !!

Quantum Tunneling !!

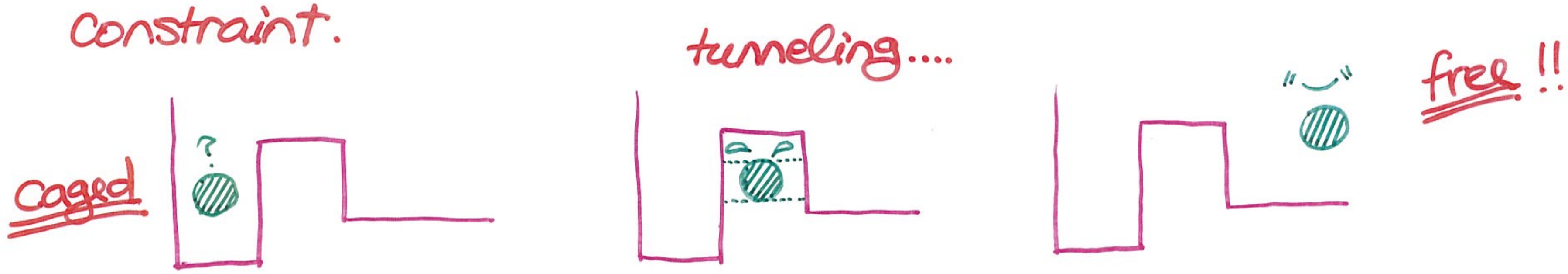
Let's look at the wave function again.

$$\psi_{I}(x) = A e^{ikx} + B e^{-ikx}$$

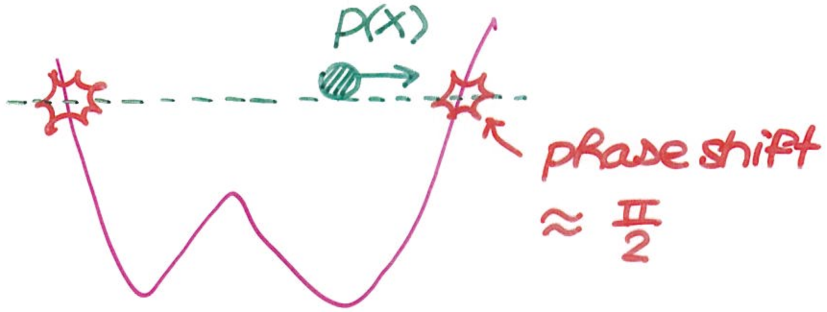
$$\psi_{II}(x) = C e^{-\alpha x} + D e^{\alpha x}$$

$$\psi_{III}(x) = E e^{ik'x} + F e^{-ik'x}$$

By matching the boundary conditions, $(\psi, \frac{d\psi}{dx})$ must be continuous $\Rightarrow$ 4 constraints. plus 1 constraint at $x=0$ $[\ \psi_{I}(0) = 0\ ]$. We can solve the constants. Remember the normalization condition gives the final 1 constraint.



Semiclassical Approximation

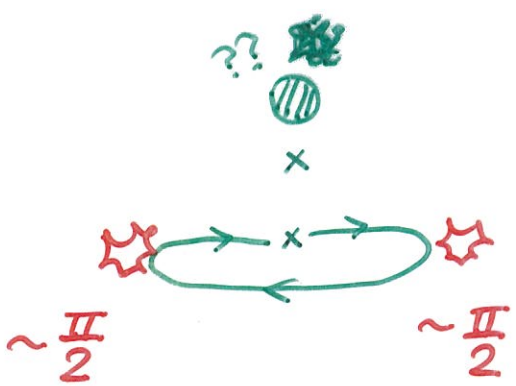


The first cute notion is $p(x)$ — the position-dependent momentum.

$$\frac{p^2}{2m} + V(x) = E, \qquad \text{smooth } V(x).$$

$$p^2(x) = 2m\left[E - V(x)\right] > 0 \quad \Rightarrow \quad p(x) = \pm\sqrt{2m\left[E - V(x)\right]}$$

The second cute notion is constructive self interference.



$$\frac{1}{\hbar}\oint p(x)\,dx - \varphi_s = 2n\pi, \qquad \varphi_s = \text{scattering phase}$$

$$\frac{1}{\hbar}\oint p(x)\,dx = 2n\pi + \varphi_s$$

$$\oint \sqrt{2m\left[E - V(x)\right]}\,dx = \hbar\,(2n\pi + \varphi_s)$$

$$\varphi_s \approx \frac{\pi}{2} + \frac{\pi}{2} = \pi$$

$$\Rightarrow \quad \oint \sqrt{2m\left[E - V(x)\right]} = 2\pi\hbar\left(n + \frac{1}{2}\right)$$

9.

A simple check.....

Does the semiclassical approximation makes sense at all ?

Let's check.... The position-dependent momentum $p(x)$ implies the wave function takes the form,

$$\psi(x,t) \approx e^{i[k(x)x-\omega t]} \qquad p(x) = \hbar k(x) = \sqrt{2m(E-V)}$$

check. ✓ $\frac{\partial \psi}{\partial t} = (-i\omega)\, e^{i(kx-\omega t)} = (-i\omega)\,\psi$

$$\frac{\partial \psi}{\partial x} = i\left(k + \frac{dk}{dx}x\right) e^{i(kx-\omega t)} = i\left(k+\frac{dk}{dx}x\right)\psi$$

$$\frac{\partial^2 \psi}{\partial x^2} = i\left(\frac{dk}{dx} + \frac{d^2k}{dx^2}x + \frac{dk}{dx}\right) e^{i(kx-\omega t)} + (i)^2\left(k+\frac{dk}{dx}x\right)^2 e^{i(kx-\omega t)}$$

$$= \left[-\left(k+\frac{dk}{dx}x\right)^2 + i\left(2\frac{dk}{dx} + \frac{d^2k}{dx^2}x\right)\right]\psi$$

Note that $\frac{dk}{dx} = \frac{1}{\hbar}\frac{dp}{dx} = \frac{1}{\hbar}\frac{-2m\frac{dV}{dx}}{2\sqrt{2m(E-V)}} \propto \frac{dV}{dx}$!! Thus, for smooth potential, we can drop all derivatives ☺

After dropping all spatial derivatives ....

$$\frac{\partial\psi}{\partial t} = (-i\omega)\,\psi \qquad \frac{\partial^2\psi}{\partial x^2} \approx -k^2\,\psi$$

plug in the Schrödinger equation $\Rightarrow$ $i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V\psi$

$$\text{left} = i\hbar\frac{\partial\psi}{\partial t} = (i\hbar)(-i\omega)\,\psi = \hbar\omega\,\psi = E\,\psi.$$

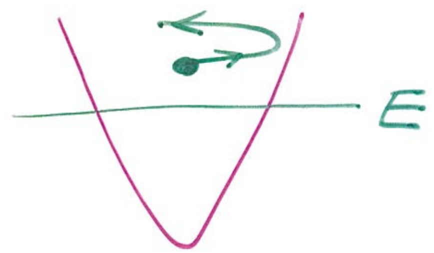
$$\text{right} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V\psi = \left[-\frac{\hbar^2}{2m}(-k^2) + V\right]\psi = \left[\frac{p^2}{2m} + V\right]\psi$$

$$= \left[\frac{\left(\sqrt{2m(E-V)}\right)^2}{2m} + V\right]\psi = \left[(E-V) + V\right] = E\,\psi.$$

The left = right $\Rightarrow$ Schrödinger equation is satisfied. Thus, as long as the potential is smooth, one can use the semiclassical approximation to compute the discrete bound-state energy.

Q: How "smooth" is smooth? Huh?

Try a simple example.



Consider a parabollic potential $V(x) = \frac{1}{2}kx^2$.

The Schrödinger equation is

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + \frac{1}{2}kx^2\psi = E\psi$$

The above differential equation certainly looks unfriendly. At least, to freshman....

Let's try to solve it by the semiclassical approach.

$$\oint p(x)\,dx = \hbar\,(2n\pi + \varphi_s) \quad \Rightarrow \quad \oint \sqrt{2m(E-V)}\,dx = 2\pi\hbar\,(n+\tfrac{1}{2})$$

How nice !! We only need to compute a simple integral.

$$\oint p(x)\,dx = 2\int_{-x_c}^{x_c} \sqrt{2mE - mkx^2}\,dx, \qquad \pm x_c: \text{turning points}$$

Some algebra....

$$\frac{1}{2}kx_c^2 = E \qquad x_c^2 = \frac{2E}{k}$$

$$2\int_{-x_c}^{x_c}\sqrt{2mE - mkx^2}\,dx = 2\sqrt{mk}\int_{-x_c}^{x_c}\sqrt{\frac{2E}{k} - x^2}\,dx$$

$$= 2\sqrt{mk}\int_{-x_c}^{x_c}\sqrt{x_c^2 - x^2}\,dx$$

change variabe $\ddot{\smile}$ $\quad x = x_c \sin\theta \qquad dx = x_c\cos\theta\, d\theta$

$$\begin{cases} x = x_c \rightarrow \theta = \frac{\pi}{2} \\ x = -x_c \rightarrow \theta = -\frac{\pi}{2} \end{cases}$$

$$= 2\sqrt{mk}\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} x_c\sqrt{1 - \sin^2\theta}\,(x_c\cos\theta\, d\theta)$$

$$= 2\sqrt{mk}\, x_c^2\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}}\cos^2\theta\, d\theta = 2\sqrt{mk}\,\frac{2E}{k}\cdot(\text{integral})$$

$$= \sqrt{\frac{m}{k}}\cdot 4E\cdot(\text{integral}) = \frac{4E}{\omega}\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}}\cos^2\theta\, d\theta$$

Now the integral ...  a piece of cake 

13.

$$\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \cos^2\theta \, d\theta = \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \frac{1+\cos 2\theta}{2} \, d\theta = \frac{\theta}{2}\Big|_{-\frac{\pi}{2}}^{\frac{\pi}{2}} + \underbrace{\cancel{\frac{1}{4}\sin 2\theta\Big|_{-\frac{\pi}{2}}^{\frac{\pi}{2}}}}_{0} = \frac{\pi}{2}$$

Finally, combine every pieces together....

$$\frac{\cancel{4}^{\,2}E}{\omega} \cdot \frac{\pi}{\cancel{2}} = \cancel{2}\pi\hbar\left(n+\frac{1}{2}\right) \Rightarrow \quad E_n = \hbar\omega\left(n+\frac{1}{2}\right)$$

☆ For a simple harmonic oscillator, the "allowed" energy is no longer continuous. In fact, the energy is quantized in unit of $\hbar\omega = h\nu$ — very similar to Einstein's notion for photons !!

charged particle

EM wave $= \underbrace{\hbar\omega + \hbar\omega + \cdots + \hbar\omega}_{N \text{ photons}}$

$= N\hbar\omega$

☆ The residual $\frac{1}{2}$ comes from .....

— Heisenberg uncertainty principle !!

The End