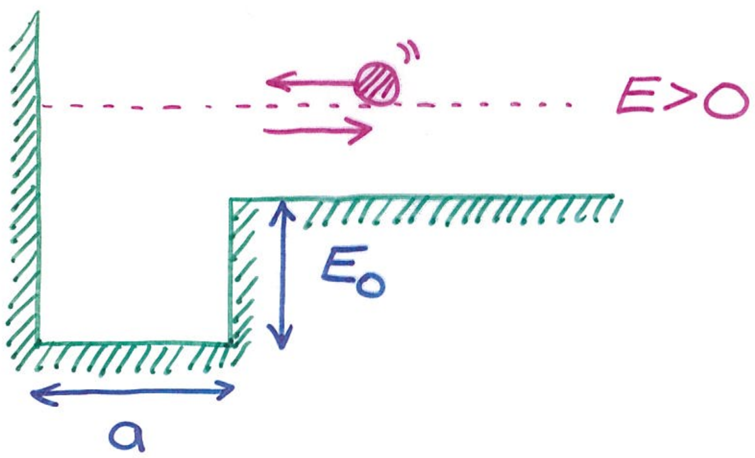
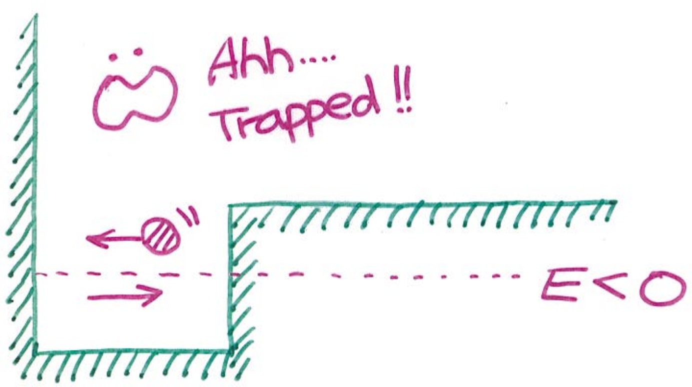
HH0135 - Quantum Tunnelling

Finite Potential Well

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





In region I :

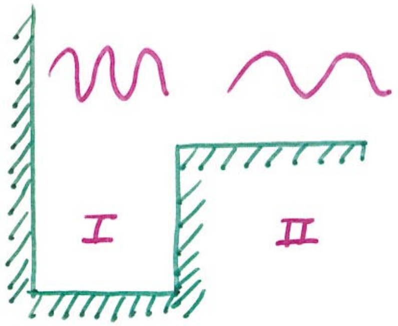
$$-\frac{\hbar^2}{2m}\frac{d^2\psi_I}{dx^2} - E_0\psi_I = E\psi_I$$

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

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

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

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:

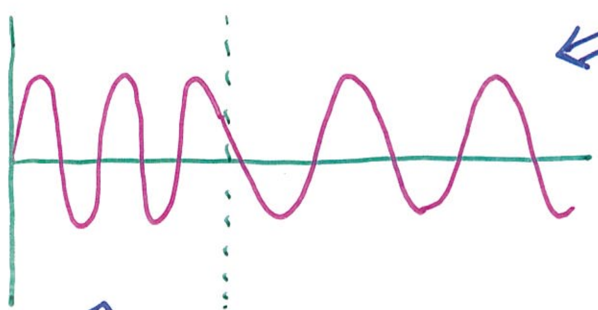
$$\frac{C\sin(k_I a)}{C k_I\cos(k_I a)} = \frac{C'\sin(k_{II}a+\delta)}{C' k_{II}\cos(k_{II}a+\delta)} \Rightarrow \frac{1}{k_I}\tan(k_I a) = \frac{1}{k_{II}}\tan(k_{II}a+\delta)$$

☆ 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 ??



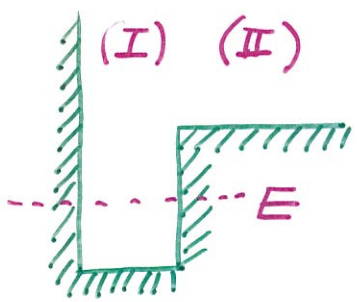
$\Leftarrow \quad \psi_{II}(x) = C' \sin(k_{II} x + \delta)$

$\Uparrow$

$\psi_I(x) = C \sin(k_I x)$

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

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

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:

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

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

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 $|E| = \mathcal{E}$

$$\hbar k_I = \sqrt{2m(E_0 - \mathcal{E})} \qquad \Rightarrow \qquad \hbar^2 k_I^2 = 2mE_0 - 2m\mathcal{E}$$

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

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

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.

energy is quantized !!

$$y = k_I a$$

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

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

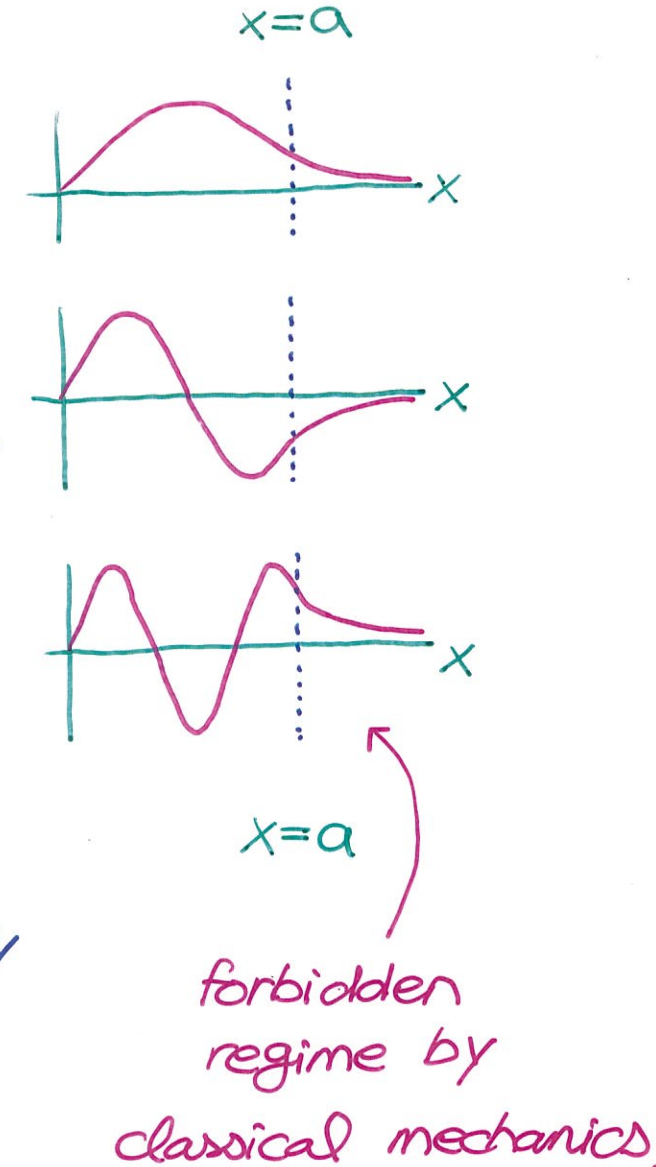
One can read off the minimum λ for the bound state to exist.

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

Quantum Leakage.

From the matching B.C.

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



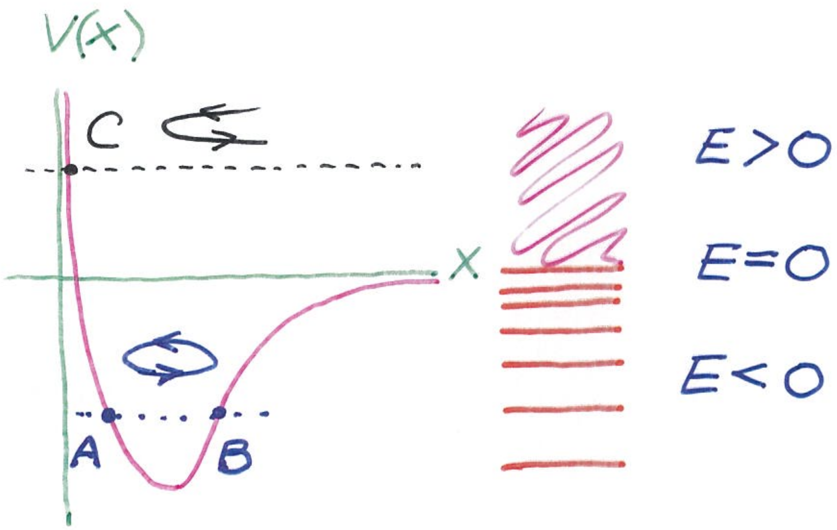
For steeper potential well, the number of bound states increase. Several important key features:

(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 $E \geq 0$
The particle moves inward until the turning point. Then, it changes direction and moves out to infinity.

Turning Point:

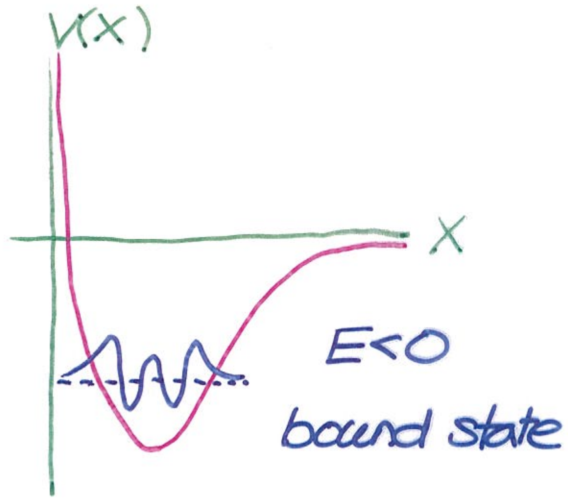
$$\cancelto{0}{\frac{p^2}{2m}} + V(x) = E$$

momentum is zero

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

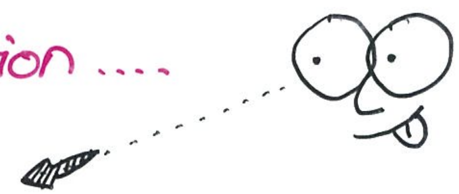
1 turning point for open
2 turning points for closed
orbits.

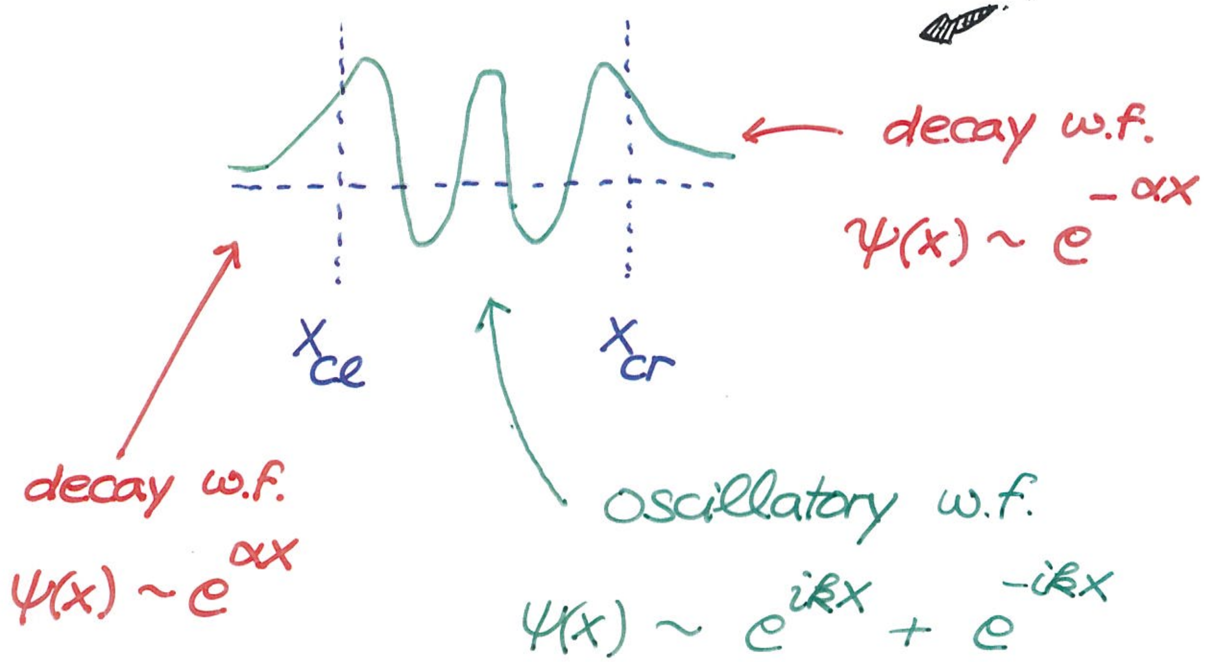
What's new is quantum physics ??



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

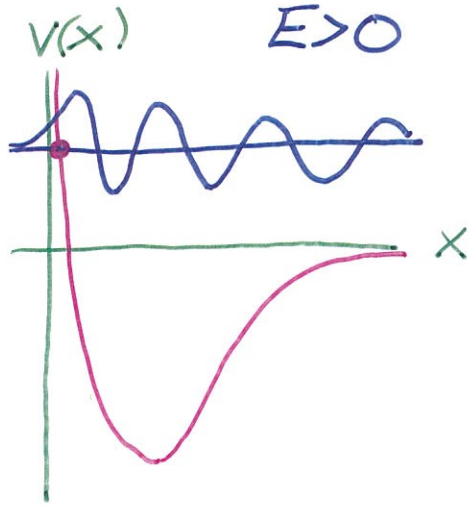
Look closer into the details of the wave function ....





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.

Continuum ....



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

Observation:

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

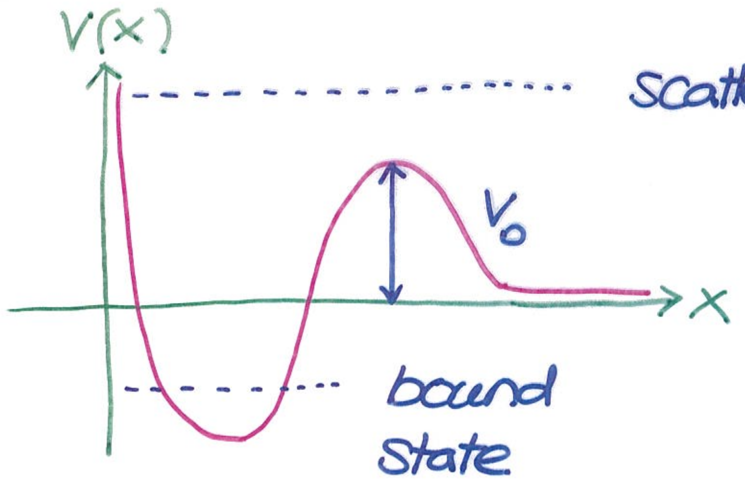
$$p(x) = \pm\sqrt{2m[E-V(x)]}$$

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

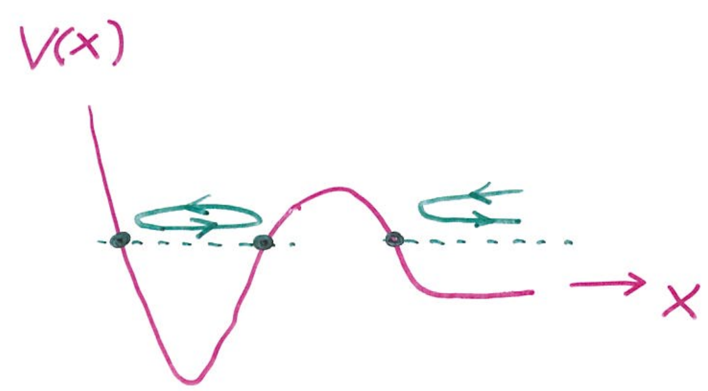
(2) $E > V_0$ Scattering state

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

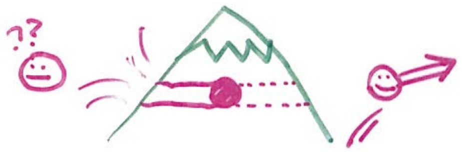
Think, think, think.... Classically, we still find either

(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 !!

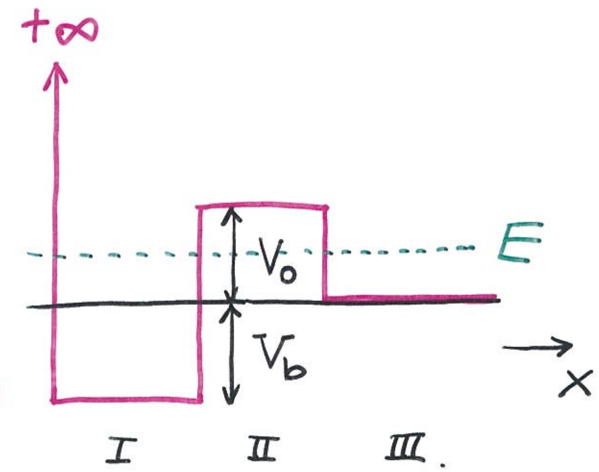


Again, what about quantum mechanics ?



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

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

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

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 !!

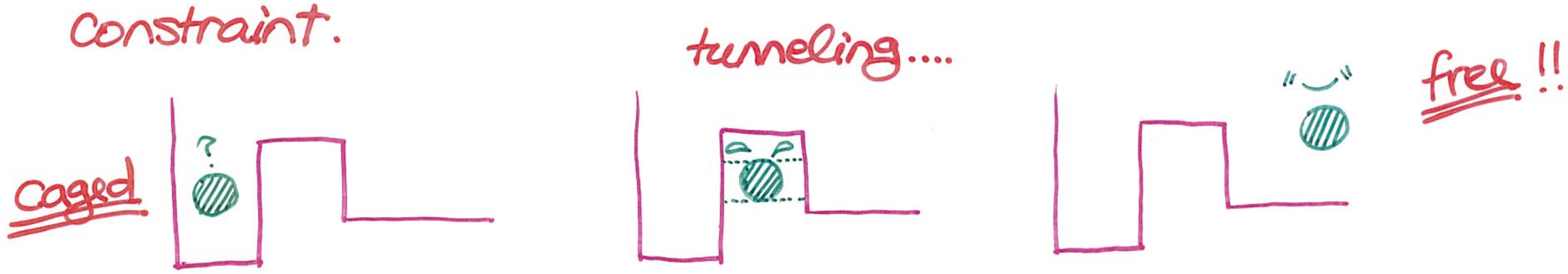
Let's look at the wave function again.

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

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

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

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.



The End