PHY2001
Quantum and Statistical Physics

Quantum Mechanics
Part-2

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Week 5-7 : Contents

1. Potential Step
2. Potential Barrier
3. Examples of quantum tunneling
4. T.I.S.E. in 2D and 3D
5. Hydrogen atom

Learning outcomes:

- To formulate solutions for matter waves in different potential functions, using boundary conditions and to obtain reflection and transmission probabilities.
- To be able to describe qualitatively and quantitatively physical examples of tunneling.
- To be able to understand the concept of degeneracy, quantum states of H-like atoms.

Textbooks - Quantum Mechanics

- Recommended – Quantum Mechanics (2nd edition) by Robert Eisberg and Robert Resnick, QC174.12 EISB

A quick overview…

Schrödinger Equation : $\hat{E}\,\Psi(r,t) = \hat{H}\,\Psi(r,t)$

- in 3D and time: $i\hbar\,\dfrac{\partial\Psi(r,t)}{\partial t} = V(r,t)\,\Psi(r,t) - \dfrac{\hbar^2}{2m}\,\nabla^2\Psi(r,t)$

- in 1D and time: $i\hbar\,\dfrac{\partial\Psi(x,t)}{\partial t} = V(x,t)\,\Psi(x,t) - \dfrac{\hbar^2}{2m}\,\dfrac{\partial^2\Psi(x,t)}{\partial x^2}$

General solution : $\Psi(x,t) = \psi(x)\,\phi(t) = \psi(x)\;e^{-iwt} = \psi(x)\,e^{-iEt/\hbar}$

$\Psi(x,t)$ is called wave function, $\psi(x)$ is called eigen function.

Schrödinger Equation,

- time independent & 1D:

(when V doesnot explicitly depends on time)

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

$$\Rightarrow \frac{\hbar^2}{2m}\,\frac{d^2\psi(x)}{dx^2} + [E - V(x)]\,\psi(x) = 0$$

A quick overview…

- **Eigen functions should be well-behaved:**

  i.e. both $\psi(x,t)$ and $d\psi(x)/dx$ should be finite, single valued & continuous

- **As T.I.S.E.** *(time-independent Schrodinger equation)* **doesnot contain $\boldsymbol{i}$,** eigen function is not necessarily complex, some examples:

  $$\psi(x) = A\sin(kx) + B\cos(kx),$$

  $$\psi(x) = A\exp(ikx) + B\exp(-ikx)$$

- **Wave function contain all the information** *that the uncertainty principle will allow us to learn* **about the associated particle**.

- **How? – Using quantum mechanical operators:**

  $$\langle G\rangle = \int_{-\infty}^{\infty} \Psi^* \, \hat{G} \, \Psi \, dx = \int_{-\infty}^{\infty} \psi^* \, \hat{G} \, \psi \, dx \ (\textit{if } \hat{G} \textit{ is time independent})$$

  Example: $\hat{x} = x; \quad \hat{p} = -i\hbar\frac{\partial}{\partial x}; \quad \hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V; \quad \hat{E} = i\hbar\frac{\partial}{\partial t}$

Typical method for solving a quantum mechanical problem using T.T.S.E :

- Define the potential $V(x)$ and regions of interest.
- Write down the T.I.S.E. for diff regions.
- Define a general form of the eigen function for each region

  (make sure the function do not diverge at any x)

- Apply boundary conditions :

  $\psi(x)$ and $\frac{d\psi(x)}{dx}$ are continuous at boundaries

- Apply normalisation to the eigen function :

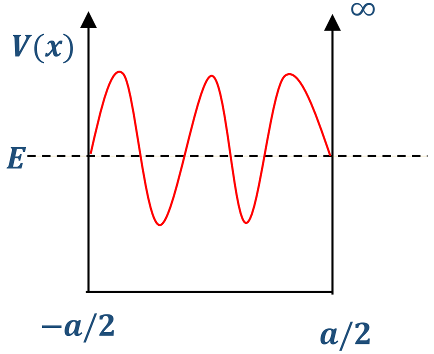
  $\int_{-\infty}^{\infty} \psi^*(x)\psi(x)dx = \int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1$

and some algebra…

Some basic quantum mechanical problems:

(single particle in different types of potential functions)

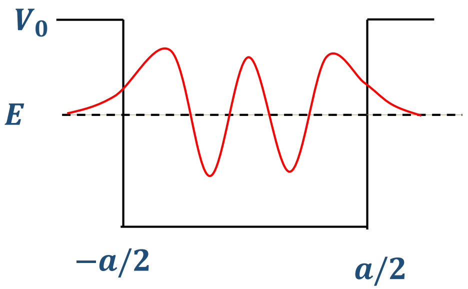
Infinite square well



- Nodes of the eigen functions at the wall
- Discrete energy levels : $E = \frac{\pi^2 \hbar^2}{2ma^2} n^2, n = 1,2,3, \dots$

  (energy quantisation)

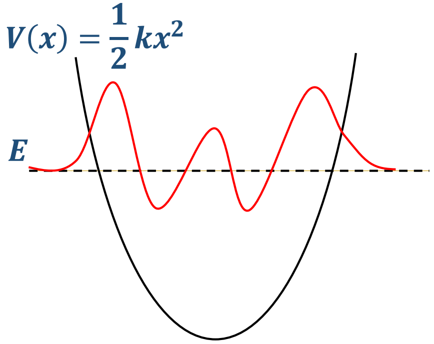
Finite square well



- Finite probability outside the wall
- Discrete energy levels, slightly less than the respective energy levels for infinite well, satisfied by

$$k \tan \frac{ka}{2} = \sqrt{\beta^2 - k^2}, \;\; k = \sqrt{\frac{2mE}{\hbar^2}} ; \beta = \sqrt{\frac{2mV_0}{\hbar^2}}$$

Simple harmonic Oscillator

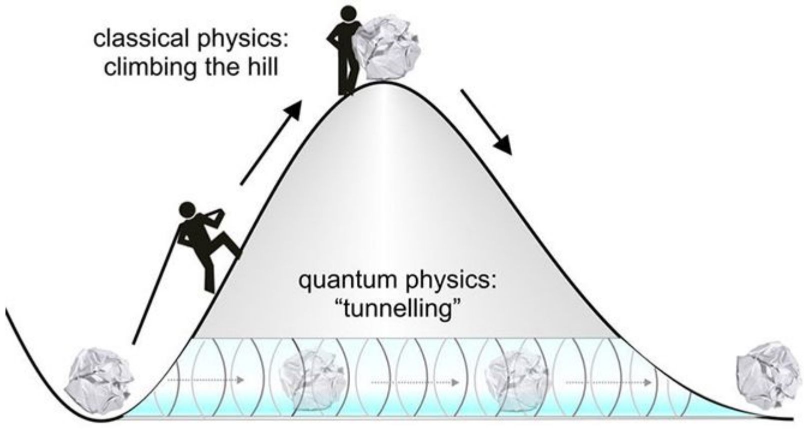


- Finite probability outside the wall
- Discrete energy levels, equally spaced,

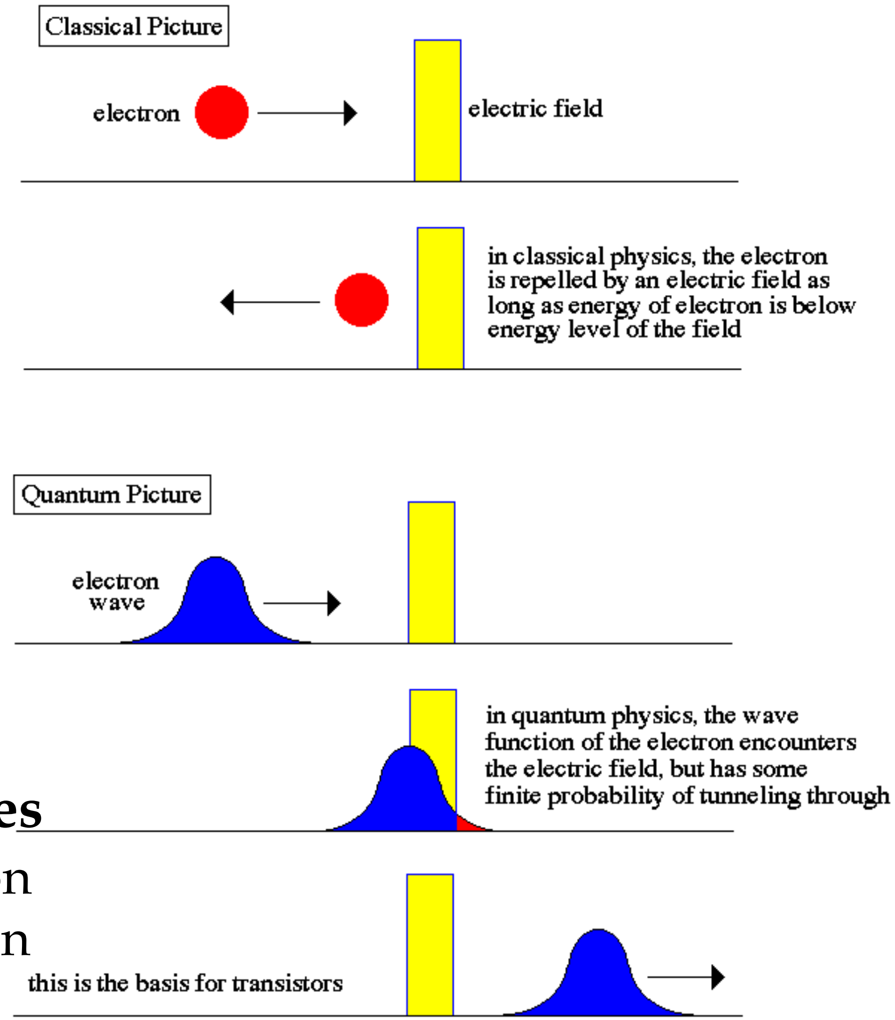
$$E = \frac{1}{2}\hbar\omega + n\hbar\omega, \qquad \text{where } n = 0,1,2,3, \dots$$

- Zero point energy : $E_0 = \frac{1}{2}\hbar\omega \neq 0$

Steps and barriers : Quantum Tunnelling



https://www.youtube.com/watch?v=cTodS8hkSDg



Classically,

- if $E < V$, 100% reflection
- if $E > V$, 100% transmission

In quantum world, particles are waves

- if $E < V$, partial reflection/transmission
- if $E > V$, partial reflection/transmission

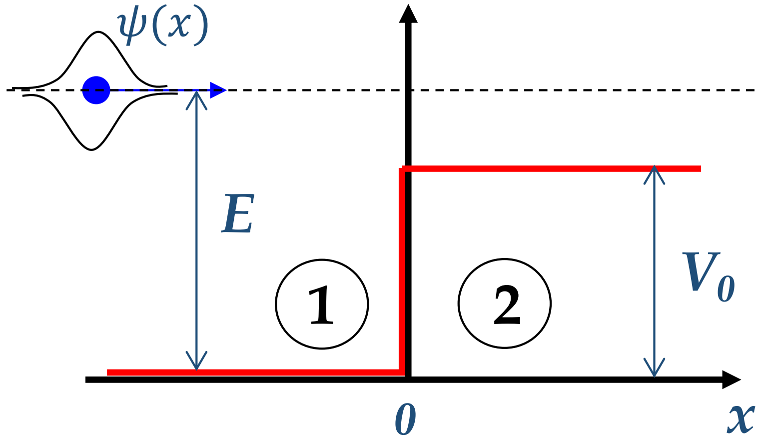
Java applet: https://phet.colorado.edu/en/simulation/legacy/quantum-tunneling

https://www.youtube.com/watch?v=RF7dDt3tVmI&t=0s&list=PLkyBCj4JhHt-80ttR5a_fwtFO4SwDAFld&index=2

Part-1
Potential Steps

Potential step : E > V_0

Aim: to find out reflection and transmission coefficients



- **define potential :**

$$V(x) = 0 \quad if\ x < 0 \quad \text{: Region 1}$$
$$= V_0 \quad if\ x > 0 \quad \text{: Region 2}$$

Region 1 | **Region 2**

- **write down T.I.S.E :**

$$\frac{\hbar^2}{2m}\frac{d^2\psi_1(x)}{dx^2} + E\,\psi_1(x) = 0$$

$$\frac{\hbar^2}{2m}\frac{d^2\psi_2(x)}{dx^2} + [E - V_0]\,\psi_2(x) = 0$$

- **define general expression for the eigen function :**

$$\psi_1(x) = \underbrace{A\exp(ik_1x)}_{+x} + \underbrace{B\exp(-ik_1x)}_{-x}$$

$$\psi_2(x) = \underbrace{C\exp(ik_2x)}_{+x} + \cancel{D\underbrace{\exp(-ik_2x)}_{-x}}$$

moving along: $+x$ $\quad$ $-x$ $\quad$ $+x$ $\quad$ $-x$

where, $k_1 = \sqrt{\frac{2mE}{\hbar^2}}$

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

A & B are amplitudes (constants)

C & D are amplitudes (constants); $\quad D = 0$

c.f. $\psi_1(x) = \underbrace{A\exp(ik_1x)}_{\text{incident}} + \underbrace{B\exp(-ik_1x)}_{\text{reflected}}$ $\psi_2(x) = \underbrace{C\exp(ik_2x)}_{\text{transmitted}}$

- **apply boundary conditions to find A, B & C:**

  ✓ $\psi_1(x)|_{x=0} = \psi_2(x)|_{x=0} \quad \Rightarrow \quad A + B = C$

  ✓ $\left.\frac{d\psi_1(x)}{dx}\right|_{x=0} = \left.\frac{d\psi_2(x)}{dx}\right|_{x=0} \quad \Rightarrow \quad Ak_1 - Bk_1 = Ck_2$

- **with some algebra, you can find**

$$\frac{B}{A} = \frac{k_1 - k_2}{k_1 + k_2} \quad \text{and} \quad \frac{C}{A} = \frac{2k_1}{k_1 + k_2}$$

- **now, reflection and transmission coefficient. What are they?**

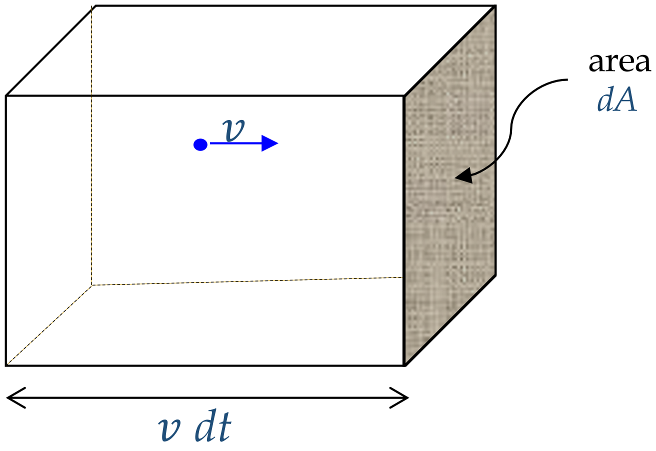
  For ex. in case of light, they are the ratio of intensities.

  For particles, they are the ratio of particle fluxes.

  In quantum mechanics, they are the ratio of ***"probability fluxes"***

probability flux or *probability current* $J(x)$

: the rate at which probability is 'flowing' past a point x



If the particle is somewhere within this volume, then by the time dt it will definitely cross the volume.

Probability per unit volume = $\Psi^*\Psi = \psi^*\psi = |\psi|^2$

Volume of the parallelepiped $= v\ dt\ dA$

$\Rightarrow$ probability of this particle crossing the surface dA

$$= |\psi|^2\ v\ dt\ dA$$

$\Rightarrow$ the probability per unit time per unit area

$$= J = v\ |\psi|^2 = \frac{p}{m}\ |\psi|^2 = \frac{\hbar k}{m}\ |\psi|^2$$

Coming back to our problem…

Incident wave: $\psi_i = A\exp(ik_1 x)$

So, incident flux : $J_I = \frac{\hbar k_1}{m}|\psi_I|^2$

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

Region 1

Similarly,

reflected flux : $J_R = \frac{\hbar k_1}{m}|\psi_R|^2$

$$= \frac{\hbar k_1}{m}B^2$$

transmitted flux : $J_T = \frac{\hbar k_2}{m}|\psi_T|^2$

$$= \frac{\hbar k_2}{m}C^2$$

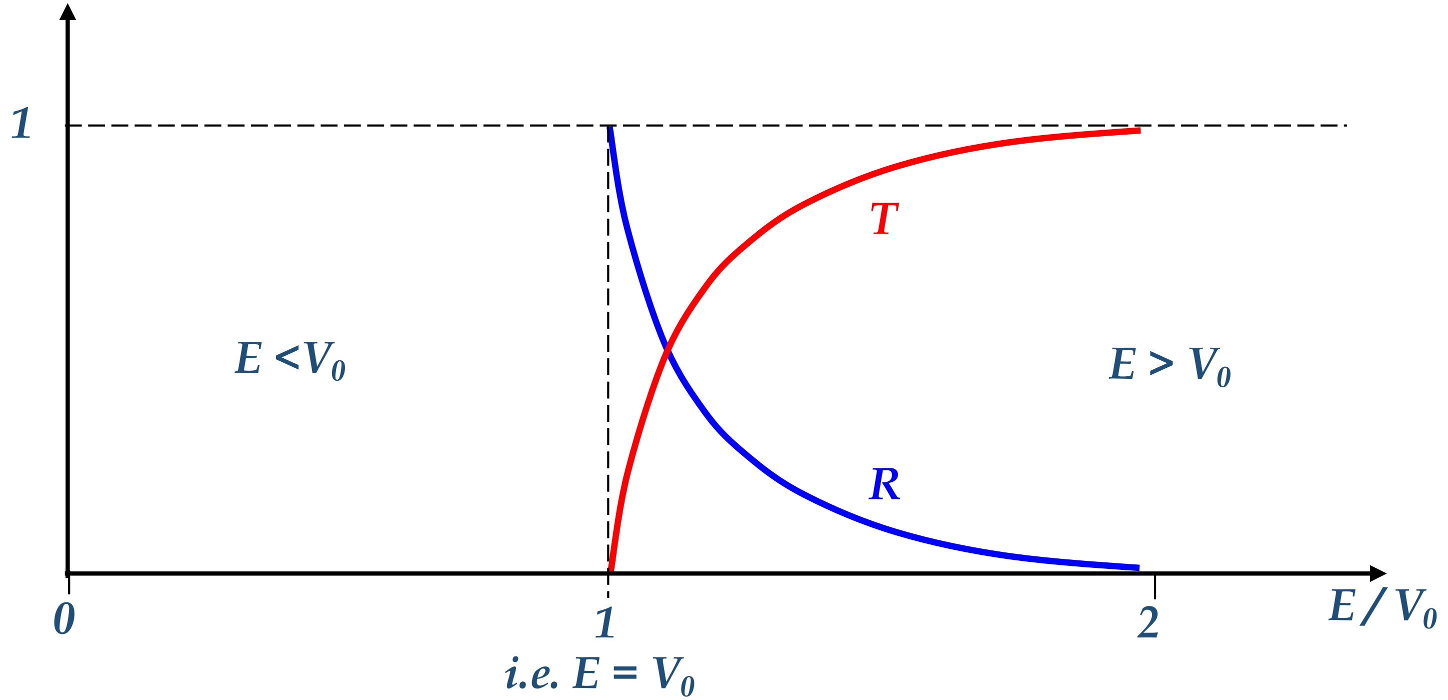
Region 2

and,

Reflection coefficient: $R = \frac{J_R}{J_I} = \frac{B^2}{A^2}$

Transmission coefficient: $T = \frac{J_T}{J_I} = \frac{k_2}{k_1}\frac{C^2}{A^2}$

Hence, $R = \frac{J_R}{J_I} = \frac{B^2}{A^2} = \left(\frac{k_1 - k_2}{k_1 + k_2}\right)^2$ and, $T = \frac{J_T}{J_I} = \frac{k_2}{k_1}\frac{C^2}{A^2} = \frac{4k_1 k_2}{(k_1 + k_2)^2}$

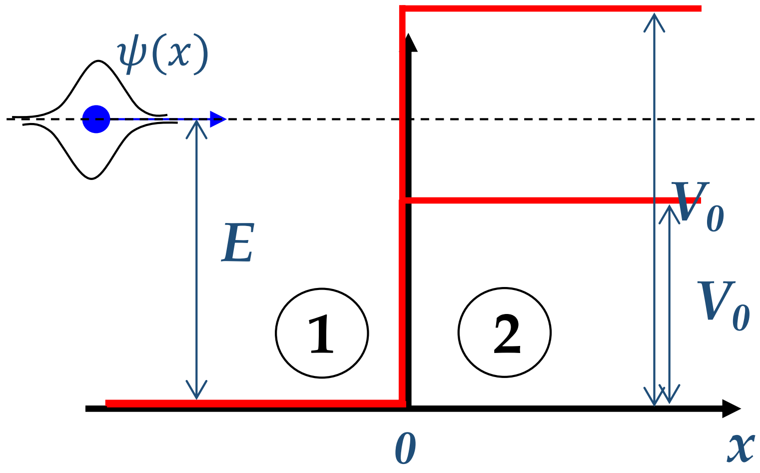


Note that $R + T = 1$, which is also true in this case (you can check ☺)

This analysis is very similar to other physical situations where waves approach a boundary. For an example, light incident normally on an interface between two media with different refractive indices.

Potential step : $E < V_0$

Aim: to find out reflection and transmission coefficients



- **define potential :**

$$V(x) = 0 \quad if\ x < 0 \quad \text{: Region 1}$$
$$= V_0 > E \quad if\ x > 0 \quad \text{: Region 2}$$

Region 1 | **Region 2**

- **write down T.I.S.E :**

Note, in this case, $[E\text{-}V_0]$ is -ve

$$\frac{\hbar^2}{2m}\frac{d^2\psi_1(x)}{dx^2} + E\,\psi_1(x) = 0$$

$$\frac{\hbar^2}{2m}\frac{d^2\psi_2(x)}{dx^2} + [E - V_0]\,\psi_2(x) = 0$$

- **define general expression for the eigen function :**

$$\psi_1(x) = A\exp(ik_1x) + B\exp(-ik_1x)$$

where, $k_1 = \sqrt{\frac{2mE}{\hbar^2}}$

A & B are amplitudes (constants)

$$\psi_2(x) = C\exp(ik_2x) + D\exp(-ik_2x)$$

where, $k_2 = \sqrt{\frac{2m(E-V_0)}{\hbar^2}} = i\sqrt{\frac{2m(V_0-E)}{\hbar^2}} = ik_2'$

C & D are amplitudes (constants)

Hence, we can rewrite the wavefunctions as

$$\psi_1(x) = \underbrace{A\exp(ik_1x)}_{\substack{+x \\ \text{Incident wave}}} + \underbrace{B\exp(-ik_1x)}_{\substack{-x \\ \text{Reflected wave}}} \qquad \psi_2(x) = \underbrace{C\exp(-k_2'x)}_{\substack{\textit{Exponential decay} \\ \text{Transmitted}}} + \cancel{\underbrace{D\exp(k_2'x)}_{\textit{Exponential growth}}}$$

moving along:

No oscillations here!

- **apply boundary conditions to find A, B & C:**

✓ $\psi_1(x)|_{x=0} = \psi_2(x)|_{x=0} \quad \Rightarrow \quad A + B = C$

✓ $\left.\frac{d\psi_1(x)}{dx}\right|_{x=0} = \left.\frac{d\psi_2(x)}{dx}\right|_{x=0} \quad \Rightarrow \quad Aik_1 - Bik_1 = -Ck_2' \qquad \Rightarrow \quad A - B = \frac{ik_2'}{k_1}C$

- **with some algebra, you can find**

$$\frac{B}{A} = \frac{k_1 - ik_2'}{k_1 + ik_2'} \quad \text{and} \quad \frac{C}{A} = \frac{2k_1}{k_1 + ik_2'}$$

Same as the $E > V_0$ case, except, replacing k_2 by ik_2'

- **Hence, the reflection coefficient is**

$$R = \frac{J_R}{J_I} = \frac{B^2}{A^2} = \frac{|k_1 - ik_2'|^2}{|k_1 + ik_2'|^2} = 1$$

and hence $T = 0$

R=1, T = 0 : What does it mean ?

- analogous to reflection of light from an ideal mirror.
- Agrees with classical concept,

  i.e. if the particle has insufficient energy, will reflect back.
- However …

  the particle will have a finite probability of penetrating into the region $x > 0$

  (called "*penetration of the classically excluded region*")

Why? : $$\psi_2(x) = C\exp(-k_2'x) = \frac{2Ak_1}{k_1+ik_2'}\exp(-k_2'x)$$

Hence the probability of the particle in the region-2 will be

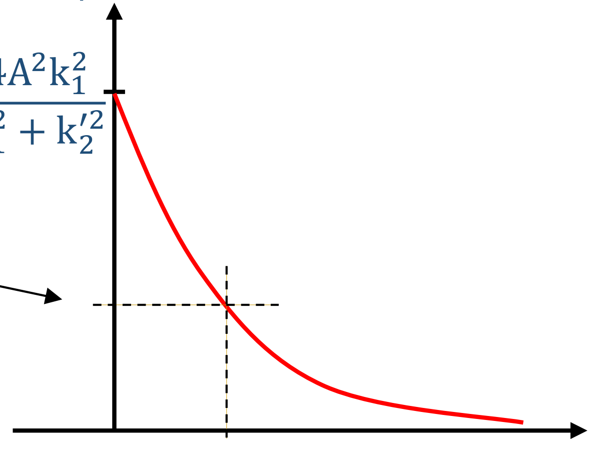
$$|\psi(x)|^2 = C^2\exp(-2k_2'x) = \underbrace{\frac{4\mathrm{A}^2\mathrm{k}_1^2}{\mathrm{k}_1^2+\mathrm{k}_2'^2}}_{\text{Real positive quantity}}\ \underbrace{\exp(-2k_2'x)}_{\text{Exponential Decay}}$$

Plotting $|\psi(x)|^2 = \frac{4A^2k_1^2}{k_1^2+k_2'^2} \exp(-2k_2'x)$

when $x = 1/2k_2'$, called "*penetration distance*" Δx

$|\psi(x)|^2$ drops to 1/e times the max.

Since $k_2' = \frac{\sqrt{2m[V_0-E]}}{\hbar} \Rightarrow \boxed{\Delta x = \frac{1}{2k_2'} = \frac{\hbar}{2\sqrt{2m[V_0-E]}}}$



which, for a macroscopic object Δx is infinitesimal ($\hbar$ too small).

Not too surprising… last time I tried, couldn't punch through a wall !!!

This penetration depth can also be regarded as the uncertainty in measuring the location of the particle.

- What about the particle energy in the region 2 ?

Using Heisenberg's Uncertainty principle,

$$\Delta p = \frac{\hbar}{2\Delta x} = \sqrt{2m[V_0 - E]},$$

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

i.e. it is no longer possible to say that the particle energy is less than the barrier – helps to overcome apparently violating conservation of energy.

Sometimes it is referred as '*Energy borrowing*'.

- Coming back to reflection and transmission coefficients…