PHY2001
Quantum and Statistical Physics

Quantum Mechanics
Part-2

Dr. Satya Kar
01.042, Main Physics Building
s.kar@qub.ac.uk; Phone : 3012

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

Over the last four weeks, you have been introduced with some basic concepts of Quantum mechanics and hopefully getting a good grasp of those. It is a different way of thinking about the particles and their behavior.

These are the topics we will cover in week 5-7, which lets say solving problems using the Schrodinger equation. The contains are a bit lengthy mathematical workouts, but once we know what we are trying to do, how we approach the problem, there is a simple template to solve it, rest is simple algebra.

A quick overview…

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

- in 3D and time:

$$i\hbar\frac{\partial\Psi(r,t)}{\partial t} = V(r,t)\,\Psi(r,t) - \frac{\hbar^2}{2m}\nabla^2\Psi(r,t)$$

- in 1D and time:

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

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)

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

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

- This should be quite familiar to you by now, the energy and the Hamiltonian operators, operating on the wavefunction of a particles, or a systems of particles.
- Note the potential V, which can be a function of time and space. This is the most important term in the Schrodinger equation that defines the problem, i.e. what is the situation/condition the particle (or the system of particles) is subjected to, which suffice to say what are the external forces acting on the system under observation. Call it the "Cause" and the wavefunction the "effect" – in a very poetic way.
- Now, the wavefunction is space and time dependent, but the space and time dependency can be exclusive, i.e. we can separate the two variables. The spatial part of the wavefunction $\psi(x)$, which does not depend on the time is called "eigen function". The time dependent part can be a simple oscillating term as $\phi(t) = e^{-i\omega t}$, which tells that the wave function is oscillating with time, with a frequency ω, which can be defined in terms of total energy : $\omega = 2\pi f = 2\pi\frac{E}{h} = E/\hbar$
- The spatial part of the wavefunction can be oscillating (next slide) in space, with a wavelength λ, that depends on the momentum as per the de-Broglie

formula $\lambda = \frac{h}{p}$. Hence we can express the wavenumber as

$k = \frac{2\pi}{\lambda} = \frac{2\pi}{h/p} = \frac{p}{\hbar}$. Then if we consider a non-relativistic particle, the p, the momentum of the particle can be related to the particle's kinetic energy, $k = \frac{p}{\hbar} = \sqrt{2m(E-V)}/\hbar$

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:**

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

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

- Again some basic points from the previous section, which are key to what we are going to do now.

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

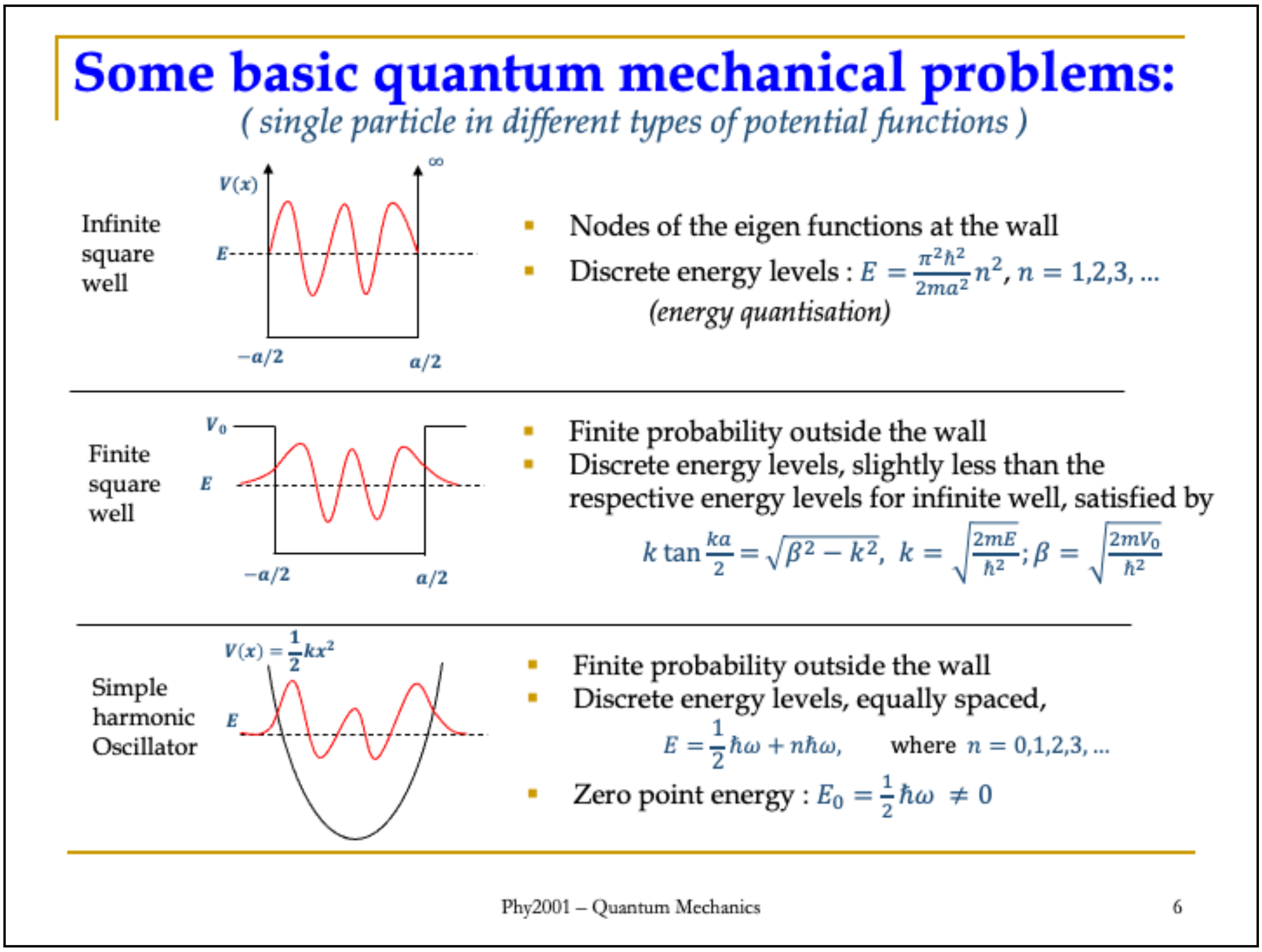
  (make sure the function do not diverge at any x)
- Apply boundary conditions :

  $\psi(x)$ and $\frac{d\psi(x)}{dx}$ are continuous at boundaries
- Apply normalisation to the eigen function :

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

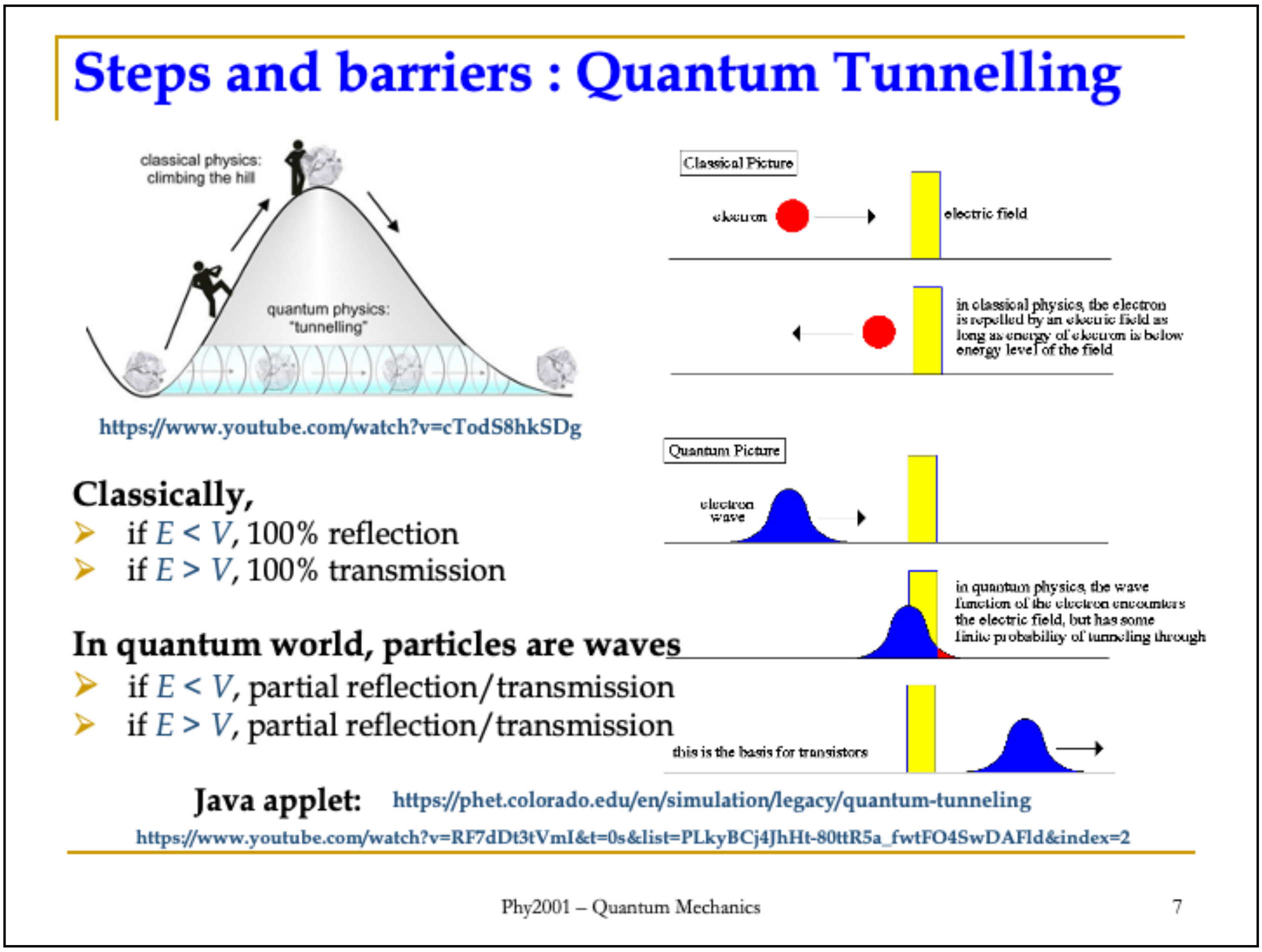
and some algebra…

- Now this is the standard recipe of anything we do in QM, although some minor variation may be necessary depending on the situation.



- Here are some problems you have already done using TISE, understanding how a particle (and associated wavefunction) manifest in a bound state.
- For instances, the concepts of energy levels, ground states (zero-point energy), wavefunction behaviour at the boundary (evanescent mode for non-infinite potential, change of wavelength and amplitude of the wavefunction at a non-uniform potential – wavelength changes due to change in kinetic energy and amplitude changes to keep the probability flux constant. We will do the Socrative quizzes around these topics to get the concepts absolutely clear.

- We will revisit the problems in this slide in 2D and 3D situations, however, first we start with some simpler problems in 1D – how a particle, or a stream of particles will behave if they encounter a force field (something they can or can't overcome).
- The term "force field" is used here to make a very generic term – for example, it can be a electric or magnetic field for an electron, a strong nuclear force field for a neutron, or simply a hill for a football.



- Now if you kick a football, it may be be able to pass over a hill to the other side depending on if he has enough kinetic energy to raise to the top of the hill – i.e. whether $\frac{1}{2}mv^2 > mgh$.
- Very similar concept for quantum mechanics, we can call the hill as a potential barrier for a quantum particle, where of course we deal more with electric/magnetic/strong forces than the earth's gravitational force.
- But the concept is similar – if the particle has a total energy=kinetic energy = E before the hill, it will have kinetic energy (E-V) at the top of the hill, where V represent the potential energy (which is mgh for the football for a hill of height h). It is the kinetic energy/momentum of the particle which defines the wavelength of the de-Broglie wave (or matter wave). For instance you can say, the wavelength of the 'football' wave is larger at the top of the hill.

- On the other hand, if the particle does not have enough energy to overcome the potential barrier, you would expect that it wont it able to penetrate it, however, here is the twist in story when you look at the problem from a quantum mechanical prospective – tunnelling, a very interesting concept, which we will go through after a few lectures.

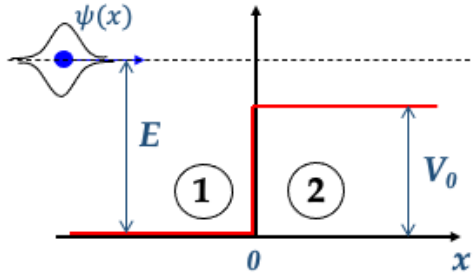
Part-1
Potential Steps

- So lets go step-by-step – the first step is potential step ☺

- It's a extremely simplified 1D problem – the space is divided into two regions, one without and other with the force field. The changeover is a delta function.

Potential step : E > V_0

Aim: to find out reflection and transmission coefficients



- **define potential :**

  $V(x) = 0 \quad if\ x < 0$ **: Region 1**

  $\quad\;\; = V_0 \quad if\ x > 0$ **: 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 :**

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

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

moving along: $+x$ $-x$ $+x$ $-x$

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); $D = 0$

- Here, we start with the case when the ‘hill’ is not too high. i.e the incoming particle has sufficient energy to overcome it. If we think of this problem from a ‘football’ prospective, we would say, it will go over the step and will roll with a lower velocity (as it had to use part of its kinetic energy to jump over the step). And this will happen, i.e. the football will never bounce back, each and every time I try this with the condition E>V.

- But if we look the problem quantum mechanically, the probability of finding the football over the hill won’t be 100%. There will be a finite(even though it is small) probability of football being bounced back. i.e. we we replace the football with a stream of electrons, each with energy higher than the energy of the barrier, there will a few electrons who will be reflecting back. This is weird to think, but its quite plausible, if you think of the small reflection of light by a transparent glass. Here the change in refractive index from air to glass can be considered as a potential step for the incoming photons.

- So our aim here is to find out the reflection and transmission probabilities/ coefficients, using TISE. We follow the recipe, in the other slide, and you can use the splited slides and summary lecture to guide you through the derivation. It should be very straightforward, but don't overlook any step.

- Although the derivation here is very detailed, there may be some trivial steps skipped here. You should try to workout the derivation by your own.

- Now going through the derivation -
- Step 1: define the problem, the step, regions, incoming particle, its energy, wavefunction.
- Step 2: the wavefunction should satisfy TISE in both regions, so write the equation separately for the two regions. In region 1, we have V=0, but we have the V term for region 2.
- Step 3: We can also postulate a general form of the wavefunction in both region.
    - We can start by assuming that we have a reflected wave in the region 1, which is the part with e^{-ikx}. In region 1, V= 0, hence the momentum of the particle is $p = \hbar k = \sqrt{2mE}$
    - But in region 2, $p = \hbar k = \sqrt{2m(E - V)}$. The other difference is that there is no wave moving along –x direction (the e^{-ikx} component) as the step is extended forever in x, no more boundary for getting a reflection. So we can assume D = 0.

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

- **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***"

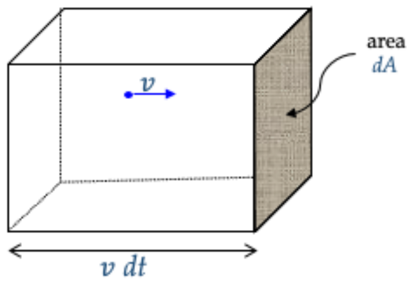
- Hence we now have general form of the wavefunctions and TISE for both appropriate to this problem.

- Step 4: But we also need to make sure the wavefunctions are well-behaved. Hence the boundary conditions. It should not be difficult to get $A + B = C$ and $Ak_1 - Bk_1 = Ck_2$
  - Hint: $\frac{d\psi_1(x)}{dx} = \frac{d}{dx}\left(Ae^{ik_1x} + Be^{-ik_1x}\right) = Aik_1e^{ik_1x} - Bik_1e^{-ik_1x}$
- Step 5: very simple algebra, to find the expression for the B and C in terms of A
  - Hint: Multiply k_1 to both side of $A + B = C$, then add this with the other equation.

- The reason we are finding the expression for $\frac{B}{A}$ and $\frac{C}{A}$ as A, B and C represent (we will see below) the probability fluxes of incident, reflected and transmitted wave, which is what we are interested to know – remember we want to check whether there will be 100% transmission as one would expect from classical mechanics viewpoint.

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: $\psi_i = A\exp(ik_1x)$

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

Similarly,

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

Region 1

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

Region 2

and,

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

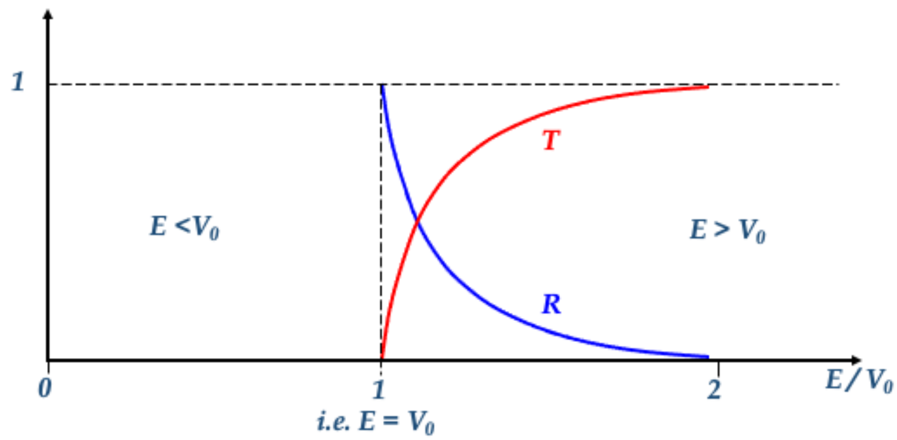
Transmission coefficient: $T = \frac{J_T}{J_I} = \frac{k_2}{k_1}\frac{C^2}{A^2}$

- Here on the left side, we see how we define the probability flux, which is probability of finding a particle per unit area and per unit time. Hence the probability flux depends on probability density $|\psi|^2$ and the velocity of the particle.

- We can then use this definition to write down the probability fluxes of the incident/reflected/transmitted wavefunctions, as written in the right hand side. Not the velocity in the region 1 is the same whether it's a incident or reflected wave, as the velocity depends on the kinetic energy, i.e. E-V, i.e. if a particle reflects, will travel backwords with the same velocity as the incident particle.

- So we can use these probability fluxes to get the reflection and transmission coefficients, as the ratio of the respective fluxes with respect to the incident one. And as you can see it depends on the ratios B/A and C/A, because of which we derived these in the previous slide.

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.

- Now here is what we get the final expression for the R and T.
- Note R and T depends on the k_1 and k_2, remember the expressions of these in the previous slide,

  $$k_1 = \sqrt{2mE}/\hbar \text{ and } k_1 = \sqrt{2m(E-V)}/\hbar$$

  So if V=0, i.e. there is no potential step, $k_1 = k_2$ => R=0 and T=1 (no reflection as long as the wave is travelling in a given medium)

  On the other hand, if E=V, $k_2 = 0$ and hence R=1 and T = 0

  And for the intermediate cases, you expect R=0 as per the classical mechanics, but quantum mechanics suggests otherwise. A finite probability of reflection – even if the football has crossed the hill, we can still feel its presence to some extent ☺ .
- Another important point is that, the reflection is not because the V increased, you will also get a reflection if the V decreases. The main reason of a reflection is that the particle experience an abrupt change in its de-Broglie wavelength.

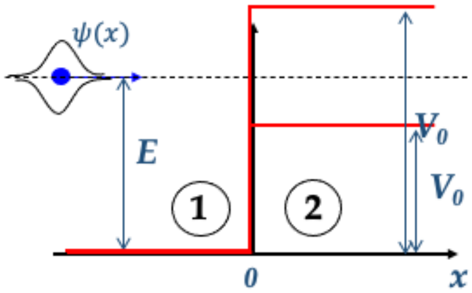
- Now you would ask, what happens the other side of the plot, when $E < V$? As we saw $R=1$ and $T=0$ for $E=V$, you would probably confidently say that the same will be the case when $V>E$.

  But, yes and no …

  again a slight twist in the story. Let's look at it now!

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**

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

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

$$\frac{\hbar^2}{2m}\frac{d^2\psi_1(x)}{dx^2} + E\,\psi_1(x) = 0 \qquad \frac{\hbar^2}{2m}\frac{d^2\psi_2(x)}{dx^2} + [E - V_0]\,\psi_2(x) = 0$$

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

$$\psi_1(x) = A\exp(ik_1x) + B\exp(-ik_1x) \qquad \psi_2(x) = C\exp(ik_2x) + D\exp(-ik_2x)$$

where, $k_1 = \sqrt{\frac{2mE}{\hbar^2}}$ where, $k_2 = \sqrt{\frac{2m(E-V_0)}{\hbar^2}} = i\sqrt{\frac{2m(V_0-E)}{\hbar^2}} = ik_2'$

A & B are amplitudes (constants) C & D are amplitudes (constants)

- Here we consider the case, when the particle does not have enough energy to overcome (classically speaking) the potential barrier.
- We can follow the exact same steps as the previous case. The difference in this case will appear when you will try to find the k_2 for the region 2, which is now an imaginary term as E<V.
- Otherwise, all same and we can continue with a substitution of $k_2 = ik_2'$

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: $+x$ / $-x$

No oscillations here!

- **apply boundary conditions to find A, B & C:**
  - ✓ $\psi_1(x)|_{x=0} = \psi_2(x)|_{x=0} \quad \Rightarrow \quad A + B = C$
  - ✓ $\left.\frac{d\psi_1(x)}{dx}\right|_{x=0} = \left.\frac{d\psi_2(x)}{dx}\right|_{x=0} \quad \Rightarrow \quad Aik_1 - Bik_1 = -Ck_2' \quad \Rightarrow \quad A - B = \frac{ik_2'}{k_1}C$
- **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 $T = 0$

- And assuming D=0, same as the previous case, as there is no reflected wave in region 2.
- Then applying boundary condition as before and finding B/A and C/A. You can see here the similarity with the previous case.
- Then we can find the R and T terms, using the definition of the probability fluxes calculated in the previous case. As expected, you would get no transmission and 100% reflection. This is good, but where is the 'twist' we talked about?

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

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

Real positive quantity

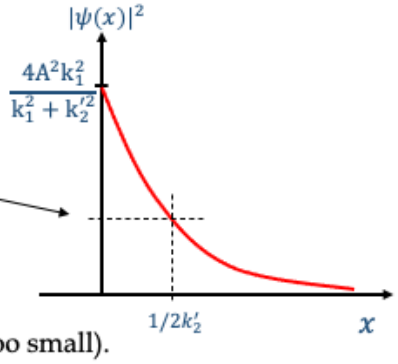
Exponential Decay

- Although R=1 and T=0, there is a finite penetration of the wave inside the force field. This is a similar concept as Evanescent mode.
- You see that the transmitted wavefunction is not oscillatory in space, as we replaced k_2 with ik_2' in its exponential term (e^{ikx})

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,

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

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

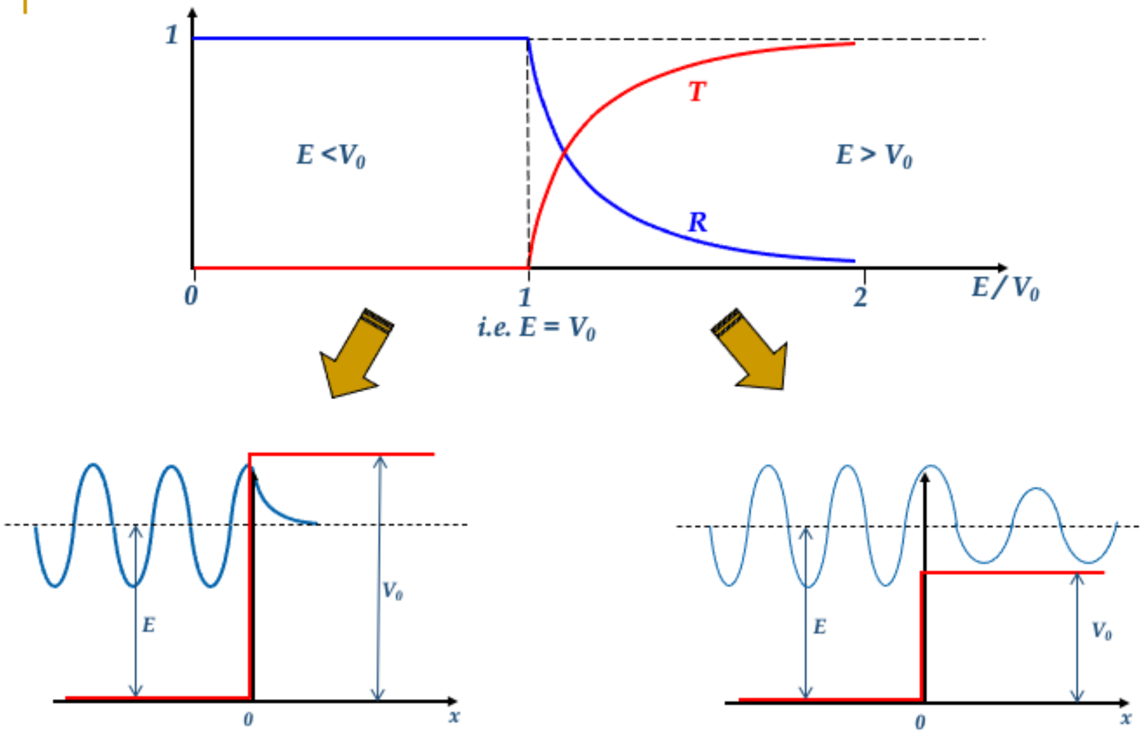
i.e. it is no longer possible to say that the particle energy is less than the barrier – helps to overcome apparently violating conservation of energy.

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

- The graph on the right shows the wavefunction inside the classically excluded region. Its only an exponentially decaying profile.
- For such an exponential profile, it is customary to define the penetration depth as the depth at which the functional value becomes 1/e times its initial value.
- Note that this depth depends on the difference between E and V. If we have too strong force field, the wavefunction penetrates a little. And in the limit V -> ∞, no penetration.
- This penetration into classically excluded region does not mean that the particle is stored in the region 2, indeed we saw R=1 and T = 0. It only says that there is an appreciable probability of finding the particle in the region between x=0 and x=Δx.
- So if we use uncertainty principle, we can see there is an uncertainty about particle energy in the region between x=0 and x=Δx, which is same as the amount V is higher than E. i.e. it is possible that the particle have the same energy as V in this region, and this by borrowing energy from the force field - hence called energy borrowing. You will perhaps learn more about this in other module.

- for more information, follow the section of the Eisberg book. For instance see the fig. in the notes of the next slide, taken from the page 192 of the book.

- Coming back to reflection and transmission coefficients…



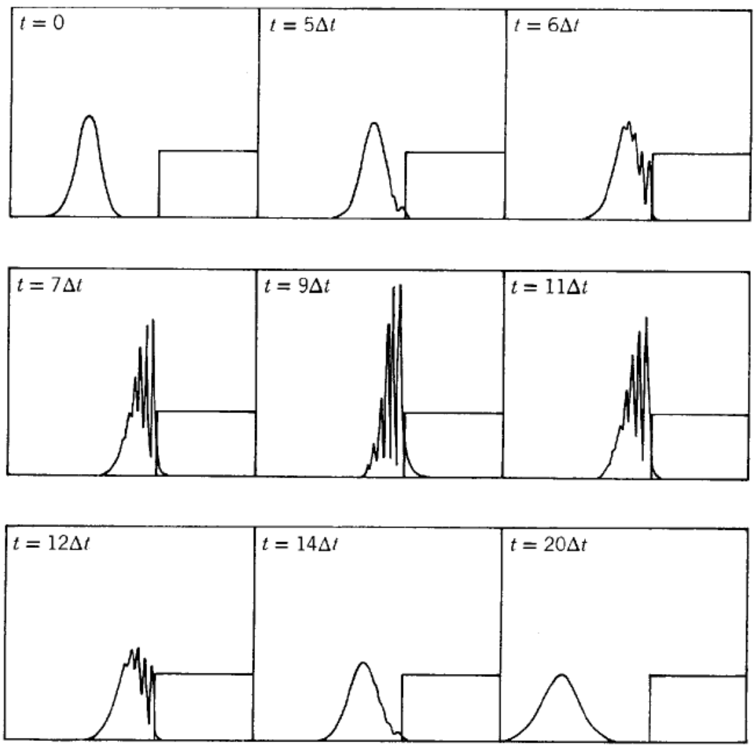


Figure 6-8 A potential step, and the probability density $\Psi^*\Psi$ for a group wave function describing a particle incident on the step with total energy less than the step height. As time evolves, the group moves up to the step, penetrates slightly into the classically excluded region, and then is completely reflected from the step. The complications of the mathematical treatment using a group are indicated by the complications of its structure during reflection.