Quantum Mechanics (P304H)
Part 2 – Lecture 12

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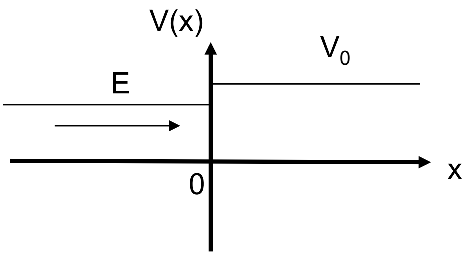
Potential step recap

$E<V_0$



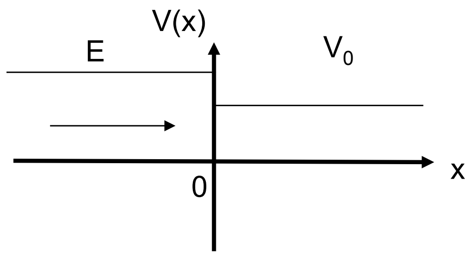
$$\frac{d^2\psi(x)}{dx^2}+k^2\psi(x)=0 \quad ,x<0$$

$$\frac{d^2\psi(x)}{dx^2}-\kappa^2\psi(x)=0 \quad ,x\geq 0$$

$$k=\sqrt{\frac{2mE}{\hbar^2}}, \quad \kappa=\sqrt{\frac{2m}{\hbar^2}(V_0-E)}$$

$$k,\kappa\in\mathbb{R}^+$$

$E>V_0$



$$\frac{d^2\psi(x)}{dx^2}+k^2\psi(x)=0 \quad ,x<0$$

$$\frac{d^2\psi(x)}{dx^2}+k'^2\psi(x)=0 \quad ,x\geq 0$$

$$k=\sqrt{\frac{2mE}{\hbar^2}}, \quad k'=\sqrt{\frac{2m}{\hbar^2}(E-V_0)}$$

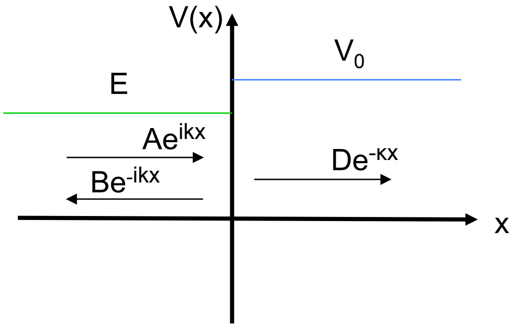
$$E>V_0 \quad k,k'\in\mathbb{R}^+$$

Potential step recap

$E<V_0$

$$\psi(x)=\begin{cases} Ae^{ikx}+Be^{-ikx} & ,x<0 \\ Ce^{\kappa x}+De^{-\kappa x} & ,x\geq 0 \end{cases}$$

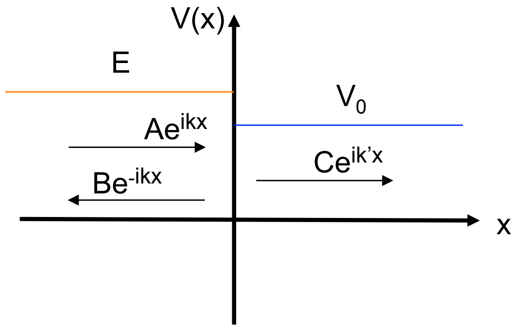
Coefficient C must be zero, else this term grows to infinity when x→∞



$E>V_0$

$$\psi(x)=\begin{cases} Ae^{ikx}+Be^{-ikx} & ,x<0 \\ Ce^{ik'x}+De^{-ik'x} & ,x\geq 0 \end{cases}$$

This would be a plane wave coming from the right, which we don't have, so D must be 0.



Potential step recap

$E<V_0$

Probability current density:

$$J(x,t)=\mathrm{Re}\left[\psi^*\frac{\hbar}{im}\frac{\partial}{\partial x}\psi\right]$$

$$\kappa\in\mathbb{R}^+,\quad |A|^2=|B|^2 \quad \leftarrow\text{Standing wave}$$

$$J(x,t)=\begin{cases} v\left(|A|^2-|B|^2\right)=0, \; x<0 \\ 0, \; x\geq 0 \end{cases}$$

Reflection and transmission coefficients:

$$R=\frac{v|B|^2}{v|A|^2}=\frac{|B|^2}{|A|^2}=1,\quad T=0$$

The wave is totally reflected, even though there is a non-zero probability of finding the particle at x>0.

$E>V_0$

Probability current density:

$$J(x,t)=\begin{cases} v\left(|A|^2-|B|^2\right), x<0, & v=\dfrac{\hbar k}{m} \\ v'|C|^2 \quad\quad ,x\geq 0, & v'=\dfrac{\hbar k'}{m} \end{cases}$$

$$k,k'\in\mathbb{R}^+,\quad J(x,t)\neq 0$$

Reflection and transmission coefficients:

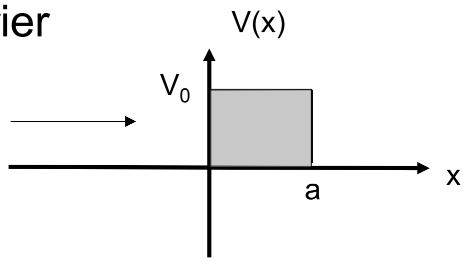
$$R=\frac{v|B|^2}{v|A|^2}=\frac{|B|^2}{|A|^2}=\frac{(k-k')^2}{(k+k')^2}$$

$$T=\frac{v'|C|^2}{v|A|^2}=\frac{4kk'}{(k+k')^2}$$

$$R+T=1$$

4. Potential Barrier

- The second example: Potential Barrier
  - The potential is defined as:



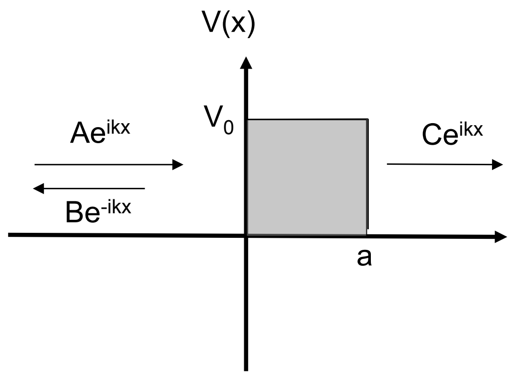
$$V(x) = \begin{cases} 0 \text{ if } x < 0 \\ V_0 \text{ if } 0 < x < a \\ 0 \text{ if } x \geq a \end{cases}$$

  - The 1D Schrödinger equation is: $\frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2}[E - V(x)]\psi(x) = 0$
  - The particle is free in the regions $x<0$ and $x>a$. We assume that the particle is incident from the left, with amplitude A, that there is a reflected wave of amplitude B from left to right, and that there is a transmitted wave of amplitude C and wave number *k*:

$$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & , x < 0 \\ Ce^{ikx} & , x > a \end{cases} \qquad k = \sqrt{\frac{2mE}{\hbar^2}}$$

4. Potential Barrier

- The probability current density is:



$$J(x,t) = \begin{cases} v\left(|A|^2 - |B|^2\right), \ x < 0 \\ v|C|^2 \qquad , x \geq a \end{cases}$$

- Reflection and transmission coefficients if $v = \frac{\hbar k}{m}$

$$R = \frac{|B|^2}{|A|^2} \quad \text{and} \quad T = \frac{|C|^2}{|A|^2}$$

(note that v is the same for *x<0* and *x>a*)

4. Potential Barrier ($E<V_0$)

What happens *within the barrier* ? Case 1: $E<V_0$

$$\frac{d^2\psi(x)}{dx^2}+\frac{2m}{\hbar^2}[E-V(x)]\psi(x)=0 \quad \text{with} \quad V(x)=V_0, 0<x<a$$

$$\Rightarrow \boxed{\psi(x)=Fe^{\kappa x}+Ge^{-\kappa x}, 0<x<a} \qquad \text{with } \kappa=\sqrt{\frac{2m(V_0-E)}{\hbar^2}}$$

– Continuity of $\psi(x)$ and $d\psi(x)/dx$ is required in both $x=0$ and $x=a$

x=0:
$$A+B=F+G$$
$$ik(A-B)=\kappa(F-G)$$

x=a:
$$Ce^{ika}=Fe^{\kappa a}+Ge^{-\kappa a}$$
$$ikCe^{ika}=\kappa\left(Fe^{\kappa a}-Ge^{-\kappa a}\right)$$

$$\Rightarrow \quad \frac{B}{A}=\frac{(k^2+\kappa^2)(e^{2\kappa a}-1)}{(\kappa+ik)^2-e^{2\kappa a}(\kappa-ik)^2}$$

$$\frac{C}{A}=\frac{4i\kappa k e^{-ika}e^{\kappa a}}{(\kappa+ik)^2-e^{2\kappa a}(\kappa-ik)^2}$$

Exercise for students: prove this result

4. Potential Barrier ($E<V_0$)

Therefore:

$$R=\frac{|B|^2}{|A|^2}=\left[1+\frac{4k^2\kappa^2}{(k^2+\kappa^2)\sinh^2(\kappa a)}\right]^{-1}=\left[1+\frac{4E(V_0-E)}{V_0^2\sinh^2(\kappa a)}\right]^{-1}$$

$$T=\frac{|C|^2}{|A|^2}=\left[1+\frac{(k^2+\kappa^2)\sinh^2(\kappa a)}{4k^2\kappa^2}\right]^{-1}=\left[1+\frac{V_0^2\sinh^2(\kappa a)}{4E(V_0-E)}\right]^{-1}$$

$$\Rightarrow \quad R+T=1$$

Remember that v is the same for $x<0$ and $x>a$ and $\sinh(\kappa a)=\dfrac{e^{\kappa a}-e^{-\kappa a}}{2}$

There is a <u>non-zero probability</u> of the particle leaking through the potential barrier (barrier penetration, or tunnel effect). This is one of the remarkable consequences of Quantum Mechanics.

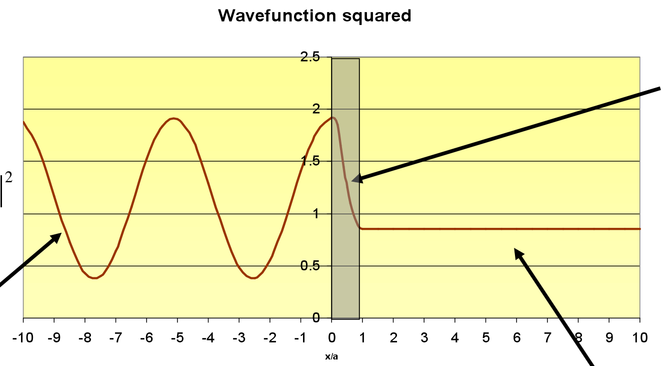
4. Potential Barrier ($E<V_0$)

Example: Plot $|\psi(x)|^2$ with $\frac{E}{V_0} = 0.75$ and opacity $\frac{mV_0 a^2}{\hbar^2} = 0.25$

$$\kappa a = \sqrt{2\left(1 - \frac{E}{V_0}\right)\frac{mV_0 a^2}{\hbar^2}} = \sqrt{\frac{1}{8}} \quad \text{and} \quad ka = \sqrt{2\frac{mV_0 a^2}{\hbar^2} - \kappa^2 a^2} = \sqrt{\frac{3}{8}}$$

We can now evaluate R=0.148, T=0.852, obtain |B| and |C|, and plot $|\psi(x)|^2$

$P(x) = |\psi(x)|^2$



$|\psi(x)|^2 = |Fe^{\kappa x} + Ge^{-\kappa x}|^2$

$|\psi(x)|^2 = |A|^2 + |B|^2 + 2|A||B|\cos(2kx)$

$|\psi(x)|^2 = |C|^2$

4. Potential Barrier ($E<V_0$)

- For small values of the energy ($E \to 0$) we have: $T \to 0$
- When the energy E approaches V_0 (the top of the barrier), then:

$$\lim_{E\to V_0} T = \lim_{E\to V_0}\left[1 + \frac{V_0^2\, 2m(V_0 - E)a^2}{4E\left(V_0 - E\right)\hbar^2}\right]^{-1} = \left[1 + \frac{mV_0 a^2}{2\hbar^2}\right]^{-1}$$

- Also, when the opacity $\frac{mV_0 a^2}{\hbar^2}$ is very large ($ka \gg 1$) then:

$$\sinh(\kappa a) \approx \frac{e^{\kappa a}}{2} \Rightarrow T \approx \frac{16E(V_0 - E)}{V_0^2} e^{-2\kappa a}$$

- This formula is important for **scanning electron microscopy**

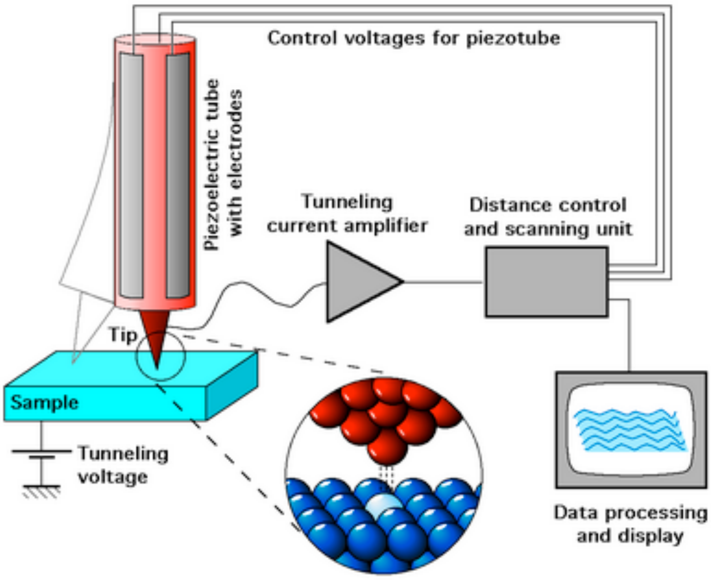
4. The Scanning Tunneling Microscope

How scanning electron microscopy works:

- A sharp needle is brought close to a metal (distance = *a*).
- Voltage applied between needle and surface creates a potential barrier.
- The energy difference between electrons in needle and metal is small, so a potential barrier of width *a* exists which electrons can tunnel.
- Current flow is dependent of the transmission coefficient *T*, which varies with *a* like

$$T \propto e^{-2\kappa a}$$

  i.e. extremely sensitive to variations in *a*
- Contour maps of accuracy 10^{-11}m can be made.



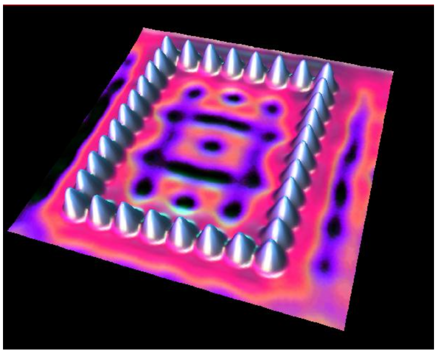
4. The STM

The scanning tunneling microscope:

Invented in 1981 by Gerd Binning and Heinrich Rohrer of IBM Zurich Labs.

Nobel prize in 1986

Reconstructed STM images:



Iron atoms on a copper surface

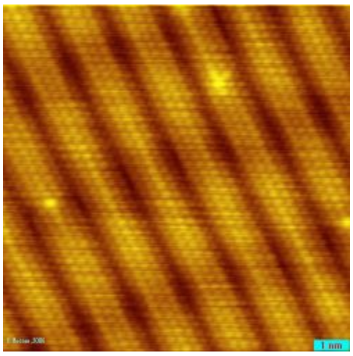
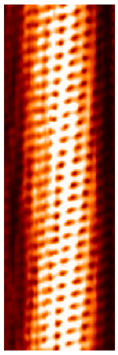


Image of an Au(100) surface



C nanotube

4. Potential Barrier (E>V_0)

- Case 2: E > V_0:

  Solution in the barrier region is similar to the case when E<V_0, but now:

$$\psi(x) = Fe^{ik'x} + Ge^{-ik'x}\ ,\ 0 < x < a \qquad \text{with } k' = \sqrt{\frac{2m(E-V_0)}{\hbar^2}}$$

  The solutions are similar to the previous case with k replaced by ik', and sinh(ka) by sin(k'a):

$$R = \frac{|B|^2}{|A|^2} = \left[1 + \frac{4k^2k'^2}{\left(k^2-k'^2\right)^2 \sin^2(k'a)}\right]^{-1} = \left[1 + \frac{4E(E-V_0)}{V_0^2 \sin^2(k'a)}\right]^{-1}$$

$$T = \frac{|C|^2}{|A|^2} = \left[1 + \frac{\left(k^2-k'^2\right)^2 \sin^2(k'a)}{4k^2k'^2}\right]^{-1} = \left[1 + \frac{V_0^2 \sin^2(k'a)}{4E(E-V_0)}\right]^{-1}$$

$$\Rightarrow R + T = 1$$

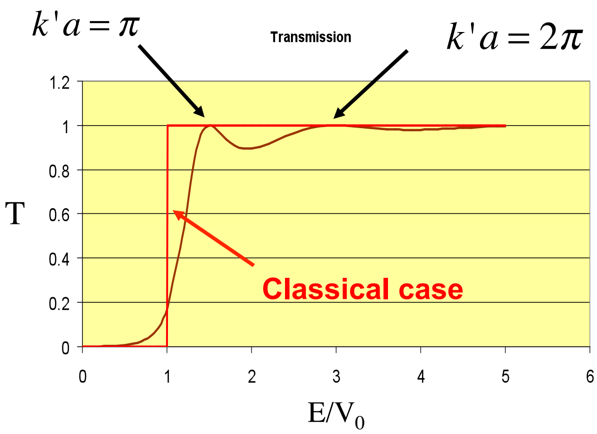
The transmission coefficient is less than unity: T ≤ 1. In classical physics, when E>V_0, the particle would always pass the barrier.

T=1 only when k'a=π, 2π, 3π, ….(when the thickness of the barrier is equal to a half-integral or integral number of de Broglie wavelengths: λ' = 2π/k'

4. Potential Barrier (E>V_0)

- Summary of transmission coefficient for potential barrier for different values of E/V_0:
- We take $\dfrac{mV_0a^2}{\hbar^2} = 10$

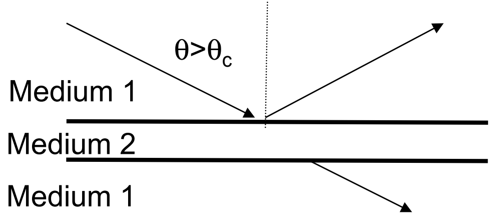
$$k'a = \sqrt{\frac{2mV_0a^2}{\hbar^2}\left(\frac{E}{V_0}-1\right)} = \sqrt{20\left(\frac{E}{V_0}-1\right)}$$



The barrier penetration phenomenon is a characteristic of waves and has an analogue in wave optics.

When reflection angle is larger than critical angle θ_c, the wave is totally reflected, and it does not propagate into the second medium.

However, the electric field penetrates into medium. If the medium 2 is thin, the wave can tunnel through.



Frustrated total internal reflection

4. Examples

1. Consider a particle incident on a potential step with V_0=10eV. Calculate the reflection and transmission coefficients when:
   a) E=5eV; b) E=15 eV and c) E=10 eV.

Answer:

a) If E = 5eV then $R = \left| e^{i\alpha} \right|^2 = 1 \quad \Rightarrow \quad T = 0$

b) If E=15eV

$$R = \frac{\left[1-\left(1-V_0/E\right)^{1/2}\right]^2}{\left[1+\left(1-V_0/E\right)^{1/2}\right]^2} = \left[\frac{1-\frac{1}{\sqrt{3}}}{1+\frac{1}{\sqrt{3}}}\right]^2 = 0.072 \quad \Rightarrow \quad T = 1 - R = 0.928$$

c) If E=10eV then $R = 1 \quad \Rightarrow \quad T = 0$

4. Examples

2. Determine the reflection and transmission coefficients a) of an electron E=1eV for a barrier potential with V_0=2eV and a = 0.1 nm b) of a proton of the same energy and same barrier potential.

Answer:

a) $V_0 - E$ = 1eV ⇒

$$\kappa = \left[\frac{2m}{\hbar^2}(V_0 - E)\right]^{1/2} = \left[\frac{2\times 9.1\times 10^{-31}\times 1.6\times 10^{-19}}{\left(1.05\times 10^{-34}\right)^2}\right]^{1/2} = 5.14\times 10^{9}\, m^{-1}$$

$\Rightarrow \kappa a = 0.514$

$$R = \left[1 + \frac{4E(V_0 - E)}{V_0^2 \sinh^2(\kappa a)}\right]^{-1} = \left[1 + \frac{4\times 1/2\times 1/2}{(0.537)^2}\right]^{-1} = 0.224 \Rightarrow T = 1 - R = 0.776$$

b) $\frac{m_p}{m_e} = 1836 \Rightarrow \kappa a = 22.0 \Rightarrow \sinh(\kappa a) = 1.8\times 10^{9}\,!! \Rightarrow R = 1 \text{ and } T = 0$