06/05/25

Lecture-31

27/11/20

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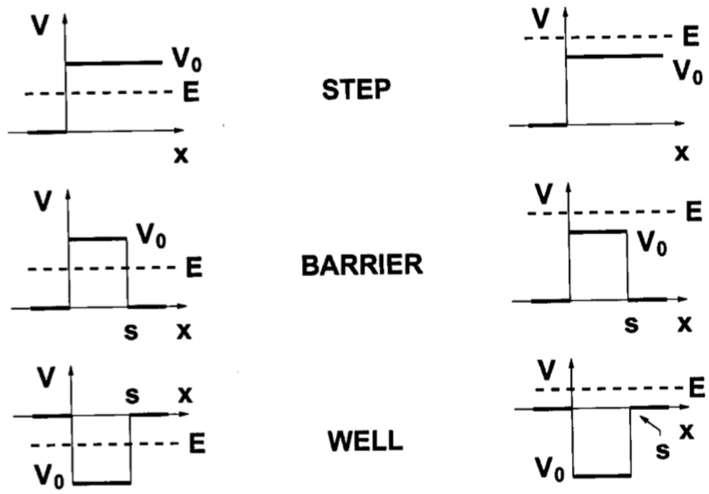
→

Piece wise constant functions



T. 14.1: Gradino, barriera e buca di energia potenziale.

→ The General Recepie for solving problems defined over sub intervals is that of solving the Schrodinger eq^n in each subinterval and then imposing the continuity conditions at the boundary from one interval to another.

(I) for STEP condition we have two intervals

$x = -ve$ & $x = +ve$

we shall solve SE in Two intervals

After solving SE wewill have two functions in which there are indeterminate coefficients and we shall find some of these coefficients by imposing continuity condition.

well we know ψ (wavefunction) is continuous & derivative of WF are continuous.

in 1D case we have two cases

(i) continuity of function in origin

(ii) derivative of function in origin

schrodinger eq^n

$$\boxed{-\frac{\hbar^2}{2m}\nabla^2\omega + V\omega = E\omega}$$

ω = wavefunction in space

schrodinger eq^n in 1D

$$\boxed{-\frac{\hbar^2}{2m}\frac{d^2\omega}{dx^2} + V\omega = E\omega}$$

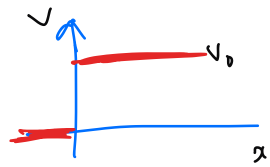
$$\frac{\hbar^2}{2m}\frac{d^2w}{dx^2} = (E-V)w$$

$$\Rightarrow \boxed{-\frac{d^2w}{dx^2} = \frac{2m}{\hbar^2}(E-V)w} \Leftrightarrow \boxed{w'' = k^2 w}$$

$$\Rightarrow k = \frac{\sqrt{2mE}}{\hbar} \quad \text{for } x<0$$

$$\alpha = \frac{\sqrt{2m(V_0-E)}}{\hbar} \quad \text{for } x>0$$

Potential Step — I



- Taking a one-dimensional case, let $V = 0$ for $x < 0$ and $V = V_0 > 0$ for $x > 0$. From the general properties of the time-independent Schrödinger equation it follows $E \geq 0$. Considering the case $0 < E < V_0$, the equation reads

$$\begin{cases} x < 0 : V=0 \quad -w'' = k^2 w\,, & k \doteq \sqrt{2mE}/\hbar \\ x > 0 : V=V_0 \quad w'' = \alpha^2 w\,, & \alpha \doteq \sqrt{2m\,(V_0 - E)}/\hbar \end{cases}$$

$$\Rightarrow \boxed{w = \begin{cases} w_- = a_1 \exp(jkx) + a_2 \exp(-jkx)\,, & x < 0 \\ w_+ = a_3 \exp(-\alpha x) + a_4 \exp(\alpha x)\,, & x > 0 \end{cases}} \Rightarrow$$

we already solved it already when Schrödinger eqn for free particle

where it must be set $a_4 = 0$ to prevent w_+ from diverging. Using
- the continuity of w and w' in the origin,

$$\boxed{\begin{cases} w_+(0) = w_-(0)\,, & a_1 + a_2 = a_3 \\ w'_+(0) = w'_-(0)\,, & jk\,(a_2 - a_1) = \alpha\, a_3 \end{cases}}$$

Eliminating a_3 yields $\alpha\,(a_1 + a_2) = jk\,(a_2 - a_1)$ whence

$$\frac{a_2}{a_1} = \frac{jk + \alpha}{jk - \alpha} = \frac{k - j\alpha}{k + j\alpha}\,, \qquad \frac{a_3}{a_1} = 1 + \frac{a_2}{a_1} = \frac{2k}{k + j\alpha}\,,$$

that determine a_2, a_3 apart from the arbitrary constant a_1. This should be expected as w is not normalizeable. because it is Non zero over infinite domain and oscillates over the infinite domain.

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→ We will find the relationship b/w a_1, a_2, a_3 by doing basic Algebra as shown above

$$\frac{a_2}{a_1} = \frac{k - j\alpha}{k + j\alpha}$$ } both are complex conjugates

$$\Rightarrow \quad |a_2| = |a_1|$$

We can further discuss the form of the solution because we can see that $a_3 \neq 0$

∴ Solution

$$\Rightarrow \quad \omega_f = a_3 \exp(-\alpha x) \neq 0$$

∴ The solution along the positive part of the x-axis decays to zero

i.e The probability of finding the particle inside the step is Non Zero

Which is in Contrast to classical case where the particle Bounces back exactly at $x = 0$

- The other issue is that the coefficient a_2 also different from zero because it is multiplied to $\exp(-ikx)$ and Here in the example we have the Total Energy 'E'
- So we may associate the Time part of the

Wavefunction ~~to~~ this solution by simply multiplying the solution by the exponential $\left(e^{-j\omega t}\right)$

where $\omega = \frac{E}{\hbar}$ and after this multiplication the

wavefunction represents PLANAR, MONOCHROMATIC WAVE that propogates in the $-ve$ part of the axis.

So, the term proportional to a_2 represents the Reflected wave. but we have to emphasise

CM : The wave is Reflected

QM : The wave is Reflected after penetrating the step for a while

- There is a physical meaning associated with the coefficients a_1, a_2, a_3.

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Potential Step — II

From $|a_2/a_1| = |k - j\alpha|/|k + j\alpha| = 1$ it is $a_2/a_1 = \exp(-j\varphi)$, with $\varphi = 2\arctan(\alpha/k)$. The time-independent wave function can then be recast as

$$w = \begin{cases} w_- = 2a_1 \exp(-j\varphi/2)\cos(kx + \varphi/2), & x < 0 \\ w_+ = [2k/(k + j\alpha)]\, a_1 \exp(-\alpha x), & x > 0 \end{cases}$$

The eigenvalues are continuous in the range $0 \le E < V_0$. The monochromatic wave function corresponding to w_k is $\psi_k(x,t) = w(x)\exp(-jE_k t/\hbar)$, with $E_k = \hbar^2 k^2/(2m)$.

The interaction of the particle with the potential step is better understood by considering a wave packet of width Δx approaching the origin from $x < 0$. The envelope has the form $A_i = A(x - u_g t)$. Before reaching the origin the particle is localized by $|\psi_i|^2 = |A_i|^2$, and crosses the origin in a time $\Delta t = \Delta x/u_g$ starting, e.g., at $t = 0$.

After a time $\Delta t + t_0$ only the reflected packet exists, described by $A_r = A[x + u_g(t - t_0)]$. The delay $t_0 \ge 0$ is unpredictable because the reflexion abscissa $u_g t_0$ is undetermined.

As the particle is eventually reflected it is $\int_{-\infty}^{0} |\psi_i|^2\, dx = \int_{-\infty}^{0} |\psi_r|^2\, dx = 1$.

- later we will see that the $\left|\frac{a_2}{a_1}\right|^2$ is the probability of reflection

for $E < V$
The particle is reflected but after penetrating the barrier.

This is situation we get if we analyze the situation considering a monochromatic case.

That is particle whose energy is fully defined and has some value.

→ We can also repeat the calculation using a wave packet

We will just discuss the outcomes without the calculations.

- for Gaussian wave packet

with standard deviation "Δx" ⇒ width of the wave packet

Assuming the wave Packet approaches the Barriar from '∞'

The wave Packet can be described by an "Envelop function" $A_i = A(x - u_g t)$

$$|\psi_i|^2 = |A_i|^2$$

when the wave packet reaches the Barrior it get extend in Space.

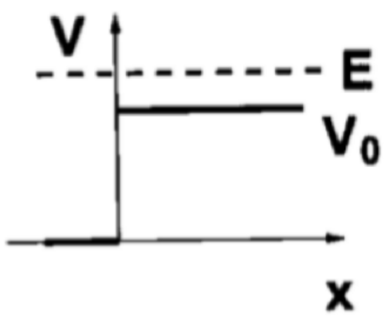
After a time $\Delta t + t_0$ only the reflected packet exists, described by $A_r = A[x + u_g(t - t_0)]$. The delay $t_0 \geq 0$ is unpredictable because the reflexion abscissa $u_g t_0$ is undetermined.

As the particle is eventually reflected it is $\int_{-\infty}^{0} |\psi_i|^2 \, dx = \int_{-\infty}^{0} |\psi_r|^2 \, dx = 1$.

incident wavepacket

Reflected wavepacket

→



Potential Step — III

- Still considering a one-dimensional case with $V = 0$ for $x < 0$ and $V = V_0 > 0$ for $x > 0$, let $E > V_0$. The Schrödinger equation reads

oscillatory behaviour

$$\begin{cases} x < 0: & -w'' = k^2 w, & k \doteq \sqrt{2mE}/\hbar \\ x > 0: & -w'' = k_1^2 w, & k_1 \doteq \sqrt{2m\,(E - V_0)}/\hbar \end{cases}$$

incoming wave from left to origin

Reflected wave

$$\Rightarrow \quad w = \begin{cases} w_- = a_1 \exp(jkx) + a_2 \exp(-jkx), & x < 0 \\ w_+ = a_3 \exp(jk_1 x) + a_4 \exp(-jk_1 x), & x > 0 \end{cases}$$

Transmitted wave

This Term can't exist if the wave is assumed to come from $+\infty$

- If the particle approaches the origin from $x < 0$ ($x > 0$) it must be set $a_4 = 0$ ($a_1 = 0$). In the classical description, the velocity decreases (increases) when the particle crosses the origin. Taking the first case ($a_4 = 0$) and using the continuity of w and w' in the origin,

$$\begin{cases} w_+(0) = w_-(0), & a_1 + a_2 = a_3 \\ w'_+(0) = w'_-(0), & k\,(a_1 - a_2) = k_1\, a_3 \end{cases}$$

Eliminating a_3 yields $k_1\,(a_1 + a_2) = k\,(a_1 - a_2)$ whence

$$\frac{a_2}{a_1} = \frac{k - k_1}{k + k_1}, \qquad \frac{a_3}{a_1} = 1 + \frac{a_2}{a_1} = \frac{2k}{k + k_1},$$

that determine a_2, a_3 apart from the arbitrary constant a_1.

Both Ratios are Non Zero.

a_2 : Reflection coefficient

a_3 : Transmission coefficient

Potential Step — IV

As $k_1 < k$ it is $a_2 \neq 0$ ($a_3 \neq 0$), namely, a probability of reflexion exists which is impossible in the classical treatment. The eigenvalues are continuous in the range $E > V_0$. The monochromatic wave function reads

$$\psi = \begin{cases} \psi_- = w_- \exp(-jE_-\,t/\hbar), & x < 0 \\ \psi_+ = w_+ \exp(-jE_+\,t/\hbar), & x > 0 \end{cases}$$

in which $E_- = E(k) = \hbar^2 k^2/(2m)$ and $E_+ = E(k_1) = \hbar^2 k_1^2/(2m) + V_0$.

The interaction of the particle with the potential step is better understood by considering a wave packet of width Δx approaching the origin from $x < 0$. The envelope has the form $A_i = A(x - u_g t)$. Before reaching the origin the particle is localized by $|\psi_i|^2 = |A_i|^2$, and crosses the origin in a time $\Delta t = \Delta x / u_g$. The reflected packet is described by

$$|\psi_r|^2 = \frac{(k_0 - k_{10})^2}{(k_0 + k_{10})^2}\,|A(x + u_g t)|^2.$$

It has the same group velocity, hence the same width, as $|\psi_i|^2$. Symbols k_0, k_{10} indicate the center of the packet for $x < 0$ and $x > 0$, respectively.

- Interestingly, we can observe

$$\boxed{\left|\frac{a_2}{a_1}\right|^2 + \left|\frac{a_3}{a_1}\right|^2 = 1}$$

Potential Step — V

The transmitted packet has the form

$$|\psi_t|^2 = \frac{(2k_0)^2}{(k_0 + k_{10})^2} \, |A(x\, k_0/k_{10} - u_g t)|^2 .$$

Its group velocity is $u_{1g} = \mathrm{d}x/\mathrm{d}t = u_g\, k_{10}/k_0 < u_g$. As all packets cross the origin in the same time interval Δt, it is

$$\frac{\Delta x}{u_g} = \frac{\Delta x_1}{u_{1g}} \quad \Longrightarrow \quad \Delta x_1 = \frac{k_{10}}{k_0} \Delta x < \Delta x .$$

This shows that the transmitted packet is slower and narrower (faster and wider) than the incident packet. From $\int_{-\infty}^{0} |\psi_i|^2 \, \mathrm{d}x = 1$ it follows

$$P_r \doteq \int_{-\infty}^{0} |\psi_r|^2 \, \mathrm{d}x = \frac{(k_0 - k_{10})^2}{(k_0 + k_{10})^2} ,$$

$$P_t \doteq \frac{k_{10}}{k_0} \int_0^{\infty} |\psi_t|^2 \, \mathrm{d}\frac{k_0 x}{k_{10}} = \frac{k_{10}}{k_0} \, \frac{(2k_0)^2}{(k_0 + k_{10})^2} = \frac{4 k_0 k_{10}}{(k_0 + k_{10})^2} .$$

The two numbers P_r, P_t fulfill the relations $0 < P_r, P_t < 1$, $P_r + P_t = 1$, and are the reflection and transmission probabilities.

$P_r + P_t = 1$

Potential Step — VI

- It is worth noting that the factor $\sqrt{2m}/\hbar$ cancels out in the expressions of P_r, P_t, yielding

$$P_r = \frac{(\sqrt{E_0} - \sqrt{E_0 - V_0})^2}{(\sqrt{E_0} + \sqrt{E_0 - V_0})^2} , \qquad P_t = \frac{\sqrt{E_0\,(E_0 - V_0)}}{(\sqrt{E_0} + \sqrt{E_0 - V_0})^2} ,$$

with E_0 the total energy corresponding to k_0 and k_{10}. Thus, the classical result $P_r = 0, P_t = 1$ cannot be recovered by letting $m \to \infty$. This is due to the Ehrenfest theorem.

- Also, the treatment for the case $E > V_0$ still holds when $V_0 < 0, E > 0$. In particular, if $V_0 < 0$ and $|V_0| \gg E$ it turns out $P_r \simeq 1$. This result has been proven experimentally.

- Finally, taking again $V = 0$ for $x < 0$ and $V = V_0 > 0$ for $x > 0$, the special case $E = V_0$ reduces the Schrödinger equation for $x > 0$ to $w'' = 0$, whence

$$w = \begin{cases} w_- = a_1 \exp(jkx) + a_2 \exp(-jkx) , & x < 0 \\ w_+ = a_3 + a_4 x , & x > 0 \end{cases}$$

with $a_4 = 0$ to prevent w_+ from diverging. Using the continuity of w and w' at $x = 0$ yields $w_- = a_3 \cos(kx)$, $w_+ = a_3$. The other special case $E = 0$ yields $w \equiv 0$.

E_0: Energy of central component of the wave function.

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Potential Barrier — I

Taking a one-dimensional case, let $V = 0$ for $x < 0, x > s$, and $V = V_0 > 0$ for $0 < x < s$. From the general properties of the time-independent Schrödinger equation it follows $E \geq 0$. Considering the case $0 < E < V_0$, the equation reads

$$\begin{cases} x < 0: & -w'' = k^2 w\,, & k \doteq \sqrt{2mE}/\hbar \\ 0 < x < s: & w'' = \alpha^2 w\,, & \alpha \doteq \sqrt{2m\,(V_0 - E)}/\hbar \\ s < x: & -w'' = k^2 w\,, & k \doteq \sqrt{2mE}/\hbar \end{cases}$$

$$\Rightarrow\ w = \begin{cases} w_- = a_1 \exp(jkx) + a_2 \exp(-jkx)\,, & x < 0 \\ w_B = a_3 \exp(\alpha x) + a_4 \exp(-\alpha x)\,, & 0 < x < s \\ w_+ = a_5 \exp(jkx) + a_6 \exp(-jkx)\,, & s < x \end{cases}$$

The sol^n inside the Barrier!

Using the continuity of w and w' in the origin,

Transmitted wave we will see as a_5 is Non zero i.e There will be Transmission which is impossible in CM (Tunnel effect)

$$\begin{cases} w_-(0) = w_B(0)\,, & a_1 + a_2 = a_3 + a_4 \\ w_-'(0) = w_B'(0)\,, & jk\,(a_1 - a_2) = \alpha\,(a_3 - a_4) \end{cases}$$

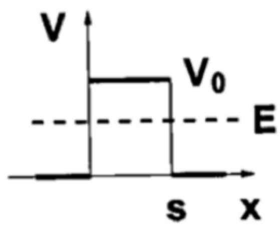
Solving for a_1, a_2 and letting $\theta \doteq 1 + j\alpha/k$ yields

$$\begin{cases} 2a_1 = \theta a_4 + \theta^* a_3 \\ 2a_2 = \theta a_3 + \theta^* a_4 \end{cases}$$

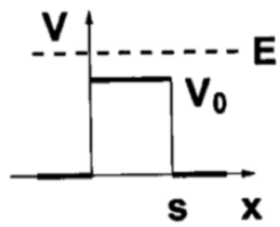
* In Potential Barrier we have 3 Regions, in Region we have to solve the 2nd order eq^n i.e the Schrodinger eq^n

$2 + 2 + 2 \Rightarrow$ There are six coefficients

However one of the '6' coefficients must be set to zero.



BARRIER



Potential Barrier — II

In the classical description, the particle is reflected at $x = 0$ ($x = s$), depending from where it approaches the origin. Here, if the particle approaches the origin from $x < 0$ ($x > 0$) it must be set $a_6 = 0$ ($a_1 = 0$). Taking the first case ($a_6 = 0$) and using the continuity of w and w' in $x = s$ yields

$$\begin{cases} w_B(s) = w_+(s)\,, & a_3\, e^{\alpha s} + a_4\, e^{-\alpha s} = a_5\, e^{jks} \\ w'_B(s) = w'_+(s)\,, & \alpha\,(a_3\, e^{\alpha s} - a_4\, e^{-\alpha s}) = jka_5\, e^{jks} \end{cases}$$

Solving for a_3, a_4 and letting $\sigma \doteq 1 + jk/\alpha$ yields

$$\begin{cases} 2a_3 = a_5\,\sigma \;\; \exp(jks - \alpha s) \\ 2a_4 = a_5\,\sigma^* \exp(jks + \alpha s) \end{cases}$$

It is worth observing that, if it were $a_5 = 0$, then it would also be $a_3 = a_4 = 0$ and $a_1 = a_2 = 0$. However, this is impossible as $w_- \neq 0$, hence it is necessarily $a_5 \neq 0$. This shows that, in contrast to the classical case, the particle can cross the barrier. The relations found so far determine a_2, a_3, a_4, a_5 apart from the arbitrary constant a_1. This should be expected as w is not normalizeable. In particular, the ratios a_2/a_1, a_5/a_1 are related to the reflected and transmitted waves, respectively.

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Potential Barrier — III

The ratio a_5/a_1 is found from

$$4\frac{a_1}{a_5} = 2\frac{a_3}{a_5}\theta^* + 2\frac{a_4}{a_5}\theta\,,$$

where the terms at the right hand side are given by

$$2\frac{a_3}{a_5} = \sigma\exp(jks - \alpha s)\,, \qquad 2\frac{a_4}{a_5} = \sigma^*\exp(jks + \alpha s)\,.$$

It is worth noting that $\mu \doteq \theta\sigma^* = 2 + j(\alpha/k - k/\alpha)$, whence

$$4\frac{a_1}{a_5}\exp(-jks) = \mu\exp(\alpha s) + \mu^*\exp(-\alpha s) =$$

$$= 4\cosh(\alpha s) + j\left(\frac{\alpha}{k} - \frac{k}{\alpha}\right) 2\sinh(\alpha s) \qquad \Longrightarrow$$

$$\left|\frac{a_1}{a_5}\right|^2 = \cosh^2(\alpha s) + \frac{1}{4}\left(\frac{\alpha}{k} - \frac{k}{\alpha}\right)^2 \sinh^2(\alpha s) =$$

$$= 1 + \left[1 + \frac{1}{4}\left(\frac{\alpha}{k} - \frac{k}{\alpha}\right)^2\right]\sinh^2(\alpha s) = 1 + \frac{1}{4}\left(\frac{\alpha}{k} + \frac{k}{\alpha}\right)^2 \sinh^2(\alpha s)$$

$\Rightarrow \alpha \propto V_0^2$

where $\cosh^2\zeta - \sinh^2\zeta = 1$ has been used. This result shows that $|a_5/a_1|^2 \to 1$ as $s \to 0$, while $|a_5/a_1|^2 \sim \exp(-2\alpha s)$ as s increases.

$s \Rightarrow$ Thickness of the Barrier

Transmission coefficient

$a_5 \neq 0 \Rightarrow$ TUNNEL EFFECT

Tunneling $\Rightarrow$ inversely proportional to 'α'
inversely proportional to 's'

Potential Barrier — IV

A similar calculation provides the ratio a_2/a_1:

$$\frac{a_1}{a_2} = \frac{\theta a_4 + \theta^* a_3}{\theta a_3 + \theta^* a_4} = \frac{\mu \exp(\alpha s) + \mu^* \exp(-\alpha s)}{\nu \exp(-\alpha s) + \nu^* \exp(\alpha s)},$$

with $\nu \doteq \theta\sigma = j(\alpha/k+k/\alpha)$. As the denominator equals $-j(\alpha/k+k/\alpha)\,2\sinh(\alpha s)$, it is found

Reflection coefficient

$$\left|\frac{a_2}{a_1}\right|^2 = \frac{(\alpha/k + k/\alpha)^2 \sinh^2(\alpha s)/4}{1 + (\alpha/k + k/\alpha)^2 \sinh^2(\alpha s)/4} = 1 - \left|\frac{a_5}{a_1}\right|^2 .$$

The eigenvalues are continuous in the range $0 \le E < V_0$.

The interaction of the particle with the barrier is better understood by considering a wave packet approaching the origin from $x < 0$. The envelope has the form $A_i = A(x - u_g t)$. Before reaching the origin the particle is localized by $|\psi_i|^2 = |A_i|^2$. After the interaction with the barrier is completed, both the reflected and transmitted packet exist, that move in opposite directions with the same velocity. Letting $P_r \doteq \int_{-\infty}^{0} |\psi_r|^2\,dx$, $P_t \doteq \int_{s}^{\infty} |\psi_t|^2\,dx$, and observing that $\int_{-\infty}^{0} |\psi_i|^2\,dx = 1$, it follows that the two numbers P_r, P_t fulfill the relations $0 < P_r, P_t < 1$, $P_r + P_t = 1$, and are the reflection and transmission probabilities.

$$\boxed{\left|\frac{a_2}{a_1}\right|^2 + \left|\frac{a_5}{a_1}\right|^2 = 1}$$

Reflection

Transmission

Potential Barrier — V

- The solution of the Schrödinger equation for the energy barrier shows that a particle with $E < V_0$, in contrast with the classical case, has a finite probability of crossing the barrier. The same result holds when the form of the barrier is more complicated than the rectangular one.

  The phenomenon is also called *tunnel effect*. Experimental evidence of the t.e. is found, for instance, in the $I - V$ curves of vacuum tubes, where the forward characteristics do not saturate at increasing bias.

- Still considering a one-dimensional case with $V = 0$ for $x < 0$, $x > s$ and $V = V_0 > 0$ for $0 < x < s$, let $0 < V_0 < E$. The Schrödinger equation reads

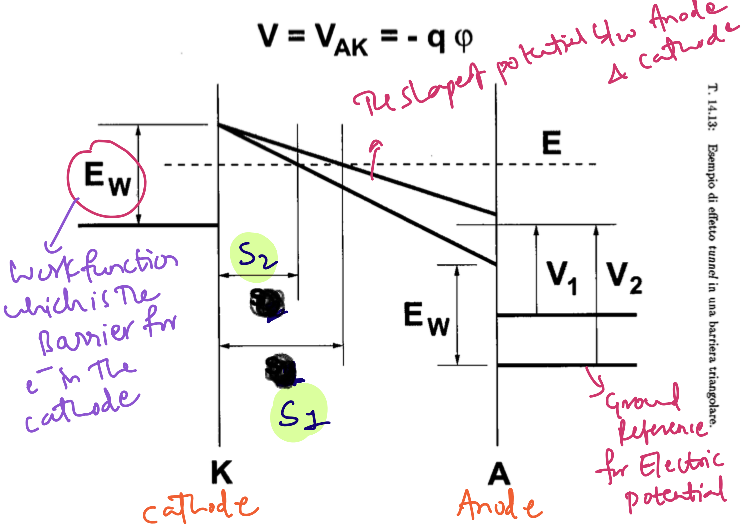
$$\begin{cases} x < 0: & -w'' = k^2 w\,, & k \doteq \sqrt{2mE}/\hbar \\ 0 < x < s: & -w'' = k_1^2 w\,, & k_1 \doteq \sqrt{2m\,(E - V_0)}/\hbar \\ s < x: & -w'' = k^2 w\,, & k \doteq \sqrt{2mE}/\hbar \end{cases}$$

$$\Rightarrow\ w = \begin{cases} w_- = a_1 \exp(jkx) + a_2 \exp(-jkx)\,, & x < 0 \\ w_B = a_3 \exp(jk_1 x) + a_4 \exp(-jk_1 x)\,, & 0 < x < s \\ w_+ = a_5 \exp(jkx) + a_6 \exp(-jkx)\,, & s < x \end{cases}$$

poisson eq^n

$\rho = 0$ because we assume negligible charge

$\nabla^2 \phi = 0$



T. 14.13: Esempio di effetto tunnel in una barriera triangolare.

V_1, V_2 are the applied Bias.

$E_W \Rightarrow$ height of barrier

$S_1, S_2 \Rightarrow$ Thickness of the barrier

$S \propto V$

which is in QM case and aids Tunneling

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Potential Barrier — VI

In the classical description, the particle is never reflected by the barrier. Here, if the particle approaches the origin from $x < 0$ ($x > 0$) it must be set $a_6 = 0$ ($a_1 = 0$). The first case ($a_6 = 0$) will be considered. The continuity relations at $x = 0$ and $x = s$ determine a_2, a_3, a_4, a_5 apart from the arbitrary constant a_1. This should be expected as w is not normalizeable. In particular, the ratios a_2/a_1, a_5/a_1 are related to the reflected and trasmitted waves, respectively; in contrast to the classical case, the particle can be reflected by the barrier.

From the solution of the Schrödinger equation it follows that w_- and w_+ are the same as in the case $0 \le E < V_0$, whereas w_B is found by replacing α with jk_1 there. Then,

$$\mu \to 2 - (k/k_1 + k_1/k)\,, \qquad \mu^* \to 2 + (k/k_1 + k_1/k)\,,$$

$$\nu \to k/k_1 - k_1/k\,, \qquad \nu^* \to k_1/k - k/k_1$$

and, using $\cosh(j\zeta) = \cos(\zeta)$, $\sinh(j\zeta) = j\sin(\zeta)$,

$$\frac{a_1}{a_5}\exp(-jks) = \cos(k_1 s) - j\frac{1}{2}\left(\frac{k}{k_1} + \frac{k_1}{k}\right)\sin(k_1 s)\,.$$

From the definition of k, k_1 it is found $k_1/k = \sqrt{1 - V_0/E}$.

k_1 = wave vector

$\lambda_1 = \dfrac{2\pi}{k_1}$

Potential Barrier — VII

- The eigenvalues are continuous in the range $E > V_0$. The above expressions yield

$$\left|\frac{a_1}{a_5}\right|^2 = \cos^2(k_1 s) + \frac{1}{4}\left(\frac{k}{k_1} + \frac{k_1}{k}\right)^2 \sin^2(k_1 s) =$$

$$= 1 + \frac{1}{4}\left(\frac{k}{k_1} - \frac{k_1}{k}\right)^2 \sin^2(k_1 s)$$

and, similarly,

$$\left|\frac{a_2}{a_1}\right|^2 = \frac{(k/k_1 - k_1/k)^2 \sin^2(k_1 s)/4}{1 + (k/k_1 - k/k_1)^2 \sin^2(k_1 s)/4} = 1 - \left|\frac{a_5}{a_1}\right|^2.$$

- This result shows that the barrier is transparent ($|a_2/a_1|^2 = 0$) for $k_1 s = i\pi$, with i any integer. Letting $\lambda_1 = 2\pi/k_1$ yields $s = i\lambda_1/2$. This is equivalent to the optical-resonance condition in a sequence of media of refractive indices n_1, n_2, n_1.
- Also, the reflection at the barrier for $k_1 s \ne i\pi$ explains why the experimental value of the Richardson constant A is lower than the theoretical one. Such constant appears in the expression $J_s = AT^2 \exp[-E_W/(k_B T)]$ of the vacuum-tube characteristics.

Potential Well

Potential Well — I

Taking a one-dimensional case, let $V = 0$ for $x < 0, x > s$, and $V = V_0 < 0$ for $0 < x < s$. From the general properties of the time-independent Schrödinger equation it follows $E \geq V_0$. Considering the case $V_0 < E < 0$, the equation reads

$$\begin{cases} x < 0: & w'' = \alpha^2 w\,, & \alpha \doteq \sqrt{-2mE}/\hbar \\ 0 < x < s: & -w'' = k^2 w\,, & k \doteq \sqrt{2m\,(E - V_0)}/\hbar \\ s < x: & w'' = \alpha^2 w\,, & \alpha \doteq \sqrt{-2mE}/\hbar \end{cases}$$

$$\Rightarrow \quad w = \begin{cases} w_- = a_1 \exp(\alpha x) + a_5 \exp(-\alpha x)\,, & x < 0 \\ w_W = a_2 \exp(jkx) + a_3 \exp(-jkx)\,, & 0 < x < s \\ w_+ = a_4 \exp(-\alpha x) + a_6 \exp(\alpha x)\,, & s < x \end{cases}$$

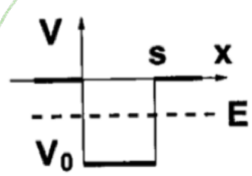
where it must be set $a_5 = a_6 = 0$ to prevent w_- and w_+ from diverging. Using the continuity of w and w' in the origin,

$$\begin{cases} w_-(0) = w_W(0)\,, & a_1 = a_2 + a_3 \\ w'_-(0) = w'_W(0)\,, & \alpha\, a_1 = jk\,(a_2 - a_3) \end{cases}$$

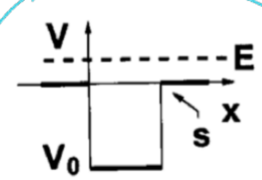
Solving for a_2, a_3 and letting $\theta \doteq 1 + j\alpha/k$ yields

$$2a_2 = \theta^* a_1\,, \quad 2a_3 = \theta a_1 \qquad \Rightarrow \qquad a_2/a_3 = \theta^*/\theta\,.$$

This is no different from the Barrier Analysis.



WELL



This is important because The particle might be trapped in the well & wavefunction is Normalizable

We can see Reflection coefficient is NONZERO.

Potential Well — II

- Using the continuity of w and w' in $x = s$ yields

$$\begin{cases} w_W(s) = w_+(s)\,, & a_4\,\mathrm{e}^{-\alpha s} = a_2\,\mathrm{e}^{jks} + a_3\,\mathrm{e}^{-jks} \\ w'_W(s) = w'_+(s)\,, & -\alpha\,a_4\,\mathrm{e}^{-\alpha s} = jk\,(a_2\,\mathrm{e}^{jks} - a_3\,\mathrm{e}^{-jks}) \end{cases}$$

Solving for a_2, a_3 :

$$\left.\begin{aligned} 2a_2 &= a_4\theta\ \exp(-\alpha s - jks) \\ 2a_3 &= a_4\theta^*\exp(-\alpha s + jks) \end{aligned}\right\} \quad \Rightarrow \quad \frac{a_2}{a_3} = \frac{\theta}{\theta^*}\exp(-2jks)\,.$$

- One sees that, if it were $a_1 = 0$ or $a_4 = 0$, then it would also be $a_2 = a_3 = 0$, which is impossible: in contrast to the classical case, the particle penetrates the boundaries of the well.
The relations found so far determine two different expressions for a_2/a_3. For them to be compatible, the following necessarily holds: $\theta^2\ \exp(-jks) = (\theta^*)^2\ \exp(jks)$, which represents the condition of a vanishing determinant of the 4×4 algebraic system for $a_1, a_2, a_3,$ and a_4. The above yields

$$\left(1 - \frac{\alpha^2}{k^2} + 2j\frac{\alpha}{k}\right)\ \exp(-jks) = \left(1 - \frac{\alpha^2}{k^2} - 2j\frac{\alpha}{k}\right)\ \exp(jks)\,,$$

$$\left(1 - \frac{\alpha^2}{k^2}\right)\ \sin(ks) = 2\frac{\alpha}{k}\ \cos(ks)\,, \qquad \frac{k^2 - \alpha^2}{2\alpha k} = \cot(ks)\,.$$

Potential Well — III

Replacing the expressions of α and k provides the transcendental equation

$$\frac{E - V_0/2}{\sqrt{E\,(E - V_0)}} = \cot\left(s\frac{\sqrt{2m}}{\hbar}\sqrt{E - V_0}\right), \qquad V_0 < E < 0\,,$$

whose roots are the eigenvalues of E. Given m, s, and V_0, let $n \geq 1$ be an integer such that

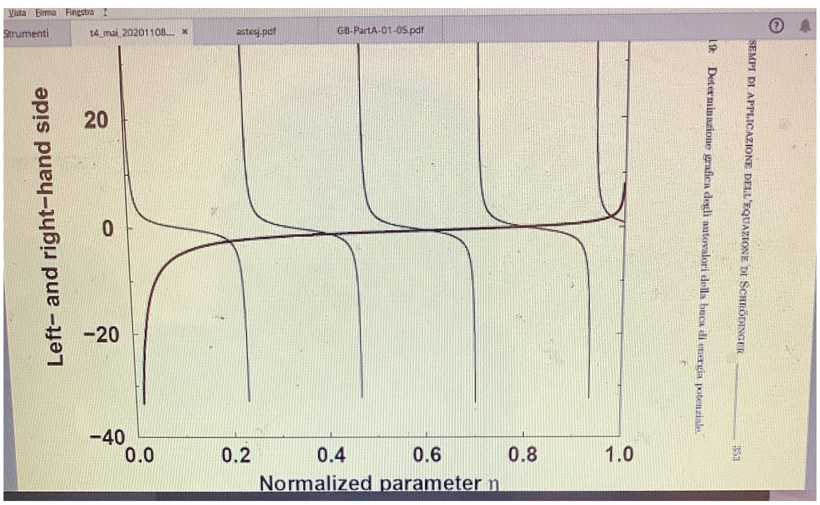
Maximum elongation

$$(n-1)\,\pi < s\sqrt{-(2m/\hbar^2)V_0} \leq n\pi\,.$$

Clearly, such an integer always exists, and indicates the number of branches of $\cot(ks)$ that belong (partially or completely) to the interval $V_0 < E < 0$. As in the same interval the left hand side increases monotonically from $-\infty$ to $+\infty$, the equation has exactly n roots $V_0 < E_1, E_2, \ldots, E_n < 0$. Each eigenvalue, say E_i, provides α_i, k_i, θ_i, whence

$$\frac{a_{i2}}{a_{i1}} = \frac{1}{2}\theta_i^*\,, \qquad \frac{a_{i3}}{a_{i1}} = \frac{1}{2}\theta_i\,, \qquad \frac{a_{i4}}{a_{i1}} = \frac{\theta_i^*}{\theta_i}\exp(\alpha_i s + j k_i s)\,.$$

The ith eigenfunction w_i can thus be expressed in terms of a_{i1} alone. The latter, in turn, is found from the normalization condition $\int_{-\infty}^{+\infty} |w_i|^2\,dx = 1$.



Quantitative Relations in Potential Well

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Let the size of the well be $s = 15$ Å $= 1.5 \times 10^{-9}$ m, its depth $-V_0 = 3$ eV $\simeq 4.81 \times 10^{-19}$ J. The maximum argument of the cotangent is found by letting $E = 0$ in $s\sqrt{2m(E - V_0)/\hbar^2}$, with $m \simeq 9.11 \times 10^{-31}$ kg, $\hbar \simeq 1.05 \times 10^{-34}$ J s. It is found

$$\gamma \doteq \frac{s}{\hbar}\sqrt{-2m\,V_0} \simeq 13.4\,, \qquad \frac{13.4}{\pi} \simeq 4.3\,, \qquad n = 5.$$

As a consequence, the cotangent has 4 complete branches and 1 incomplete branch in the interval $V_0 < E < 0$, corresponding to 5 eigenvalues $E_1, \dots, E_5$. Using the normalized parameters

$$0 < \eta \doteq \sqrt{1 - \frac{E}{V_0}} < 1\,,$$

the equation to be solved reads

$$\frac{\eta^2 - 1/2}{\eta\sqrt{1 - \eta^2}} = \cot(\gamma\,\eta)\,.$$

Over the η axis, the 5 branches belong to the intervals $(0, \pi/\gamma)$, $(\pi/\gamma, 2\pi/\gamma)$, $(2\pi/\gamma, 3\pi/\gamma)$, $(3\pi/\gamma, 4\pi/\gamma)$, $(4\pi/\gamma, 1)$.

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EBIT, Unibo
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