Stationary States

The time dependent Schrodinger equation in 1D:

$$i\hbar\frac{\partial}{\partial x}\psi(x,t) = \left[\frac{\hbar^2}{2m}\nabla^2 + V(x,t)\right]\Psi(x,t) = H\,\Psi(x,t)$$

H : the Hamiltonian

V(x) : the potential , assumed to be time independent

Let us calculate the solutions of this equation by using the method of separation of variables : ψ(t,x) = ψ(x)f(t)

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

Divide by $\psi(x)f(t)$

$$\frac{1}{f(t)}\,i\hbar\frac{\partial f(t)}{\partial t} = -\frac{1}{\psi(x)}\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} + V(x)$$

left hand side is only t dependent and the right hand side x dependent. So both sides must be equal to a constant, E (say). We can thus solve each side independently. The left side yields

$$\frac{1}{f(t)}\,i\hbar\frac{\partial f(t)}{\partial t} = E \quad\rightarrow\quad \frac{\partial f}{f} = -\frac{i}{\hbar}E\partial t \quad\rightarrow\quad f(t) = const.\,e^{-iEt/\hbar}$$

The constant in Eq. (4.4) will later on be absorbed into ψ(x).

The right side yields

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]\psi(x) = E\,\psi(x) \quad\rightarrow\quad H\,\psi(x) = E\,\psi(x)$$

This is time independent Schrodinger equation.

The Solution of time dependent Schrodinger equation is called **stationary state**, if it is represented by the wave function ψ(x,t) = ψ(x)e−iEt/ħ .

Why are they so called?

because the probability density of the states do not depend on time

$$|\Psi(x,t)|2 = \Psi^*(x,t)\Psi(x,t)$$

$$= (\Phi(x)e - iEt/\hbar)^*\Phi(x)e - iEt/\hbar$$

$$= \Phi^*(x)eiEt/\hbar)\Phi(x)e - iEt/\hbar$$

$$= \Phi^*(x)\Phi(x) = |\Phi(x)|2$$

The dependence on t has gone ⇒ Particle can stay there for ever unless disturbed.

The expectation values of observables A(x,p) are time independent

$$\langle A(x,p)\rangle = \int dx\,\psi^*(x)e^{\frac{iEt}{\hbar}}A\left(x,-i\hbar\frac{\partial}{\partial x}\right)\psi e^{\frac{-iEt}{\hbar}} = \int dx\,\psi^*(x)\,A\left(x,-i\hbar\frac{\partial}{\partial x}\right)\psi$$

(time dependence disappears)

Just take H(x,p) instead of A(x,p)………

The eigenvalues of the Hamiltonian, which are the possible energy levels of the system, are clearly time independent.

***Some interesting features about stationary states :

1. The normalization of the wavefunction will restrict the possible values of the constant E, the energy of the system in the Schrodinger equation.

2. For normalized solutions ψ(x) of the Schrodinger equation the energy E must be real.

3. Solutions ψ(x) of the time-independent Schrodinger equation can always be chosen to be real.

4. The parity operator P acting on a function f(x) changes the sign of its argument: Pf(x) = f(−x).

Try to prove yourselves…

We conclude that even and odd functions are eigenfunctions of the parity operator

Pψeven = +ψeven and Pψodd = −ψodd , which we will use later on.

Try to prove……

5.The time-independent Schrodinger equation is an eigenvalue equation. The stationary states ψi are eigenvectors/eigenfunctions of the Hamiltonian H with eigenvalues E. It implies stationary state has a precisely defined energy. Calculating the expectation value of the Hamiltonian for a stationary system just gives

$$\langle E \rangle = \int dx\, \psi^*(x)\, H\, \psi(x) = \int dx\, \psi^*(x)\, E\, \psi(x) = E \int dx\, \psi^*(x)\, \psi(x) = E$$

Consequently, there is no uncertainty in energy $\Delta E = 0$

6.The eigenvalues of hermitian operators are real and the eigenvectors corresponding to different eigenvalues are orthogonal. H is Hermitian and its eigenvectors corresponding to different eigenvalues are orthogonal.

7. For a symmetric potential $V(x) = V(-x)$, a basis of states ϕ_i can be chosen such that there is a family of even and odd solutions, which we will call $\psi(+)(x)$ and $\psi(-)(x)$

Try to prove……

EXPANSION INTO STATIONARY STATES

According to spectral theorem we can then expand a given state into a complete orthonormal system of energy eigenstates ϕ_n

$$\psi(x) = \sum_n c_n\, \phi_n(x)$$

Where $\int \psi^* \phi_i dx = \int \sum c_n{}^* \, \phi_n{}^* \phi_i dx = \int \sum c_n{}^* \delta_{ni} dx = c_i{}^* = c_i$

We can now extend the expansion from the time independent case to the time dependent one. We just remember the time dependent Schrodinger equation

$$i\hbar \frac{\partial}{\partial x} \Psi(x,t) = H\, \Psi(x,t)$$

with a particular solution $\psi_n(x,t) = \psi_n(x) e^{-iEt/\hbar}$

The general solution is then a superposition of particular solutions

$$\Psi_n(x,t) = \sum_n \psi_n(x) e^{-iEt/\hbar}$$

The expansion coefficients can easily be computed by setting t = 0 and taking the scalar product with $\psi_m(x)$

$$\int \psi_m{}^*(x)\,\Psi(x,0)dx = \int dx\,\psi_m{}^*(x)\sum_n c_n\ \phi_n(x)e^{-iE\frac{0}{\hbar}}$$

$$= \sum_n c_n \int dx\,\psi_m{}^*(x)\ \phi_n(x).1 = \sum_n c_n\,\delta_{mn} = c_m$$

Physical interpretation of the expansion coefficients:

- If a system is in an eigenstate Ψ_n of this observable A the expectation value in this state is equal to the corresponding eigenvalue a_n $A\,\Psi_n = a_n\,\Psi_n$
- The uncertainty of the observable vanishes for this state $\Delta A = 0$.
- The measurement leaves the state unchanged, the system remains in the eigenstate Ψ_n.

- If the system is in a general state ψ_i, which is a superposition of eigenstates ϕ_n,(ϕ_n is eigenstates of A), the expectation value is given by the sum of all eigenvalues, weighted with the modulus squared of the expansion coefficients

$$\langle A\rangle = \int \Psi^* A\Psi\,dx$$

$$= \sum_n\sum_m \int dx c_n{}^*\phi_n{}^*\,A\,c_m\phi_m$$

$$= \sum_n\sum_m c_n{}^*c_m \int dx\phi_n{}^*\,a_m\,\phi_m = \sum_n\sum_m c_n{}^*c_m a_m \int dx\phi_n{}^*\ \phi_m$$

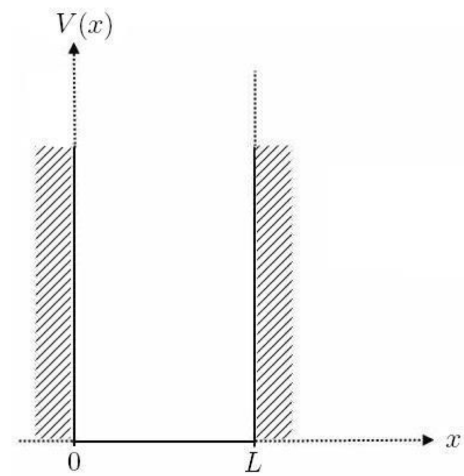
$$= \sum_n\sum_m c_n{}^*c_m a_m\delta_{nm} = \sum_n c_n{}^2 a_n$$

- The expansion coefficients c_n can thus be regarded as a probability amplitude for the transition from a state ψ to an eigenstate ϕ_m when the corresponding observable is measured. The actual transition probability is given by its modulus squared $|c_n|^2$, the probability for measuring the result a_n
- $\sum_n |c_n|^2 = 1$
- measurement of an observable in a general state changes the state to one of the eigenstates of the observable. This process is often called the reduction or collapse of the wave function $\Psi \xrightarrow{A} \phi_n$.

now we will calculate the energy eigenvalues and eigenfunctions for several Hamiltonians, i.e. for several potentials.

A. Infinite Potential Well

$$V(x) = \begin{cases} 0, & 0 \le x \le L \\ \infty, & otherwise \end{cases}$$



The quantum object is limited to a certain region between x = 0 and x = L where it moves freely but cannot leave.

The potential is infinite outside the interval [0 , L] and vanishes inside. Therefore the only physically allowed region for a particle is inside the interval.

Furthermore, for the wave function to be continuous we have to require that it vanishes at the boundaries x = 0 and x = L

$$\psi = 0 \ at \ x = 0 \ and \ x = L$$

The particles behave like free particles inside the well. Therefore we need to solve the time-independent Schrodinger equation with above mentioned boundary conditions .

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x) = E\psi(x) \qquad \text{Where } k^2 = \frac{2mE}{\hbar^2}$$

i.e $\frac{\partial^2}{\partial x^2}\psi(x) + k^2\psi(x) = 0$, whose general solution is

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

Here A and B are some constants that are yet to be determined by the boundary conditions, starting with ψ (0) = 0

$\Rightarrow$ 0=A sin(0)+Bcos(0) $\Rightarrow$ B=0 Therefore, $\psi(x) = A\sin(kx)$

Using the second boundary condition $\psi(x = L) = 0$, we get

0 = A sin (kL) $\Rightarrow$ kL=nπ $\Rightarrow$ $k_n = n\pi/L$

Therefore, $\psi_n(x) = A_n \sin(k_n x)$ $\Rightarrow \psi_n(x) = A_n \sin(n\pi x/L)$

where n = 1, 2, 3,….. can be any natural number.

$$E_n = \frac{k^2\hbar^2}{2m} = \frac{n^2\pi^2\hbar^2}{2mL^2} \quad \text{i.e energy is quantized}$$

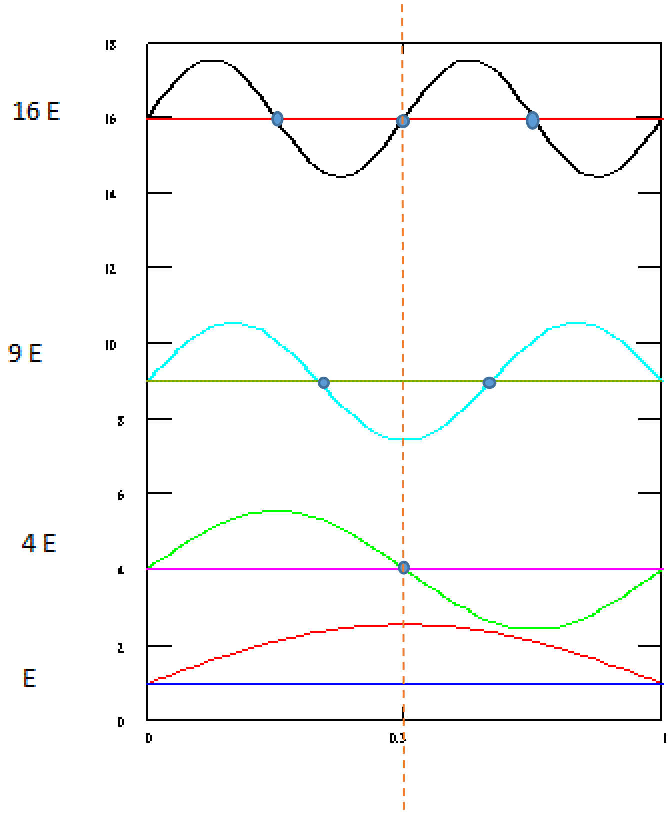
Normalization constant of wave function

$$\int_0^L dx|\psi|^2 = 1 \quad \Rightarrow \quad |a|^2\int_0^L dx\, sin^2(n\pi x/L) = 1 \quad \Rightarrow \quad |a|^2 = \frac{2}{L}$$

Thus the bound states of the infinite potential well are then given by

$$\psi_n(x) = \sqrt{\frac{2}{L}}\sin(n\pi x/L)$$

n	Energy values	Wave functions
1# ground state	E	$\sqrt{2/L}\,\sin(\pi x/L)$
2 # 1st excited state	4E	$\sqrt{2/L}\,\sin(2\pi x/L)$
3 # 2nd excited state	9E	$\sqrt{2/L}\,\sin(3\pi x/L)$
4 # 3rd excited state	16E	$\sqrt{2/L}\,\sin(4\pi x/L)$



We note a few features:

1. The ground state n = 1 has no nodes. A node is a zero of the wave function in $0 < x < L$. The zeroes at x = 0 and x = a do not count as nodes. Clearly $\psi_1(x)$ has no nodes.

It is in fact true that any normalizable ground state of a one-dimensional potential does not have nodes.

2. The first excited state, n = 2 has one node. It is at x = L/2, the midpoint of the interval. The second excited state, n = 3 has two nodes. The pattern in fact continues. The n-th excited state will have n nodes.

3. In the figure the dotted vertical line marks the interval midpoint x = L/2. We note that the ground state is symmetric under reflection about x = L/2. The first excited state is antisymmetric, indeed its node is at x = L/2. The second excited state is again symmetric. Symmetry and antisymmetry alternate forever.

4. The symmetry just noted is not accidental. It holds, in general for potentials V (x) that are even functions of x: V (-x) = V (x). Our potential, does not satisfy this equation, but this could have been changed easily. We could shift the origin s.t well extends from –L/2 to +L/2 , then it would be symmetric about the origin x = 0 . It

is in fact true that the bound states of a one-dimensional even potential are either even or odd!

5. The wavefunctions $\psi_n(x)$ with n = 1,2,... form a complete set that can be used to expand any function in the interval [0,L] that vanishes at the endpoints. If the function does not vanish at the endpoints, the convergence of the expansion is delicate, and physically such wavefunction would be problematic as one can verify that the expectation value of the energy is infinite.

B. Finite Potential Well

Its a similar problem only with the change that the potential walls are no longer infinitely high.

Classically, a particle is trapped within the box, if its energy is lower than the height of the walls, then it has zero probability of being found outside the box. We will see here that, quantum mechanically, the situation is different.

As before we will start with the time-independent Schrodinger equation and insert the following potential V (x) into our Hamiltonian

$$V(x) = \begin{cases} -V_0, -L \leq x \leq L & \Rightarrow\ |x| \leq L \\ \ \ 0, \qquad outside & \Rightarrow\ |x| > L \end{cases}$$

Suppose energy of the particle be negetive i.e -E $> -V_0 \Rightarrow E < V_0$

we consider separately the two energy regions,

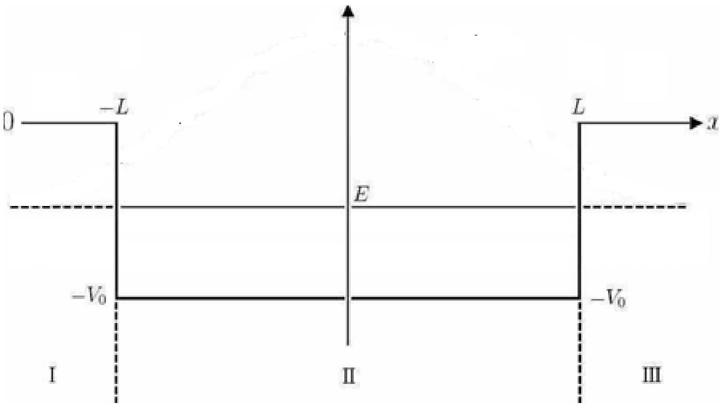
1. $-E$ **greater than** $-V_0 \quad \Rightarrow$ **the bound states**
2. **E > 0** $\Rightarrow$ **the scattered states.**

Lets split the whole x-range into the three regions I, II, and III, and solve the equations separately.

Region :1 $\Rightarrow \quad x < -L$

Region :II $\Rightarrow$ $-L \leq x \leq L \Rightarrow |x| \leq L$

Region :III $\Rightarrow$ $x > L$



Lets solve for Bound states

Region :1 $\boldsymbol{x < -L}$, **V = 0**

Time independent SE:

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x) = -E\,\psi(x)\,, \qquad \text{Where } k^2 = -\frac{2mE}{\hbar^2}$$

Or, $\frac{\partial^2}{\partial x^2}\psi(x) - k^2\psi(x) = 0$, whose general solution is

$$\psi(x) = Ae^{kx} + Be^{-kx}$$

Here A and B are some constants that are yet to be determined by the boundary conditions.

Since we are in the region where x < -L the exponent of the second term would diverge with ever decrease for x . In order to keep the wave function normalizable we must demand that the constant B be identically zero, and we get as solution for region I

$$\psi(x) = Ae^{kx}$$

Region :II $\boldsymbol{-L \leq x \leq L} \Rightarrow \boldsymbol{V(x) = -V_0}$

Time independent SE:

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x) - V_0\,\psi(x) = -E\,\psi(x)\ ,$$

Or, $\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x) + V_0\,\psi(x) = E\,\psi(x)$

Or, $\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x) + (V_0 - E)\,\psi(x) = 0$

Here $\frac{2m(V_0-E)}{\hbar^2} > 0$, since $E < V_0$ so call $\frac{2m(V_0-E)}{\hbar^2} = q^2$

Or, $\frac{\partial^2}{\partial x^2}\psi(x) + q^2\psi(x) = 0$, whose general solution is

$$\psi(x) = C\sin(qx) + D\cos(qx)$$

Region :1 $\boldsymbol{x > L}$ $\Rightarrow$ **V = 0**

Same as Region :1

$$\psi(x) = Ge^{kx} + Fe^{-kx}$$

Here A and B are some constants that are yet to be determined by the boundary conditions.

Since we are in the region where x > L the exponent of the first term would diverge with ever increase for x . In order to keep the wave function normalizable we must demand that the constant G be identically zero, and we get as solution for region I

$$\psi(x) = Fe^{-kx}$$

Therefore for bound state, E<0 and -V_0 < -E < 0

$$\psi(x) = \begin{cases} Ae^{kx}\ , & for\ \boldsymbol{x < -L},\ \boldsymbol{Region: I} \\ C\sin(qx) + D\cos(qx), & for - \boldsymbol{L \le x \le L}\ ,\boldsymbol{Region: II} \\ Fe^{-kx}\ , & for\ \ \boldsymbol{x > L}\ \ ,\boldsymbol{Region: III} \end{cases}$$

Remark: The motion of a classical particle with energy E < 0 is strictly confinned to region II. A quantum mechanical particle, however, can

penetrate into the classically forbidden regions I and III, i.e. the probability density is non-vanishing, $|\psi(x)|^2 \neq 0$.**How far the particle can penetrate depends on the respective energy**, it can reach a depth of about

$$\Delta x \; \alpha \; \frac{1}{k} = \frac{\hbar}{\sqrt{2mE}} \rightarrow 0 \; as \; E \rightarrow infinity$$

Thus, penetration vanishes for large energies in deep potentials. Accordingly, there exists a momentum uncertainty which a classical particle would need to overcome the potential barrier

$$\Delta p \quad \alpha \quad \frac{\hbar}{\Delta x} = \sqrt{2mE}$$

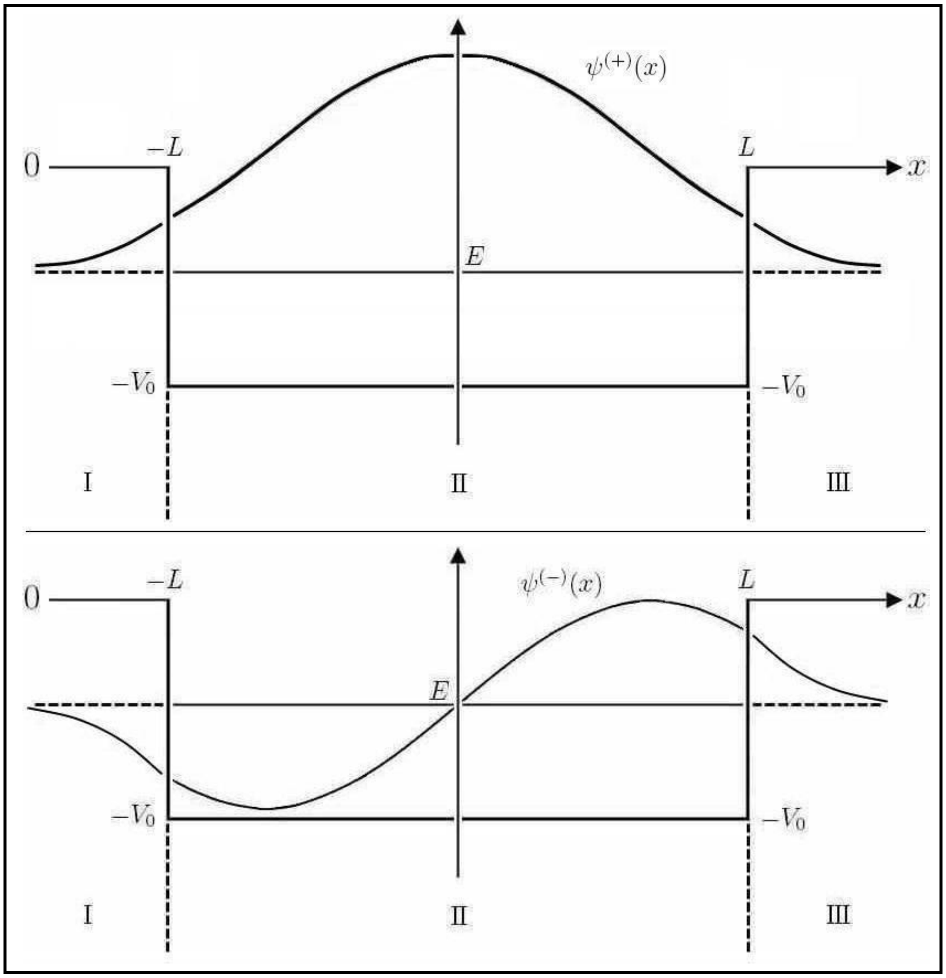
Lets remember a we pointed earlier for a symmetric potential V(x) =V(-x), a basis of states ϕ_i can be chosen such that there is a family of even and odd solutions, which we will call $\psi_{(+)}(x)$ and $\psi_{(-)}(x)$

Here V(x) is symmetrical, we should have a set of even solution, $\psi_{(+)}(x)$ and a set of odd solution, $\psi_{(-)}(x)$

$$\psi_+(x) = \begin{cases} Ae^{kx}, \boldsymbol{Region}: \boldsymbol{I} \\ D\cos(qx), \boldsymbol{Region}: \boldsymbol{II} \\ Ae^{-kx}, \boldsymbol{Region}: \boldsymbol{III} \end{cases}$$

$$\psi\_(x) = \begin{cases} -Ae^{kx}, \boldsymbol{Region}: \boldsymbol{I} \\ C\sin(qx), \boldsymbol{Region}: \boldsymbol{II} \\ Ae^{-kx}, \boldsymbol{Region}: \boldsymbol{III} \end{cases}$$

At the boundaries of the potential well the functions that are solutions in their respective areas need to merge smoothly into each other. Mathematically this means, that the total wave function needs to be smooth, i.e. the values as well as the first derivatives of the respective partly solutions must match at ±L.



We can summarize these two requirements into the statement, that the logarithmic derivative of the wave function must be continuous

Logarithmic derivative: $\frac{d}{dx}\, ln\psi(x) = \frac{\psi'(x)}{\psi(x)}$ *must be continuous*

It does not matter here whether one chooses the boundary between regions I and II or II and III, the result is the same.

For even solution, $\psi_+(x)$, $\left.\frac{\psi_+'(x)}{\psi_+(x)}\right|_{x\to L} = \frac{-Dq sin(qL)}{Dcos(qL)} = \frac{-Ake^{-kL}}{Ae^{-kL}}$

$$\Rightarrow \quad \boldsymbol{q tan(qL) = k}$$

We know q and k depend on energy. $\boldsymbol{q tan(qL) = k}$ **is quantisation formula for energy i.e it gives permitted energies only.**

For odd solution, $\psi_-(x)$, **the quantisation formula for energy :** $\boldsymbol{q\cot(qL) = -k}$

Graphical solution: $\boldsymbol{q\tan(qL) = k}$ and $\boldsymbol{q\cot(qL) = -k}$ are called transcendental equations, which means that they can only be written in implicit form. Solutions to these equations can be found numerically or graphically, but not analytically. However before we do so, we will introduce new (dimensionless) variables z and z_0 to simplify the calculation

$\boldsymbol{z = qL}$ **and** $\boldsymbol{z_0 = \frac{L}{\hbar}\sqrt{2mV_0}}$

$$k^2 + q^2 = \frac{2mE}{\hbar^2} + \frac{2m(V_0 - E)}{\hbar^2} = \frac{2mV_0}{\hbar^2}$$

Now, $(k^2 + q^2)L^2 = \frac{2mV_0}{\hbar^2}L^2 = {z_0}^2$

$$\Rightarrow (k^2L^2 + q^2L^2) = {z_0}^2 \Rightarrow \frac{k^2L^2}{q^2L^2} + 1 = \frac{{z_0}^2}{q^2L^2} = \frac{{z_0}^2}{z^2} \Rightarrow \frac{k^2L^2}{q^2L^2} = \frac{{z_0}^2}{z^2} - 1$$

$$\Rightarrow \frac{k}{q} = \sqrt{\frac{{z_0}^2}{z^2} - 1}$$

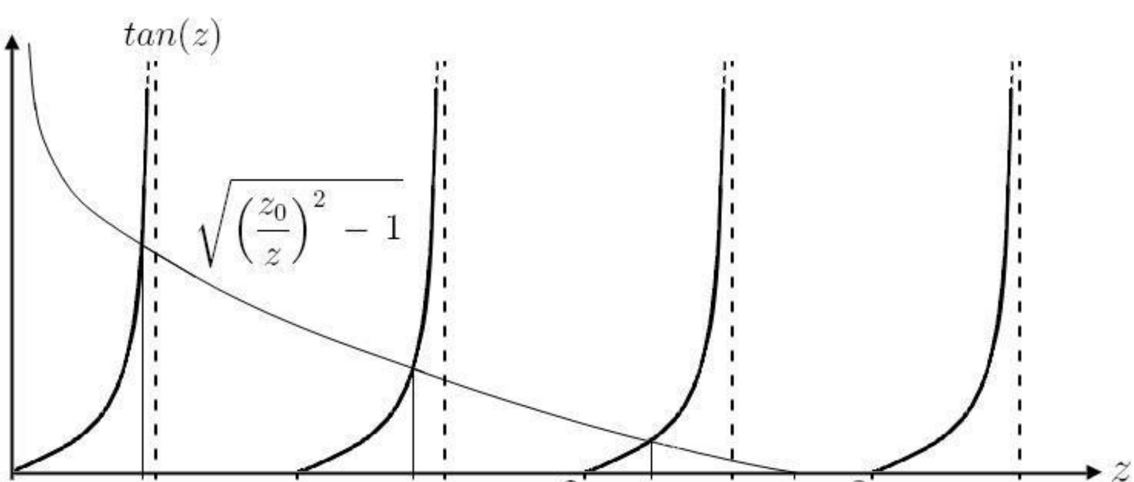
Therefore, quantisation formulae for energy :

$$\boldsymbol{\tan z} = \sqrt{\frac{{z_0}^2}{z^2} - 1}, \quad \textit{for} \text{ even solution, } \psi_+(x)$$

$$\boldsymbol{\cot z} = -\sqrt{\frac{{z_0}^2}{z^2} - 1}, \quad \textit{for} \text{ odd solution, } \psi_-(x)$$

We can now study this graphically by plotting both the left hand and the right hand function for given values of z_0, e.g. for L, m and V_0 . Below I am plotting two equations:

$$y = \boldsymbol{\tan z} \qquad \boldsymbol{and} \qquad \boldsymbol{y = \sqrt{\frac{{z_0}^2}{z^2} - 1}}, \quad \text{for} \quad z_0 = 8 \Rightarrow \frac{L}{\hbar}\sqrt{2mV_0}$$



The intersections lead to the allowed values of

For the chosen parameter we have three solutions $z_1 = 0.8\pi/2$, $z_2 = 2.6\ \pi/2_2$ and $z_3 = 4.25\pi/2$.

$$\boldsymbol{z_n = q_n L} = \sqrt{\frac{2m(V_0 - E_n)}{\hbar^2}}\ L = \frac{L}{\hbar}\sqrt{2m(V_0 - E_n)}$$

This gives allowed values of E_n.

For increasing parameters L and V_0 the value of z_0 increases and we obtain more bound states.

You please repeat the same procedure for the odd states by replacing tan z with -cot z and find the energies of the odd solutions at Home.

Special cases: Let us now study some limits of the graphical solutions, where we can find analytical approximations to our problem.

Case I: Broad & deep potential well:

For big values for L and V_0 the quantity z_0 becomes high and the intersections with the tan-curves are closer to $(2n+1)\pi/2$, where n=0,1,2…….

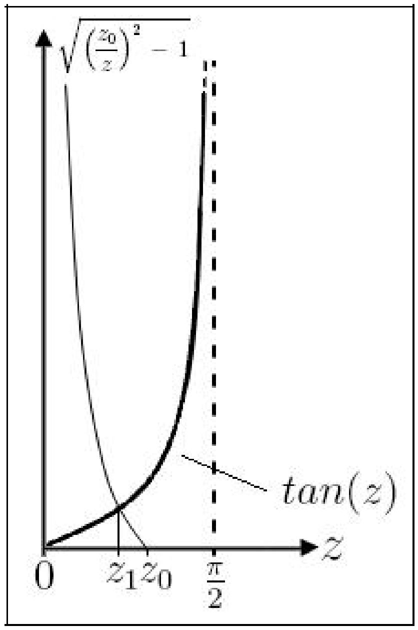
$$\boldsymbol{z_n = (2n+1)\pi/2}$$

$$\boldsymbol{z_n}^{\mathbf{2}} = \frac{2m(V_0 - E_n)}{\hbar^2}\ L^2 = \boldsymbol{(2n+1)^2\pi^2/4}$$

$$-E_n \approx\ -V_0 + \frac{\boldsymbol{(2n+1)^2\pi^2}\hbar^2}{\boldsymbol{8}mL^2}$$

Case I: Narrow & small potential well:

Here L and V_0 values are small, z_0 less, much less than $\pi/2$



However small the parameter z_0, an intersection of the functions always remains, but intersecting points are less. Here we are getting only one intersecting point $\Rightarrow$ there is only one bound state i.e even bound state.

There may not be odd bound state.

At least one even bound state we must get…..

Summary

$\boldsymbol{tanz} = \sqrt{\frac{{z_0}^2}{z^2} - 1}$ is for even solution, $\psi_+(x)$, exist for z= 0 to π/2, π to 3π/2, 2π to 5π/2 and so on

$-\boldsymbol{cotz} = \sqrt{\frac{{z_0}^2}{z^2} - 1}$ is for odd solution, $\psi\_(x)$, exist for z= π/2 to π, 3π/2 to 2π, 5π/2 to 3π and so on.=

Ground state is even function, Ist excited state is an odd function, 2^{nd} excited state is again even function….

Let us now return again to the even and odd wavefunctions, where we still have to determine the constants A, C and D. We first use the continuity of ψ_+ and $\psi\_$ at x = L

$$\psi_+(x)\big|_{x=L} = \psi_+(x)\big|_{x=L}, \quad \text{which gives} \quad D\cos(q_n L) = Ae^{-k_n L}$$

Therefore, $D = A\dfrac{e^{-k_nL}}{\cos(q_nL)}$

And

$\psi\_(x)\big|_{x=L} = \psi\_(x)\big|_{x=L}$, which gives $C\sin(q_nL) = Ae^{-k_nL}$

Therefore, $C = A\dfrac{e^{-k_nL}}{\sin(q_nL)}$

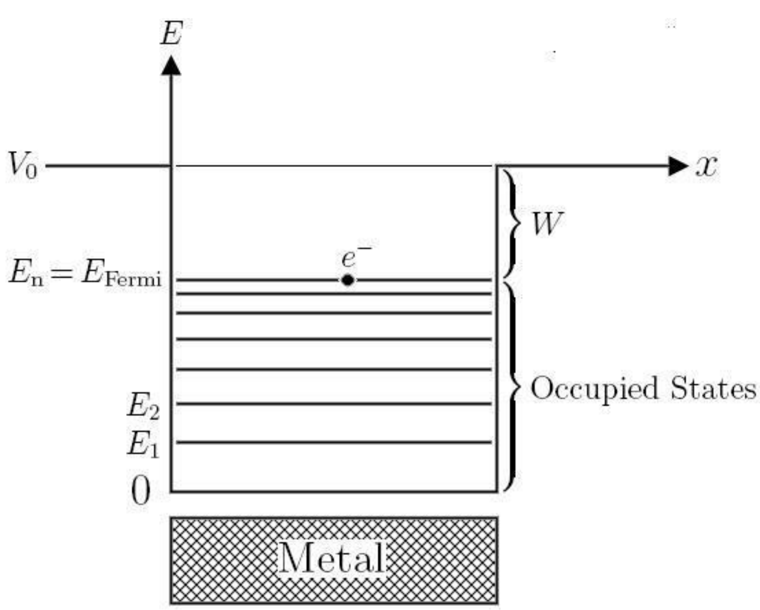
A can be obtained from normalization,

$$A_n = \frac{\cos\,(q_nL)}{\sqrt{1+k_nL}}e^{k_nL} \Rightarrow C_n = D_n = \frac{1}{\sqrt{1+k_nL}}$$

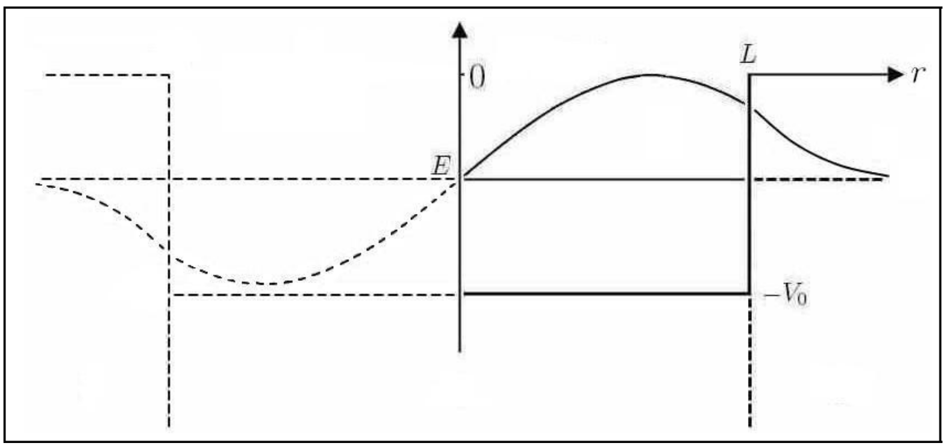
Physical interpretation of the finite potential well: An application for the finite potential well is the model for free electrons in metal, used in solid state physics. There the atoms of the metal crystal **share** the electrons which are free to move inside the metal, but face a potential barrier, which keeps them inside. Thus in a first approximation, the finite (square) potential well is a good model for the situation.

To release one electron from the metal, the energy W must be invested. This is the work function, which we can calculate3 with the formula $W = V_0 - E_n$,

Keep in mind, that we rescaled the energy here in contrast to our previous calculations, the potential V_0 as well as the energies of the bound states are positive here.



Though we solved a 1D problem, the square well represents a 3D problem as well. Consider for example a spherical well in 3D: The potential is zero inside a region of radius a and is V_0 for r > a. Then we can rewrite the time independent Schrodinger equation in 3D for this potential in spherical coordinates and use separation of variables ({r, ϑ, ϕ}). Because of symmetry, the wavefunction is a constant in ϑ and ϕ, thus we will have to solve just a single differential equation for the radial variable, very similar to what found here. We must then choose the odd-parity solution in order to obtain a finite wavefunction at r = 0. Thus in 3D, only the odd solutions are possible and we need a minimum potential well depth in order to find a bound state which is the equivalent of the first excited state of 1D.



B. Suppose the energy of the particle be E > 0 i.e lets investigate Scattered States

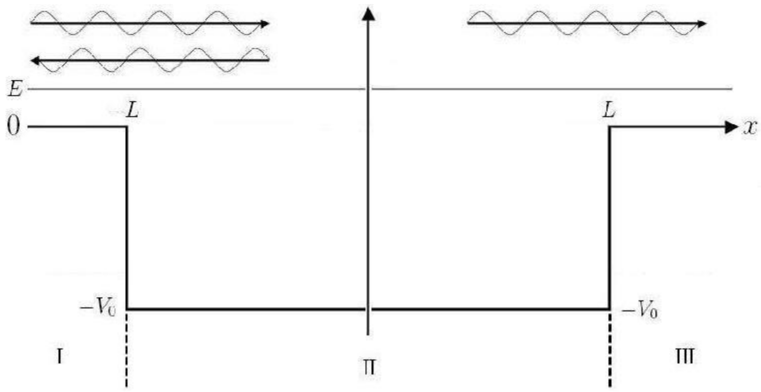
As before we will split our problem for the regions I, II and III

Region :1 $\Rightarrow$ $x < -L$

Region :II $\Rightarrow$ $-L \leq x \leq L \Rightarrow |x| \leq L$

Region :III $\Rightarrow$ $x > L$

We will assume that an initial plane wave travels from $x = -\infty$ to our potential and study the possible states that are not bound but scattered, i.e. transmitted or reflected by the potential



Region :1 $\boldsymbol{x < -L}$ $\Rightarrow$ **V = 0**

Time independent SE:

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\,\psi(x) = +E\,\psi(x)\ , \qquad \text{Where } k^2 = \frac{2mE}{\hbar^2}$$

Or, $\frac{\partial^2}{\partial x^2}\psi(x) + k^2\psi(x) = 0$, whose general solution is

$$\psi(\mathrm{x}) = \underbrace{\mathrm{A}e^{ikx}}_{incoming} + \underbrace{\mathrm{B}e^{-ikx}}_{reflected}$$

Here A and B are some constants that are yet to be determined by the boundary conditions.

Region :II $\boldsymbol{-L \le x \le L}$ $\Rightarrow$ $\boldsymbol{V(x) = -V_0}$

Time independent SE:

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\,\psi(x) - V_0\,\psi(x) = E\,\psi(x)\ ,$$

Or, $\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\,\psi(x) + V_0\,\psi(x) = -E\,\psi(x)$

Or, $\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\,\psi(x) + (V_0 + E)\,\psi(x) = 0$

Here $\frac{2m(V_0+E)}{\hbar^2} > 0$, so call $\frac{2m(V_0+E)}{\hbar^2} = q^2$

Or, $\frac{\partial^2}{\partial x^2}\psi(x) + q^2\psi(x) = 0$, whose general solution is

$$\psi(\mathrm{x}) = \mathrm{C}\sin(qx) + \mathrm{D}\cos(qx)$$

Region :1 $\boldsymbol{x > L}$ $\Rightarrow$ **V = 0**

Same as Region :1

$$\psi(\mathrm{x}) = \mathrm{G}e^{ikx} + \mathrm{F}e^{-ikx}$$

Here A and B are some constants that are yet to be determined by the boundary conditions. Since no wave is coming from infinity i.e from right to left F=0

$$\psi(\mathrm{x}) = \mathrm{G}e^{ikx}$$

Lets summerize,
$$\psi(\mathrm{x}) = \begin{cases} \mathrm{A}e^{ikx} + Be^{-ikx} & : I \\ \mathrm{C}\sin(qx) + \mathrm{D}\cos(qx) & : II \\ \mathrm{G}e^{ikx} & : III \end{cases}$$

We apply the boundary conditions, i.e. the continuity of the wave function and its first derivative at the edges of the potential wall

At x= -L: $\mathrm{A}e^{-ikL} + Be^{ikL} = -\mathrm{C}\sin(qL) + \mathrm{D}\cos(\mathrm{qL})$

and $ik\left(\mathrm{A}e^{-ikL} - Be^{+ikL}\right) = q(C\cos(qL) + Dsin(qL))$

At x= L: $\mathrm{C}\sin(qL) + \mathrm{D}\cos(\mathrm{qL}) = Ge^{ikL}$

and $q(C\cos(qL) - Dsin(qL)) = ike^{+ikL}$

Together with the normalization condition we thus have 5 equations for our 5 variables A, B, C, D and F.

$$D = \left(cos(qL) - i\frac{k}{q}sin(qL)\right)Ge^{ikL}$$

$$C = \left(sin(qL) + i\frac{k}{q}cos(qL)\right)Ge^{ikL}$$

$$2B = i\left(\frac{q}{k} - \frac{k}{q}\right)\sin(2qL)\ G$$

$$\Rightarrow \quad \frac{B}{G} = i\left(\frac{q^2-k^2}{2qk}\right) sin(2qL) \quad \Rightarrow \quad \frac{Reflection\ Amplitude}{\text{Transmission Amplitude}}$$

To get the probability for the reection or transmission we have to normalize each part by the amplitude of the incoming wave and to take the modulus squared of each expression. We also want to express the quantities q and k by the more familiar constants m, ħ and V_0

$$.q^2 - k^2 = \frac{4m^2{V_0}^2}{\hbar^4}\ , \qquad (2qk)^2 = 4\frac{4m^2}{\hbar^4}E(E+V_0)$$

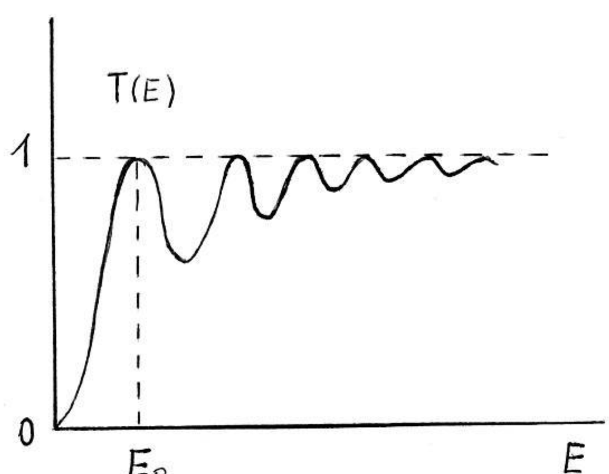
Thus we find for the reflection coefficient R(E) describing the probability of reflection

$$Reflection\ Coeff., R = \frac{|B|^2}{|A|^2} = \frac{{V_0}^2}{4E(E+V_0)}\ sin^2(2qL)\frac{|G|^2}{|A|^2}$$

Transmission amplitude: $\frac{G}{A} = e^{-2ikL}\left[\cos(2qL) - i\frac{q^2+k^2}{2qk}\sin\,(2qL)\right]^{-1}$

$$Transmission\ coeff., T = \frac{|G|^2}{|A|^2} = \left[1 + \frac{{V_0}^2}{4E(E+V_0)}\sin^2(2qL)\right]^{-1}$$

$$R + T$$



Transmission coefficient is plotted as a function of the energy showing the positions E_R of the resonances.

$$T = 1 \quad for \sin(2qL) = 0$$

i.e $for \quad 2qL = n\pi \quad \Rightarrow \quad \frac{2L}{\hbar}\sqrt{2m(E+V_0)} = n\pi \Rightarrow \mathbf{E}_n = \frac{n^2\pi^2\hbar^2}{8mL^2} - V_0$

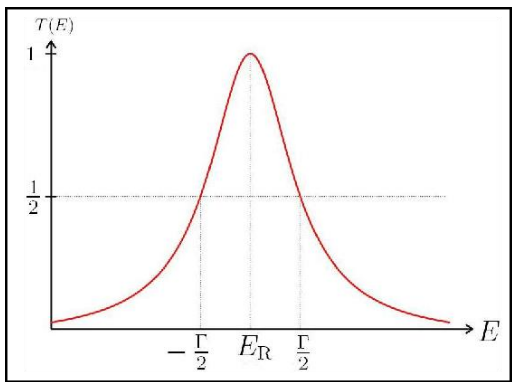
Maximum allowed transmission energy is $\mathbf{E}_R = \frac{n^2\pi^2\hbar^2}{8mL^2} - V_0$

Transmission is minimum for

$$\sin(2qL) = \pm 1 \Rightarrow 2\mathrm{qL} = (2n+1)\frac{\pi}{2} \Rightarrow \frac{2L}{\hbar}\sqrt{2m(E+V_0)} = (2n+1)\frac{\pi}{2}$$

Minimum allowed transmission energy is $\mathbf{E}_{min} = \frac{(2n+1)^2\pi^2\hbar^2}{32mL^2} - V_0$

It can be shown that Transmission coefficient falls off from max value like resonance curve.



This is the well-known Breit–Wigner distribution, also known as Lorentz- or Cauchy distribution, which describes resonance phenomena. The quantity Γ represent the width at half maximum of the distribution

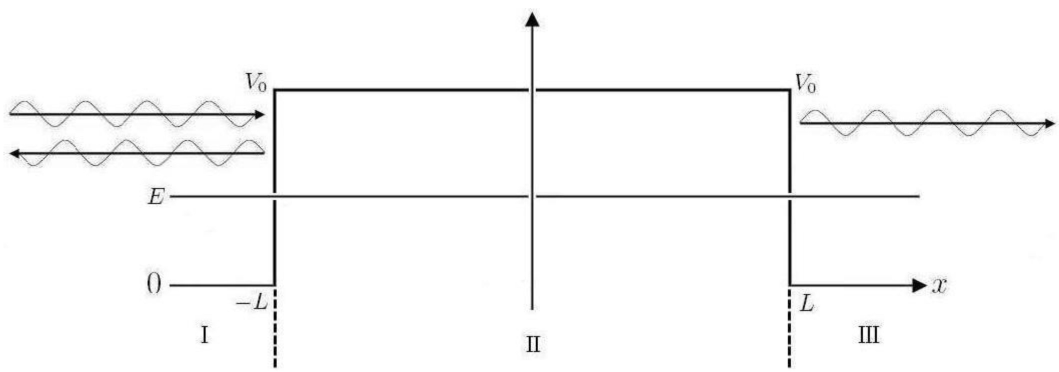
Ramsauer-Townsend experiment

The resonance of transmission can be nicely seen in the scattering of slow electrons in a noble gas (e.g. Ne, Ar, Xe) which has been studied independently by C. Ramsauer and J.S. Townsend in the 1920's. The probability for the electrons to collide with the gas particles, which classically should decrease monotonically for increasing energy, is observed to reach local minima for certain energies. This experiment is in total agreement with the quantum mechanical prediction of transmission of energy through potential well.

Tunnel Effect

The so-called tunnel effect of quantum mechanics can be derived from a special case of the potential well, by changing $-V_0$ into $+V_0$, thus creating a potential barrier.

$$V(x) = \begin{cases} +V_0, -L \leq x \leq L & \Rightarrow \ |x| \leq L \\ \quad 0, \qquad outside & \Rightarrow \ |x| > L \end{cases}$$



For a given potential barrier with height V_0 the solutions of the Schrodinger equation with energy $E < V_0$ still have a nonvanishing probability density in region III, which allows them to "tunnel" through the barrier although this would classically be forbidden.

Classically, a particle with less energy than the potential barrier could only be reflected. But in quantum mechanics, due to continuity the wave function decreases exponentially in the forbidden region II, resulting in a nonvanishing probability density in region III. It allows the particle to pass the barrier as if it was through a tunnel, this linguistic illustration gives rise to the name tunnel effect.

Region :1 $\boldsymbol{x < -L}$ $\Rightarrow$ **V = 0**

Time independent SE:

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x) = +E\,\psi(x)\ , \qquad \text{Where } k^2 = \frac{2mE}{\hbar^2}$$

Or, $\frac{\partial^2}{\partial x^2}\psi(x) + k^2\psi(x) = 0$, whose general solution is

$$\psi(\mathrm{x}) = \mathrm{A}e^{ikx} + \mathrm{B}e^{-ikx}$$

Here A and B are some constants that are yet to be determined by the boundary conditions.

Region :II $\boldsymbol{-L \le x \le L} \quad \Rightarrow \quad \boldsymbol{V(x) = V_0}$

Time independent SE:

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x) + V_0\,\psi(x) = E\,\psi(x)\,,$$

Or, $\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x) - V_0\,\psi(x) = -E\,\psi(x)$

Or, $\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x) - (V_0 - E)\,\psi(x) = 0$

Here $\frac{2m(V_0-E)}{\hbar^2} > 0$, so call $\frac{2m(V_0-E)}{\hbar^2} = q^2$

Or, $\frac{\partial^2}{\partial x^2}\psi(x) - q^2\psi(x) = 0$, whose general solution is

$$\psi(\mathrm{x}) = \mathrm{C}\sinh(qx) + \mathrm{D}\cosh(qx)$$

Region :1 $\boldsymbol{x > L} \quad \Rightarrow \quad$ **V = 0**

Same as Region :1

$$\psi(\mathrm{x}) = \mathrm{G}e^{ikx} + \mathrm{F}e^{-ikx}$$

Here A, B, C and D are some constants that are yet to be determined by the boundary conditions. Since no wave is coming from infinity i.e from right to left F=0

$$\psi(\mathrm{x}) = \mathrm{G}e^{ikx}$$

Lets summerize,

$$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & : I \\ C\, e^{-qx} + D\, e^{qx} & : II \\ Ge^{ikx} & : III \end{cases}$$

Where $k = \frac{\sqrt{2mE}}{\hbar}$ and $\frac{\sqrt{2m(V_0-E)}}{\hbar} = q$

Applying continuity conditions of $\psi(x)$ and its first derivative at boundaries, +L and -L

For the transmission amplitude we get the result

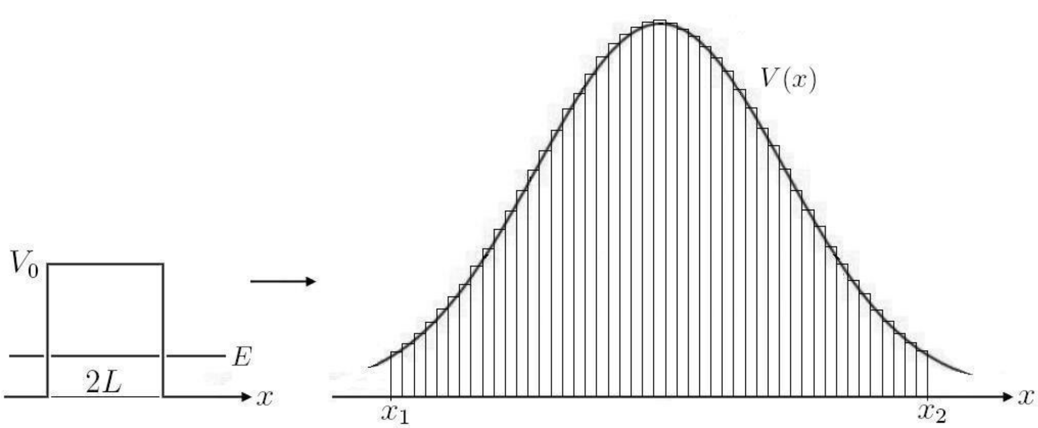
$$\frac{F}{A} = e^{-2ikL}\left[\cosh(2qL) - i\frac{q^2-k^2}{2qk}\sinh(2qL)\right]^{-1}$$

$$Transmission\ coeff.,T = \frac{|F|^2}{|A|^2} = \left[1 + \frac{(k^2+q^2)}{4k^2q^2}\sinh^2(2qL)\right]^{-1}$$

$$= \left[1 + \frac{{V_0}^2}{4E(V_0-E)}\sinh^2(2qL)\right]^{-1}$$

$$\approx \frac{16E((V_0-E)}{{V_0}^2}e^{-\frac{4L}{\hbar}\sqrt{2m(V_0-E)}}, \quad \text{if qL>>>1}$$

We now have a good approximation for the transmission probability of a single potential step, constant in certain interval and vanishing outside. This potential is of course a very crude approximation of real life potentials, which usually are more complicated functions of x. To meet these concerns we can generalize the transmission coefficient to the so called Gamow factor by "chopping" a given potential in infinitesimal potential steps with constant values and integrating over a reasonable range $[x_1, x_2]$.



$$T \approx e^{-\frac{2}{\hbar}\int_{x1}^{x2} dx\sqrt{2m(V(x)-E)}}$$

Physical Examples of Tunneling

Tunneling between conductors: Imagine two conducting materials, separated by a thin insulating material, The tunnel effect then allows the electrons to tunnel through that barrier, creating a current. This effect is also observed for superconducting materials, where it is named Josephson effect.

Cold emission

If we consider the electrons in a metal at 0K temperature, we know that a certain amount of energy (work function) is necessary to bring the electron out of the metal. In this condition the electrons are not escaping and they are trapped by an approximate square barrier. Electrons can be removed by heating the metal, or transferring energy through photons (photoelectric effect) or applying an external electric field. In this case the potential seen by the electrons is not *perfect rectangular barrier* but slightly different. This includes, *e*, the charge of the electron, *E,* the intensity of the electric field, imperfection of the metal. And when an electron leaves the surface an image positive charge is created and this attracts the escaping electron. That effect is also included in the barrier potential.

We use

$$T \approx e^{-\frac{2}{\hbar}\int_{x1}^{x2} dx\sqrt{2m(V(x)-E)}}$$

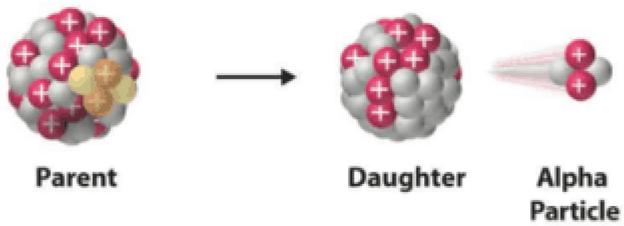
substitute the new potential in the formula and calculate the new transition coefficient:

$$T \approx \exp\left(-\frac{8\pi^2\sqrt{2mV}}{\hbar^2}\left(\frac{V}{eE}\right)\right.$$

This is called Fowler-Norheim formula and describes the emission only qualitatively.

Alpha decay

It is the disintegration of a parent nucleus to a daughter through the emission of the nucleus of a helium atom.



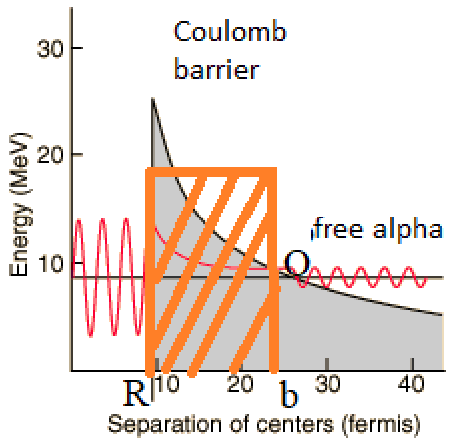
$${}^{A}_{Z}X \quad \rightarrow \quad {}^{A-4}_{Z-2}Y + {}^{4}_{2}He$$

Alpha decay is a quantum tunneling process. In order to be emitted, the alpha particle must penetrate a potential barrier. The height of the **Coulomb barrier** for nuclei of A « 200 is about **20-25 MeV.** By 1928, **George Gamow** (and independently by **Ronald Gurney** and **Edward Condon**) had solved the theory of **alpha decay** via **quantum tunneling**. They assumed that the alpha particle and the daughter nucleus exist within the parent nucleus prior to its dissociation,. The alpha particle is trapped in a potential well by the parent nucleus. Classically, it is forbidden to escape, but according to the quantum mechanics, it has a tiny (but non-zero) probability of "tunneling" through the barrier and appearing on the other side to escape the nucleus. Using the tunneling mechanism, Gamow, Condon and Gurney calculated the penetrability of the tunneling α particle through the Coulomb barrier, using the following formula and found the lifetimes of some α emitting nuclei.

$$Transmission\ coeff., T = \frac{16E((V_0 - E)}{{V_0}^2} e^{\frac{-4L}{\hbar}\sqrt{2m(V_0-E)}},$$

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

The main success of this model was the reproduction of the semi-empirical Geiger-Nuttall law that expresses the lifetimes of the α emitters in terms of the energies of the released α particles



Actual Barrier: shaded ash colour

We consider an equivalent rectangular barrier, bordered yellow. Point O is very important. This determines the width of equivalent barrier.

2L=R-b

R : Nuclear radius

$b = 2Ze^2/E$

E: energy of alpha particle

V_0=16MeV

Ref: pg 186, Introduction to Quantum Mechanics by S N Ghoshal (for alpha decay)