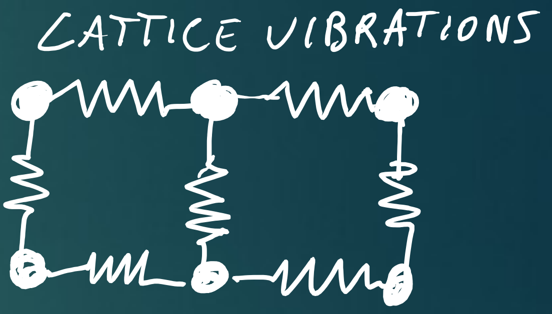
UNIVERSITÀ DEGLI STUDI DI MILANO BICOCCA

One-Dimensional Potentials II

(with extension to the 3D case)

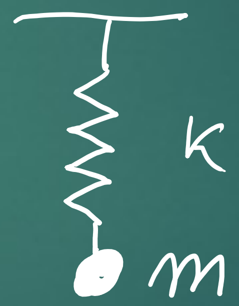
Harmonic Oscillator

Harmonic oscillators are ubiquitous and appear every time when one is dealing with a system that can oscillate around its equilibrium state (e.g. atoms, molecules, solids, electromagnetic field, etc).



The typical classical representation of the armonic oscillator is a mass m attached to a spring.

Acoording to the Hooke's law:



$$F = -kx = m\frac{\mathrm{d}^2 x}{\mathrm{d}t^2}$$

The solution has the form:

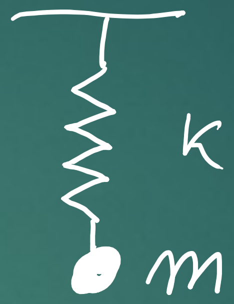
$$x(t) = A\sin(\omega t) + B\cos(\omega t)$$

with $\omega \equiv \sqrt{\dfrac{k}{m}}$ Angular frequency of oscillations

Harmonic Oscillator

According to the Hooke's law:

$$F = -kx = m\frac{d^2x}{dt^2}$$



The solution has the form:

$$x(t) = A\sin(\omega t) + B\cos(\omega t)$$

with $\omega \equiv \sqrt{\dfrac{k}{m}}$ — Angular frequency of oscillations

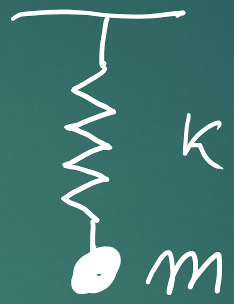
The potential energy is:

$$V(x) = \frac{1}{2}kx^2 = \frac{1}{2}m\omega^2x^2$$

Harmonic Oscillator

According to the Hooke's law:

$$F = -kx = m\frac{\mathrm{d}^2 x}{\mathrm{d}t^2}$$



The solution has the form:

$$x(t) = A\sin(\omega t) + B\cos(\omega t)$$

with $\omega \equiv \sqrt{\frac{k}{m}}$ Angular frequency of oscillations

The potential energy is:

$$V(x) = \frac{1}{2}kx^2 = \frac{1}{2}m\omega^2 x^2$$

Harmonic Oscillator

Let's imagine that we are studying a particle moving in one dimension, subject to a conservative force with a corresponding potential energy function U (x). V

For small $(x - x_0)$

$$E_T = V + E_k$$

Expansion in Taylor series around x_0

$$V(x) \cong V(x_0) + V'(x_0)(x - x_0) \quad + \frac{1}{2}V''(x_0)(x - x_0)^2$$

0

Like a harmonic oscillator potential

$$V(x) = \frac{1}{2}kx^2$$

Harmonic Oscillator

The quantum problem is to solve the S.E. for the potential:

$$V(x) = \frac{1}{2} K x^2 = \frac{1}{2} m\omega^2 x^2$$

Thus, the Hamiltonian will be:

$$H = \frac{p^2}{2m} + \frac{1}{2} K x^2$$

While the T.I.S.E. for a particle moving in a simple harmonic oscillator:

$$\frac{d^2\psi}{dx^2} = \frac{2m}{\hbar^2}\left(\frac{1}{2} K x^2 - E\right)\psi$$

With $k = \omega^2 m$

$$= \frac{2m}{\hbar^2}\left(\frac{1}{2} m\omega^2 x^2 - E\right)\psi$$

We can write:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = \left(E - \frac{1}{2} m\omega^2 x^2\right)\psi$$

or

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2} m\omega^2 x^2\right)\psi = E\,\psi$$

Harmonic Oscillator

We can write:

$$-\frac{2}{\hbar\omega}\left(-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}+\frac{1}{2}m\omega^2x^2\right)\psi=-\frac{2}{\hbar\omega}E\,\psi$$

Then $\frac{\hbar}{m\omega}\frac{d^2\psi}{dx^2}-\frac{m\omega}{\hbar}x^2\psi=-\frac{2}{\hbar\omega}E\,\psi$

With $\xi=\sqrt{\frac{m\omega}{\hbar}}x,\quad \epsilon=\frac{2E}{\hbar\omega}$

We can apply the chain rule to get higher order derivatives:

$$\frac{dy}{du}=\frac{dx}{du}\cdot\frac{dy}{dx}$$

$$\frac{d^2y}{du^2}=\frac{d^2x}{du^2}\cdot\frac{dy}{dx}+\left(\frac{dx}{du}\right)^2\cdot\frac{d^2y}{dx^2}$$

We have: $\frac{d^2\psi}{d\xi^2}-(\xi^2-\epsilon)\psi=0$

Harmonic Oscillator

Materials Science

UNIVERSITÀ DEGLI STUDI DI MILANO BICOCCA

We can write:

$$\frac{\hbar}{m\omega}\frac{d^2\psi}{dx^2} - \frac{m\omega}{\hbar}x^2\psi = -\frac{2}{\hbar\omega}E\,\psi$$

With $\xi = \sqrt{\frac{m\omega}{\hbar}}\,x$, $\epsilon = \frac{2E}{\hbar\omega}$

$$\frac{d\psi}{dx} = \frac{d\xi}{dx}\cdot\frac{d\psi}{d\xi}$$

$$\frac{d\xi}{dx} = \sqrt{\frac{m\omega}{\hbar}}$$

$$\frac{d^2\psi}{dx^2} = \frac{d^2\xi}{dx^2}\cdot\frac{d\psi}{d\xi} + \left(\frac{d\xi}{dx}\right)^2\cdot\frac{d^2\psi}{d\xi^2} = 0 + \frac{m\omega}{\hbar}\frac{d^2\psi}{}$$

Harmonic Oscillator

Materials Science
UNIVERSITÀ DEGLI STUDI DI MILANO BICOCCA

We can write:

$$\frac{\hbar}{m\omega}\frac{d^2\psi}{dx^2} - \frac{m\omega}{\hbar}x^2\psi = -\frac{2}{\hbar\omega}E\,\psi$$

With $\xi = \sqrt{\frac{m\omega}{\hbar}}x, \quad \epsilon = \frac{2E}{\hbar\omega}$

$$\frac{d\xi}{dx} = \sqrt{\frac{m\omega}{\hbar}}$$

$$\frac{d^2\psi}{dx^2} = \frac{m\omega}{\hbar}\frac{d^2\psi}{d\xi^2}$$

$$\frac{\hbar}{m\omega}\frac{m\omega}{\hbar}\frac{d^2\psi}{d\xi^2} - \xi^2\psi = -\varepsilon\psi$$

$$\frac{d^2\psi}{d\xi^2} - (\xi^2 - \varepsilon)\psi = 0$$

Harmonic Oscillator

We can write:

$$\frac{d^2\psi}{d\xi^2} - (\xi^2 - \epsilon)\psi = 0$$

And for $|\xi| \gg 1$ (it means very large x)

$$\frac{d^2\psi}{d\xi^2} \approx \xi^2\psi$$

With approximate solutions:

$$\psi(\xi) \simeq A\, e^{-\xi^2/2} + B\, e^{+\xi^2/2}$$

The second term with B cannot be normalized thus,

because

$$e^{+\xi^2} \rightarrow \infty$$

for $\xi \rightarrow \infty$

let's consider: $\psi(\xi) = h(\xi)\, e^{-\xi^2/2}$

And hope that $h(\xi)$ will be a function simpler than $\psi(\xi)$

Harmonic Oscillator

The second derivative of

$$\psi(\xi) \simeq h(\xi)\, e^{-\xi^2/2}$$

Is:

$$\frac{d^2\psi}{d\xi^2} = \left[\frac{d^2h}{d\xi^2} - 2\xi\frac{dh}{d\xi} + (\xi^2 - 1)h\right] e^{-\xi^2/2}$$

And $\frac{d^2\psi}{d\xi^2} - (\xi^2 - \epsilon)\psi = 0$ becomes:

$$\left[\frac{d^2h}{d\xi^2} - 2\xi\frac{dh}{d\xi} + (\xi^2 - 1)h\right] e^{-\xi^2/2} - (\xi^2 - \epsilon)h e^{-\xi^2/2} = 0$$

$$\Rightarrow \quad \frac{d^2h}{d\xi^2} - 2\xi\frac{dh}{d\xi} + (\epsilon - 1)h = 0$$

Harmonic Oscillator

$$\frac{d^2h}{d\xi^2} - 2\xi\frac{dh}{d\xi} + (\epsilon - 1)h = 0$$

Let's try with a solution of the form of a power series in ξ:

$$h(\xi) = a_0 + a_1\xi + a_2\xi^2 + \cdots = \sum_{i=0}^{\infty} a_i\xi^{\mathrm{i}}$$

$$\frac{dh}{d\xi} = a_1 + 2a_2\xi + 3a_3\xi^2 + \cdots = \sum_{i=0}^{\infty} i\, a_i\xi^{\mathrm{i}-1}$$

$$\frac{d^2h}{d\xi^2} = 2a_2 + 2\cdot 3\, a_3\,\xi + 3\cdot 4a_4\xi^2 + \cdots = \sum_{i=0}^{\infty}(i+1)(i+2)\, a_{i+2}\,\xi^{\mathrm{i}}$$

Harmonic Oscillator

$$\frac{\mathrm{d}^2 h}{\mathrm{d}\xi^2} - 2\xi \frac{\mathrm{d}h}{\mathrm{d}\xi} + (\epsilon - 1)h = 0$$

$$h(\xi) = \sum_{i=0}^{\infty} a_i \xi^{\mathrm{i}}$$

$$\frac{\mathrm{d}h}{\mathrm{d}\xi} = \sum_{i=0}^{\infty} i\, a_i \xi^{\mathrm{i}-1}$$

$$\frac{\mathrm{d}^2 h}{\mathrm{d}\xi^2} = \sum_{i=0}^{\infty} (i+1)(i+2)\, a_{i+2}\, \xi^{\mathrm{i}}$$

We can re-write the S.E. as:

$$\sum_{i=0}^{\infty} (i+1)(i+2)\, a_{i+2}\, \xi^{\mathrm{i}} - 2\xi\, i\, a_i \xi^{\mathrm{i}-1} + (\epsilon - 1) a_i \xi^{\mathrm{i}} = 0$$

Thus: $$\sum_{i=0}^{\infty} [(i+1)(i+2)\, a_{i+2} - 2\, i\, a_i + (\epsilon - 1) a_i] \xi^{\mathrm{i}} = 0$$

...the coefficient of each power of ξ must vanish!

Harmonic Oscillator

$$\sum_{i=0}^{\infty}[(i+1)(i+2)\,a_{i+2} - 2\,i\,a_i + (\epsilon - 1)a_i]\xi^{i} = 0$$

...the coefficient of each power of ξ must vanish!

$$(i+1)(i+2)\,a_{i+2} - 2\,i\,a_i + (\epsilon - 1)a_i = 0$$

⇓

$$a_{i+2} = \frac{2i + 1 - \epsilon}{(i+1)(i+2)}a_i$$

This recursion formula is entirely equivalent to the Schrödinger equation itself.

Harmonic Oscillator

$$h(\xi) = a_0 + a_1\xi + a_2\xi^2 + \cdots = \sum_{i=0}^{\infty} a_i \xi^i$$

$$a_{i+2} = \frac{2i + 1 - \epsilon}{(i+1)(i+2)} a_i$$

Starting with a given a_0

$$a_2 = \frac{1-\epsilon}{2} a_0$$

$$a_4 = \frac{5-\epsilon}{12} a_2 = \frac{(5-\epsilon)(1-\epsilon)}{24} a_0 = \frac{(5-\epsilon)(1-\epsilon)}{4!} a_0$$

Harmonic Oscillator

$$h(\xi) = a_0 + a_1\xi + a_2\xi^2 + \cdots = \sum_{i=0}^{\infty} a_i \xi^{\mathrm{i}}$$

$$a_{i+2} = \frac{2i + 1 - \epsilon}{(i+1)(i+2)} a_i$$

Given a_1

$$a_3 = \frac{3 - \epsilon}{6} a_1 \qquad a_5 = \frac{(7-\epsilon)}{20} a_3 = \frac{(7-\epsilon)(3-\epsilon)}{5!} a_1$$

Thus, given a_0 and a_1 I can generate a_n and hence h, which is a sum of "even" and "odd" functions:

$$h(\xi) = h_{\mathrm{o}}(\xi) + h_{\mathrm{e}}(\xi)$$

Harmonic Oscillator

$$\sum_{i=0}^{\infty}[(i+1)(i+2)\, a_{i+2} - 2\, i\, a_i + (\epsilon - 1)a_i]\xi^{\mathrm{i}} = 0$$

…not all solution are acceptable:

$$a_{i+2} = \frac{2i + 1 - \epsilon}{(i+1)(i+2)} a_i$$

For very large i, $1 - \epsilon$ can be neglected w.r.t. $2i$.

$$\Rightarrow \qquad a_{i+2} \approx \frac{2}{i} a_i$$

When applied recursively N times, and considering only even indexes

$$a_{2i+2\mathrm{N}} \approx \frac{2^{2N}}{2i(2i+2)\ldots(2i+2N)} a_{2i} = \frac{2^N}{i(i+1)\ldots(i+N)} a_{2i}$$

Harmonic Oscillator

For very large i, $1-\epsilon$ can be neglected w.r.t. $2i$.

$$\Rightarrow \qquad a_{i+2} \approx \frac{2}{i} a_i$$

When applied recursively N times, and considering only even indexes

$$a_{2i+2\mathrm{N}} \approx \frac{2^{2N}}{2i(2i+2)\dots(2i+2N)} a_{2i} = \frac{2^{N}}{i(i+1)\dots(i+N)} a_{2i}$$

Although I was considering very large indexes i, I can extend the expression above to all indexes because this will not affect the asymptotic behavior, of h thus

$$a_i \approx \frac{a_0}{\left(\frac{i}{2}\right)!}$$

Harmonic Oscillator

For very large i, $1-\epsilon$ can be neglected w.r.t. $2i$.

$$a_i \approx \frac{a_0}{\left(\frac{i}{2}\right)!}$$

Then:

$$h(\xi) = \sum_{i=0}^{\infty} a_i \xi^{i} \approx a_0 \sum_{i=0}^{\infty} \frac{1}{\left(\frac{i}{2}\right)!} \xi^{i} \approx a_0 \sum_{i=0}^{\infty} \frac{1}{i!} \xi^{2i} \approx C\, e^{\xi^2}$$

Harmonic Oscillator

$$h(\xi) \approx C\, e^{\xi^2}$$

But we were looking for:

$$\psi(\xi) \approx h(\xi)\, \mathrm{e}^{-\xi^2/2}$$

Thus, for high values of ξ it would be:

$$\psi(\xi) \approx C\, \mathrm{e}^{\xi^2/2}$$

But this cannot be accepted for the normalization problem.
The only way in which we can avoid that $\psi \rightarrow \infty$ as $\xi \rightarrow \infty$ is to stop power series at some finite value of i.
This implies, from the recursion relation that:

$$\epsilon = 2n + 1$$

where n is a non-negative integer.

Harmonic Oscillator

This implies, from the recursion relation $a_{i+2} = \frac{2i+1-\epsilon}{(i+1)(i+2)} a_i$ that:

$\epsilon = 2n+1$

But: $\epsilon = \frac{2E}{\hbar\omega}$

Thus:

$$E = \left(n + \frac{1}{2}\right)\hbar\omega$$

Here, the quantization of energy is also evident!

We conclude that a particle moving in a harmonic potential has quantized energy levels that are equally spaced by an energy $\hbar\omega$, where ω is the classical oscillation frequency.

The lowest energy state (n=0) has energy (1/2)$\hbar\omega$, called zero-point energy.

Hermite polynomials

What about the w.f.?

$$\psi(\xi) \simeq h(\xi)\, e^{-\xi^2/2}$$

The $h(\xi)$ functions are polynomials of degree n in ξ either entirely odd or entirely even.

They are the so called Hermite polynomials

One can write the normalized w.f. as:

$$\psi_n(\xi) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} H_n(\xi) e^{-\xi^2/2}$$

Hermite polynomials

$$H_0 = 1$$
$$H_1(\xi) = 2\xi$$
$$H_2(\xi) = 4\xi^2 - 2$$
$$H_3(\xi) = 8\xi^3 - 12\xi$$
$$H_4(\xi) = 16\xi^4 - 48\xi^2 + 12$$

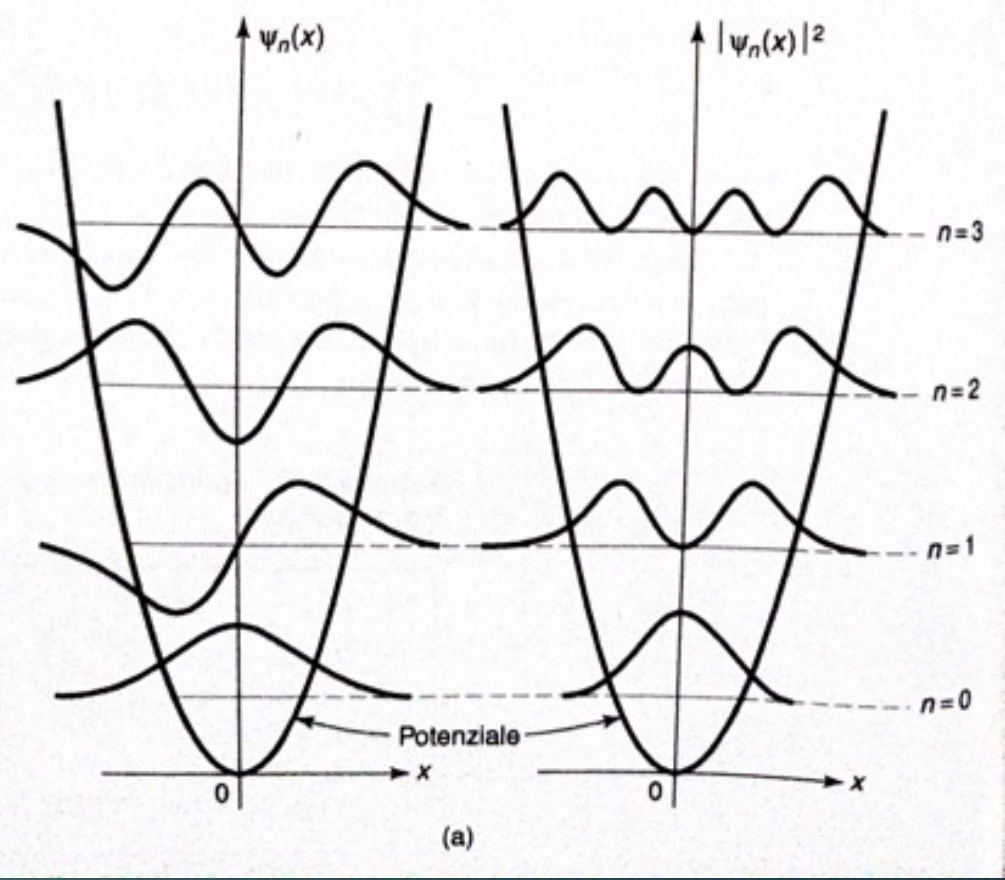
Harmonic Oscillator

solutions

$$\psi_n(\xi) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} H_n(\xi) e^{-\xi^2/2}$$

$$E = \left(n + \frac{1}{2}\right) \hbar\omega$$

The allowed energy levels are equally spaced, separated by an amount $\hbar\omega$, with ω the classical oscillation frequency.

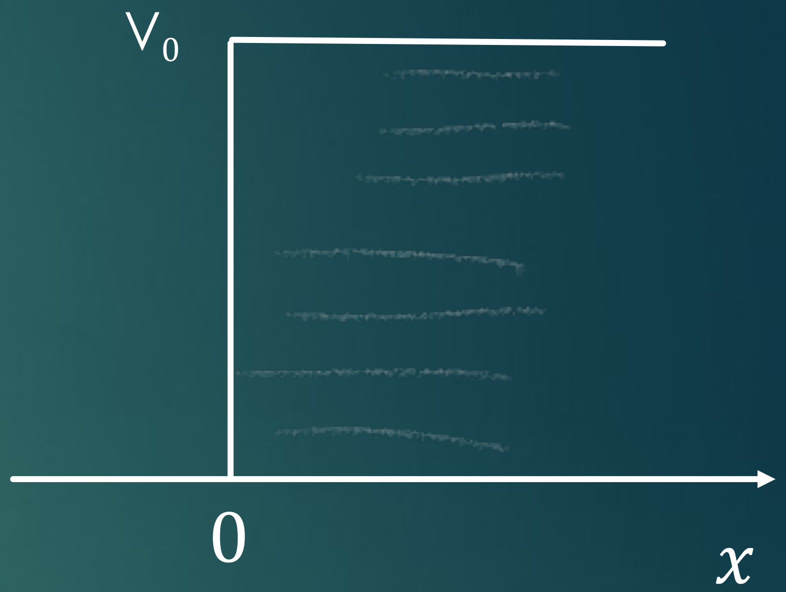


Like the potential well, there is also a "zero point energy" the first allowed state is not at zero energy, but instead here at $\hbar\omega/2$ compared to the classical minimum energy.

Infinitely thick barrier (or potential step)

Consider a particle of mass m and energy E moving in the following potential:

$$V(x) = \begin{cases} V_0, & for \quad x \geq 0 \\ 0, & \text{otherwise} \end{cases}$$



The quantum mechanical wave is incident from the left on the barrier

It can be reflected from the barrier into the region on the left.

General solutions of the equation on the left side:

$$\psi_{left}(x) = C\, e^{ikx} + De^{-iKx}$$

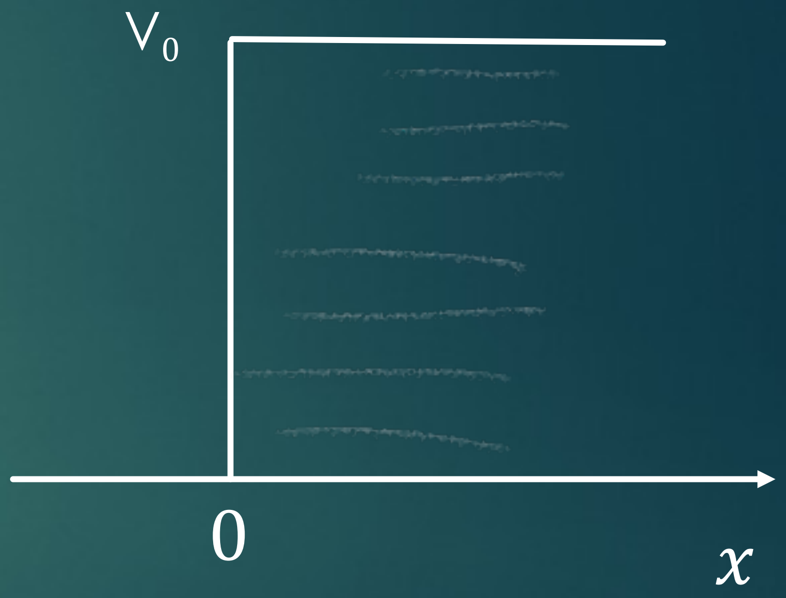
As for the infinite square well

$$k = \frac{\sqrt{2mE}}{\hbar}$$

Infinitely thick barrier (or potential step)

Let's consider $E < V_0$

i.e., the particle does not have enough energy to get over this barrier.



The t.i. S.E. inside the barrier will be:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = -[V_0 - E]\,\psi$$

General solutions of the equation on the right side:

$$\psi_{right}(x) = F\,e^{\kappa x} + G e^{-\kappa x}$$

Now $\kappa = \frac{\sqrt{2m(V_0 - E)}}{\hbar}$

Infinitely thick barrier (or potential step)

Let's consider $E < V_0$

i.e., the particle does not have enough energy to ge

The t.i. S.E. inside the barrier will be:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = -[V_0 - E]\,\psi$$

General solutions of the equation on the right side:

$$\psi_{right}(x) = F\,e^{\kappa x} + Ge^{-\kappa x}$$

$$\mathrm{E} = \frac{p^2}{2m} + V_0 = \frac{k^2\hbar^2}{2m} + V_0$$

$\Downarrow$

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

$\Downarrow$

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

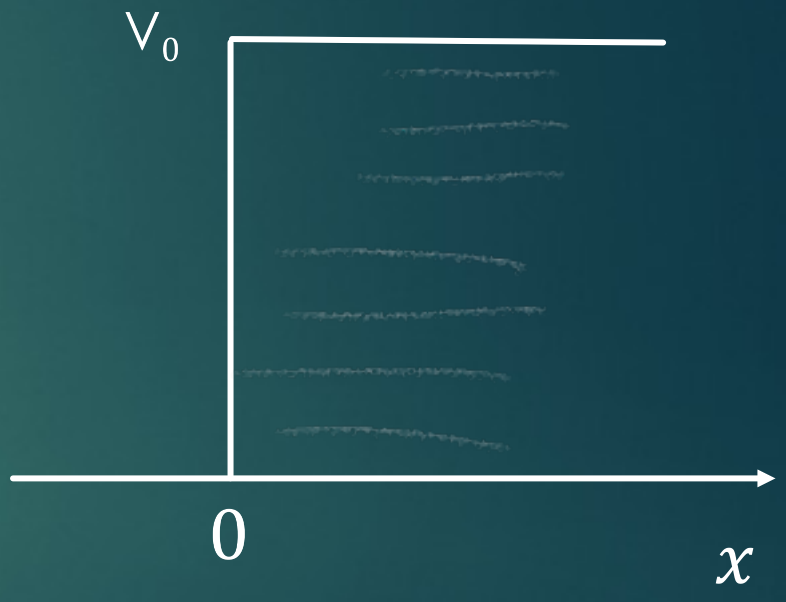
Now $\kappa = \frac{\sqrt{2m(V_0 - E)}}{\hbar}$

Is real, while K should be imaginary

Infinitely thick barrier (or potential step)

Let's consider $E < V_0$

i.e., the particle does not have enough energy to get over this barrier.



The t.i. S.E. inside the barrier will be:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = -[V_0 - E]\,\psi$$

General solutions of the equation on the right side:

$$\psi_{right}(x) = F\,e^{\kappa x} + Ge^{-\kappa x}$$

F=0 to have a square-integrable wavefunctions

$$\psi_{right}(x) = Ge^{-\kappa x}$$

*This is an exponential function, not really a wave function

Infinitely thick barrier (or potential step)

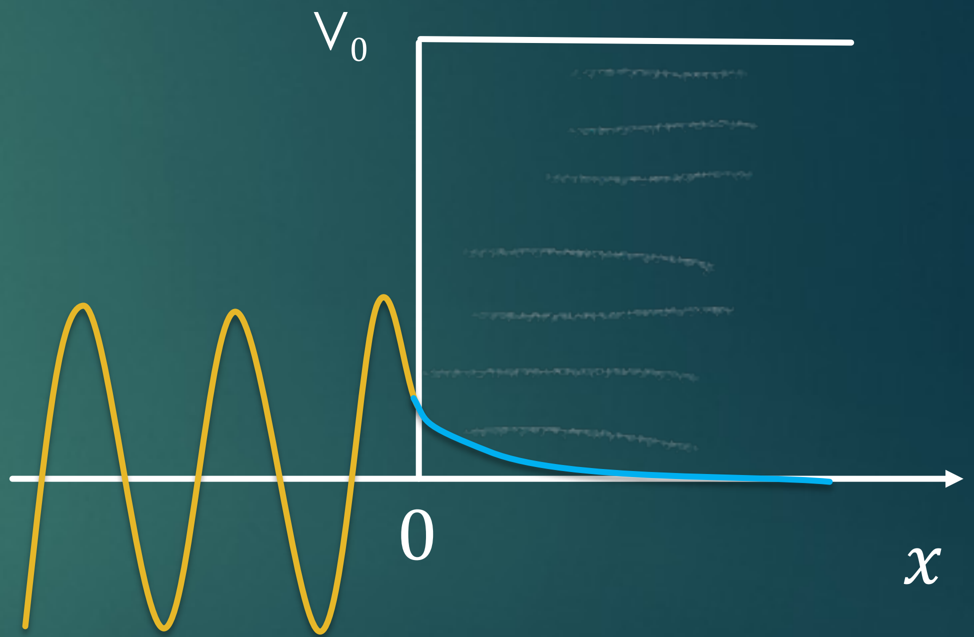
Let's consider $E < V_0$

i.e., the particle does not have enough energy to get over this barrier.

General solutions of the S.E. on the right side:

$$\psi_{right}(x) = Ge^{-\kappa x}$$

This solution means that the wave inside the barrier is not zero, but it falls off exponentially!



So there must be a probability of finding the particle inside the barrier.

This phenomena is often called tunneling.

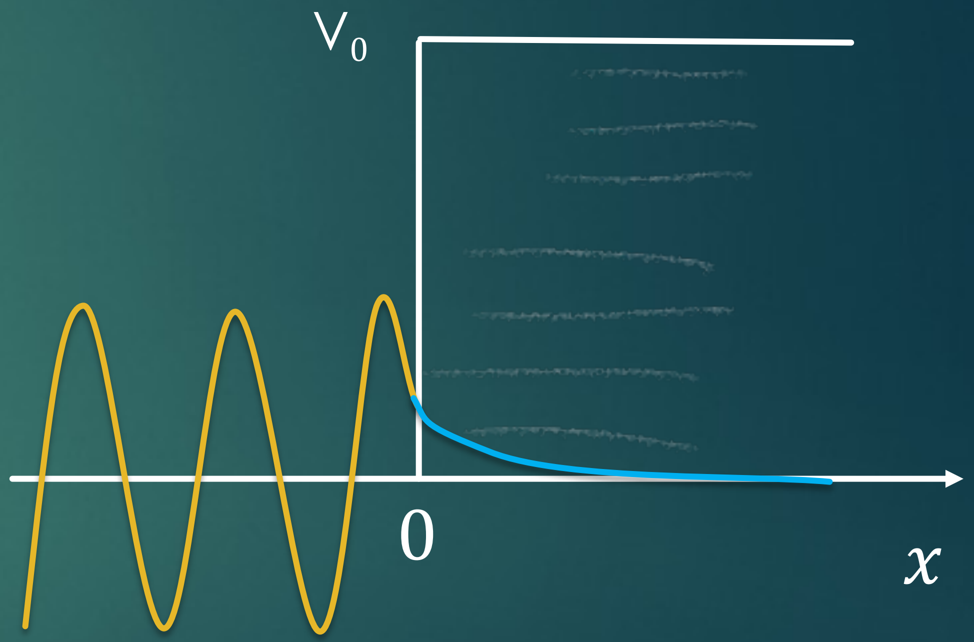
Infinitely thick barrier (or potential step)

Let's consider boundary conditions:

- Continuity of the wavefunction and its derivative at x=0 gives us two equations:

$C+D=G$

$ik(C-D)=-\kappa G.$



which we can solve for the ratios

$$\frac{D}{C}=\frac{k-i\kappa}{k+i\kappa} \qquad \frac{G}{C}=\frac{2k}{k+i\kappa}$$

Thus

$$\left|\frac{D}{C}\right|^2=1 \qquad or \qquad |D|^2=|C|^2$$

We have total reflection of the wavefunction!