Section 3: 1D Schrödinger Equation

In these slides we will cover:

- The time-independent Schrödinger equation
- Boundary and continuity conditions for $\psi(x)$
- Solutions for an infinite potential well
- Solutions for bound states of a finite potential well
- Solutions for a harmonic oscillator
- Ladder operators for the harmonic oscillator
- Representation of a free particle in 1 dimension
- Beams of particles incident on a potential step or barrier

Square potential wells

The time-independent Schrödinger equation

- We saw in the last Section that solutions to the Schrödinger equation for a particle moving in a 1D potential $V(x)$ are,

$$\Psi(x,t) = \psi_n(x)\, e^{-iE_n t/\hbar}$$

- Here, $\psi_n(x)$ are solutions to the **time-independent Schrödinger equation**:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_n(x)}{dx^2} + V(x)\,\psi_n(x) = E_n\,\psi_n(x)$$

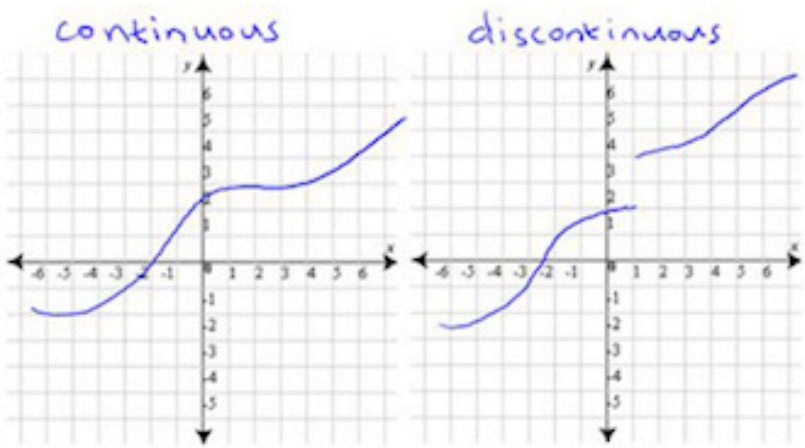
- This equation is just $\hat{H}\psi_n = E_n\psi_n$ in terms of the Hamiltonian $\hat{H}$, i.e. $\psi_n(x)$ are **energy eigenfunctions** with eigenvalues E_n

Square potential wells

Boundary and continuity conditions for ψ

- The solutions of a differential equation (such as the Schrödinger equation) always require **boundary conditions**

- For the Schrödinger equation, there are 2 boundary conditions:



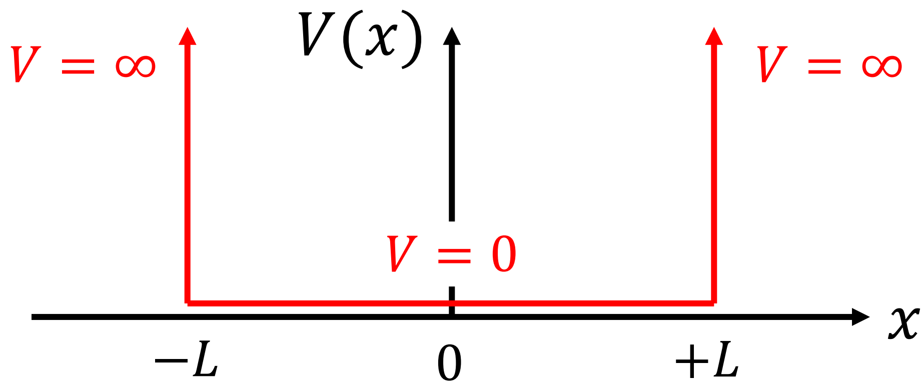
1. The **wavefunction ψ must be a continuous function** – that is, include no sudden jumps – since it represents a probability

2. If ψ is continuous, then the Schrödinger equation implies that $\frac{d\psi}{dx}$ **must also be continuous**, except at an infinite jump in $V(x)$

Square potential wells

Infinite square well: eigenfunctions and eigenvalues

- The classical example of a potential well is the **infinite square well** you have met before. Let's recap it …



- The Schrödinger Equation for $|x| < L$, where $V = 0$, is $-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\,\psi$, which has solutions $\psi = N\sin kx$ or $\psi = N\cos kx$, where $k^2 = 2mE/\hbar^2$
- Since $V = \infty$ for $|x| > L$ there is zero probability in this region so, since ψ is continuous, the wavefunctions must satisfy $\psi = 0$ at $x = \pm L$
- Hence $kL = \frac{1}{2}n\pi$, where $n = 1,3,\ldots$ (for $\cos kx$) or $n = 2,4,\ldots$ (for $\sin kx$)
- Normalising, we find $\psi_n = \frac{1}{\sqrt{L}} \begin{matrix}\cos\\ \sin\end{matrix}\left(\frac{n\pi x}{2L}\right)$ with energy eigenvalues $E_n = \frac{n^2\pi^2\hbar^2}{8mL^2}$

Square potential wells

Infinite square well: eigenfunctions and eigenvalues

- Here are the shapes of the energy eigenfunctions for the infinite potential well (Each one is offset along the y-axis for clarity)

- They are $\sin kx$ or $\cos kx$ functions, which always satisfy $\psi = 0$ at the edges

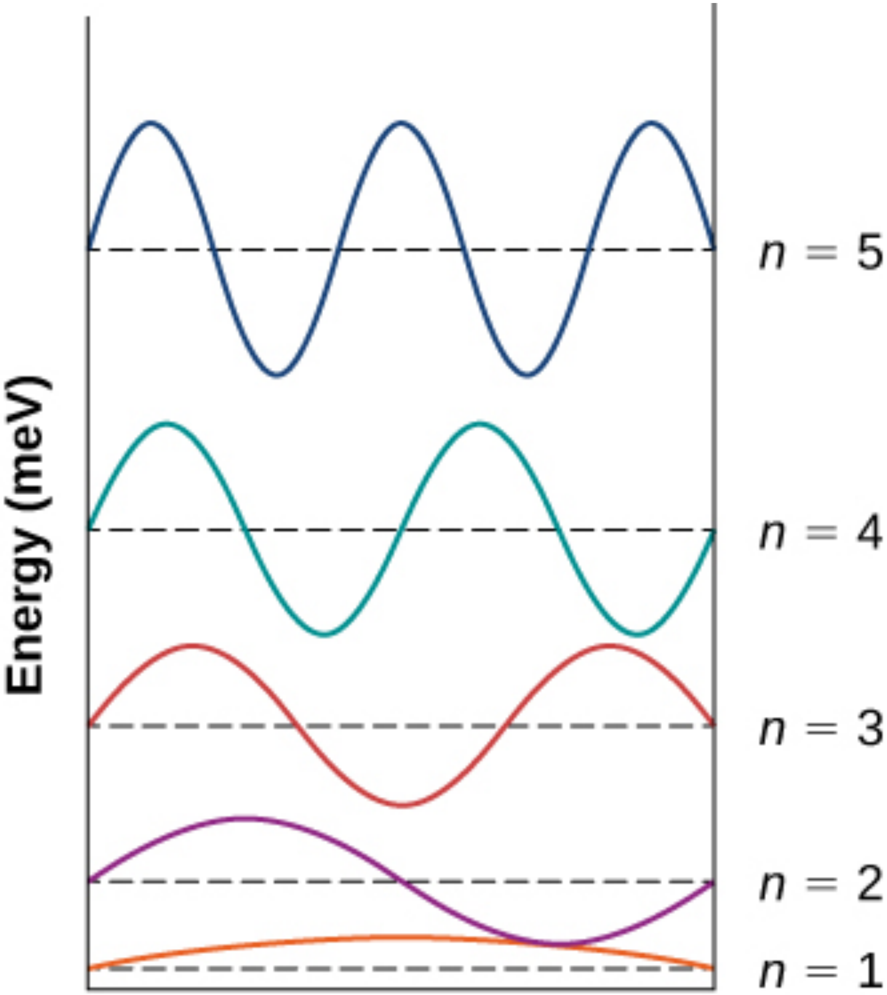
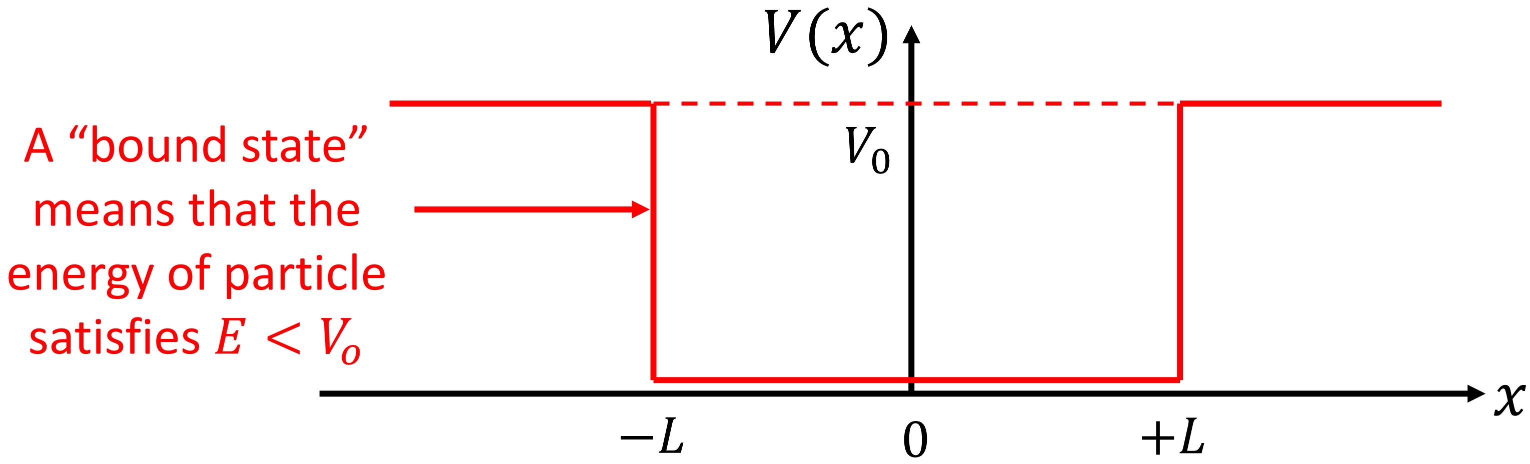


Image credit: https://opentextbc.ca/universityphysicsv3openstax/chapter/the-quantum-particle-in-a-box/

Square potential wells

Bound states of a finite square well

- Now let's consider a particle with energy E in a finite square potential well of depth V_0 (where $E < V_0$), which looks like:



- Classically speaking, the particle would not cross into $|x| > L$, since $E < V_0$. However, this is not true in Quantum Mechanics – **particles can appear in the forbidden region**!

Square potential wells

Bound states of a finite square well

- We can determine the wavefunction by **solving the Schrödinger equation** and **applying the boundary conditions**

In the region $|x| < L$:

- $V = 0$, so $\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + E\psi = 0$
- Solutions are $\psi = A\cos kx$ or $\psi = A\sin kx$
- $k^2 = 2mE/\hbar^2$
- There is hence a family of **even solutions** (symmetric in x, $\cos kx$) and **odd solutions** (anti-symmetric in x, $\sin kx$)

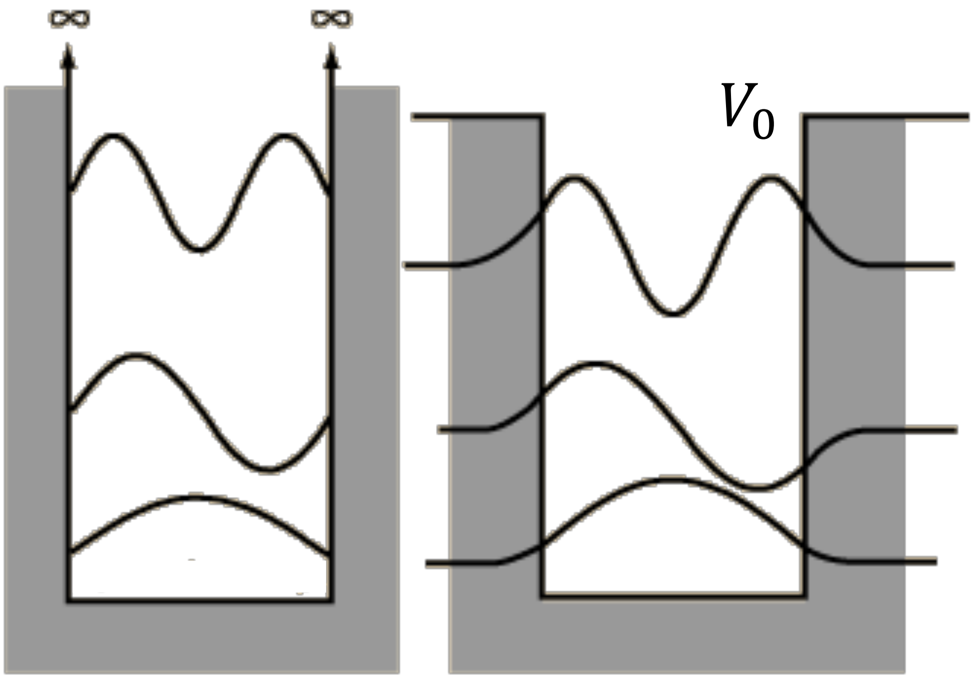
In the region $|x| > L$:

- $V = V_0$, so $\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} - (V_0 - E)\psi = 0$ *(note the sign change compared to $|x| < L$, since $V_0 > E$)*
- Solutions are $\psi = Ae^{lx}$ or $\psi = Ae^{-lx}$
- $l^2 = 2m(V_0 - E)/\hbar^2$
- Since $\psi \to 0$ as $x \to \pm\infty$ if ψ tells us probability, we need $\psi \propto e^{-lx}$ for $x > L$ and $\psi \propto e^{lx}$ for $x < -L$

Square potential wells

Bound states of a finite square well

- We can determine the wavefunction by **solving the Schrödinger equation** and **applying the boundary conditions**



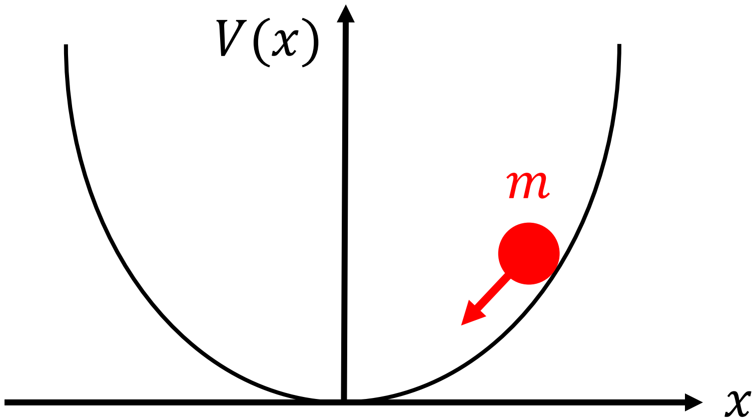
Comparing the lowest energy eigenfunctions of the infinite potential well and finite potential well (Image credit: http://hyperphysics.phy-astr.gsu.edu)

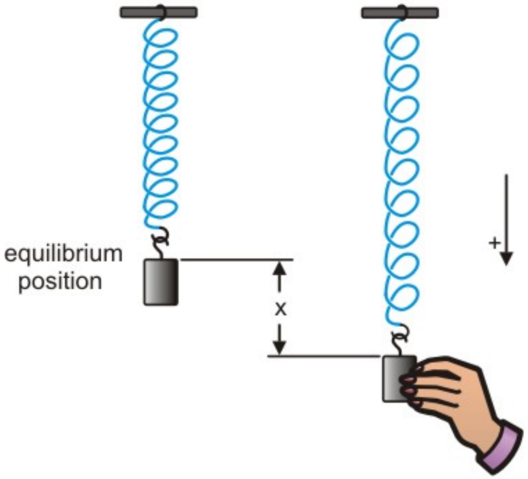
- For example, the even solutions: $\psi_A(x) = A\cos kx$ for $|x| < L$ and $\psi_B(x) = Be^{-lx}$ for $x > L$
- ψ is continuous at $x = L \rightarrow \psi_A(L) = \psi_B(L) \rightarrow A\cos kL = Be^{-lL}$
- $\frac{d\psi}{dx}$ is continuous at $x = L \rightarrow$ $\frac{d\psi_A}{dx}(L) = \frac{d\psi_B}{dx}(L) \rightarrow$ $kA\sin kL = lBe^{-lL}$
- Combining these $\rightarrow k\tan kL = l$ from which we can find the energy

The harmonic oscillator

Definition of the harmonic oscillator

- The **harmonic oscillator** is a particle moving in a 1D potential $V(x) = \frac{1}{2}kx^2$ – classically, this is like a mass on a spring





- Classically, a particle would oscillate to-and-fro with "simple harmonic motion" $x(t) = A\cos\omega t$, where $\omega^2 = k/m$, and its motion would be restricted to $|x| < A$, where $A = \sqrt{2E/k}$

The harmonic oscillator

The Schrödinger equation for the harmonic oscillator

- In Quantum Mechanics, the particle does not have a definitive location, it can be found outside the classically-permitted region, and its energy is restricted to discrete values!

- The energy eigenfunctions $\psi(x)$ of the particle satisfy the time-independent Schrödinger equation (using $\omega^2 = k/m$):

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

- By simple substitution we find that $\psi_1(x) \propto e^{-ax^2}$ is a solution of this equation with energy $E_1 = \frac{1}{2}\hbar\omega$, where $a = m\omega/2\hbar$. This is actually the **ground state (lowest energy state)**

The harmonic oscillator

Ladder operators for the harmonic oscillator

- A cunning method of finding the other energy eigenfunctions, whilst using the concept of operators from the previous Section, is to introduce the **ladder operators** $\hat{A}_+$ and $\hat{A}_-$:

$$\hat{A}_+ = \sqrt{\frac{m\omega}{2\hbar}}\hat{x} - \frac{i}{\sqrt{2mw\hbar}}\hat{p} = \sqrt{a}\,x - \frac{1}{2\sqrt{a}}\frac{d}{dx}$$

$$\hat{A}_- = \sqrt{\frac{m\omega}{2\hbar}}\hat{x} + \frac{i}{\sqrt{2mw\hbar}}\hat{p} = \sqrt{a}\,x + \frac{1}{2\sqrt{a}}\frac{d}{dx}$$

- In the above equations, $\hat{x} = x$ and $\hat{p} = -i\hbar\frac{d}{dx}$ are the usual operators for position and momentum, and we have used the constant $a = m\omega/2\hbar$ from the previous slide

The harmonic oscillator

Ladder operators for the harmonic oscillator

- For example, the result of applying the operator $\hat{A}_+$ on a function $f(x)$ is the new function $\hat{A}_+ f = \sqrt{a} x f - \frac{1}{2\sqrt{a}} \frac{df}{dx}$
- Again by substitution, we find that the function $\psi_2(x) = \hat{A}_+ \psi_1(x) \propto x\, e^{-ax^2}$ is also a solution of the Schrödinger equation for the harmonic oscillator, with energy $E_2 = \frac{3}{2} \hbar\omega$
- You can show that $\psi_1(x) \propto \hat{A}_- \psi_2(x)$ and $\int_{-\infty}^{\infty} \psi_1^* \, \psi_2 \, dx = 0$
- The operator $\hat{A}_+$ creates energy eigenfunctions of higher energy, and $\hat{A}_-$ creates eigenfunctions of lower energy – we are moving up and down the "ladder" of energy states

The harmonic oscillator

Ladder operators for the harmonic oscillator

- The energy levels of the harmonic oscillator are given by $E_n = \left(n - \frac{1}{2}\right)\hbar\omega$ where $n = 1,2,3, \ldots$

- Here is an illustration of the ladder of states including another gratituous picture of a cat:

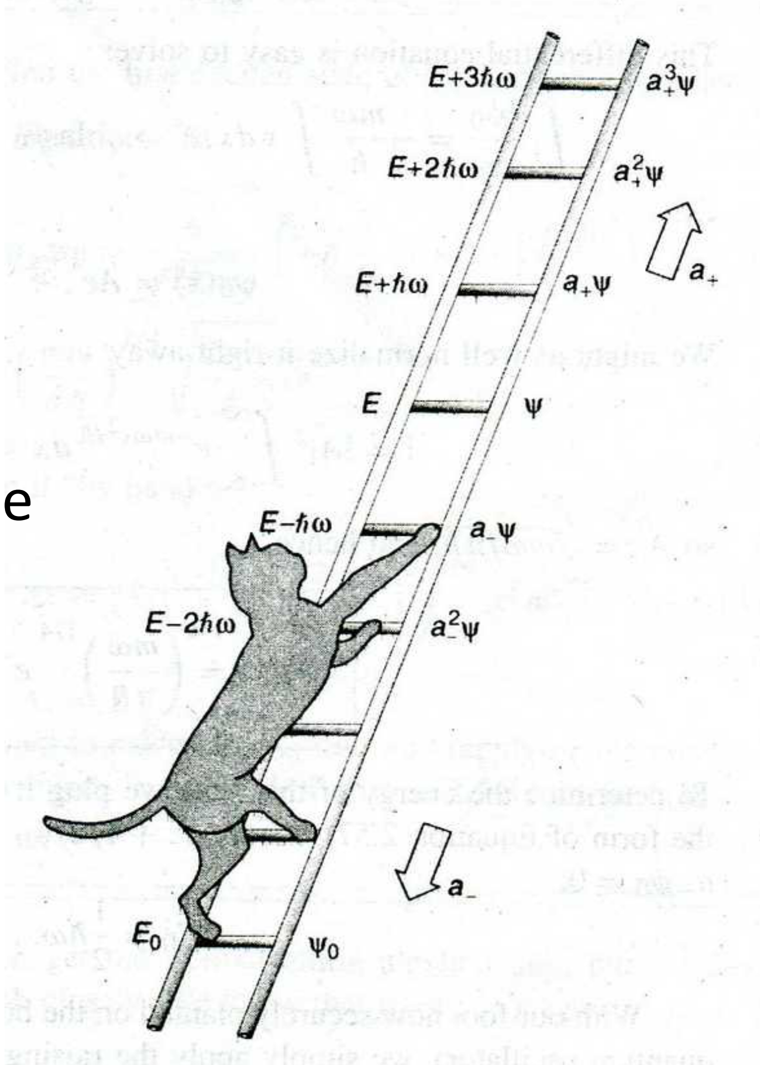


Image credit: https://www.lessthanepsilon.net/second-quantization/

The harmonic oscillator

Harmonic oscillator summary

- Here's a representation of the first few energy eigenfunctions:

Again, the energy eigenfunctions are alternating even (symmetric) functions and odd (anti-symmetric) functions of x

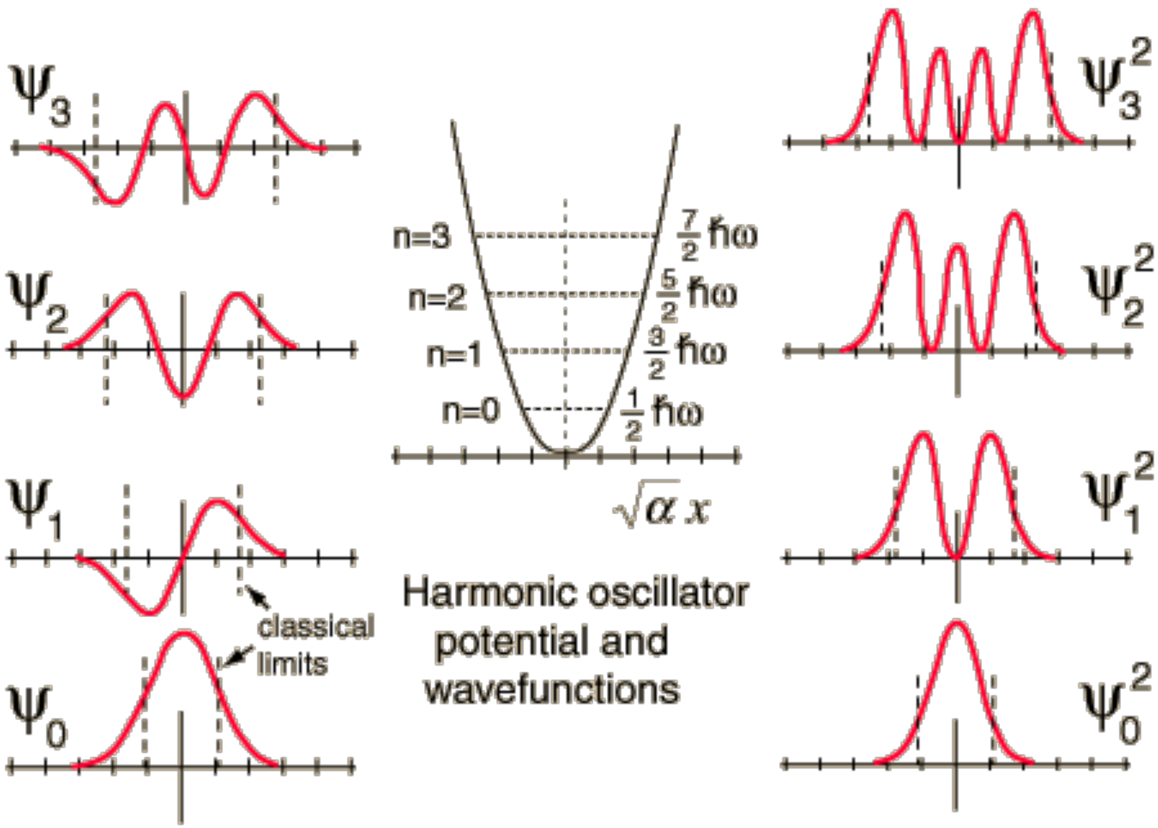


Image credit: http://hyperphysics.phy-astr.gsu.edu/hbase/quantum/hosc5.html

The harmonic oscillator

Commutation relations and energy levels

- Non-examinable: We can use some operator relations to prove the general result that $\hat{A}_+\psi$ is the eigenfunction of the next energy level up. We start with some useful relations we can show using the forms of $\hat{A}_+$ and $\hat{A}_-$:

$$\hat{H} = \hbar\omega\left(\hat{A}_+\hat{A}_- + \frac{1}{2}\right) \qquad\qquad [\hat{A}_-, \hat{A}_+] = 1$$

- This then enables us to find (using $[\hat{A}\hat{B}, \hat{C}] = \hat{A}[\hat{B}, \hat{C}] + [\hat{A}, \hat{C}]\hat{B}$)

$$[\hat{H}, \hat{A}_+] = \hbar\omega[\hat{A}_+\hat{A}_-, \hat{A}_+] = \hbar\omega[\hat{A}_-, \hat{A}_+]\hat{A}_+ = \hbar\omega\hat{A}_+$$

- If ψ is an energy eigenfunction ($\hat{H}\psi = E\psi$), let's then consider

$$\hat{H}(\hat{A}_+\psi) = [\hat{H}, \hat{A}_+]\psi + \hat{A}_+\hat{H}\psi = \hbar\omega\hat{A}_+\psi + E\hat{A}_+\psi = (E + \hbar\omega)\hat{A}_+\psi$$

- Hence, $\hat{A}_+\psi$ is an energy eigenfunction with energy $E + \hbar\omega$, proving our initial statement

Unbound particles in 1D

Representation of a free particle

- We now consider **1D unbound problems**, where "unbound" means that particles are able to escape to infinity
- We first note that a solution of the time-dependent Schrödinger equation for a "free particle" (in a region where $V(x) = 0$) is

$$\Psi(x,t) = e^{i(kx-\omega t)}$$

e^{ikx} implies a wave travelling in the $+x$ direction – e^{-ikx} would be travelling towards $-x$

- (This satisfies $-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} = i\hbar\frac{\partial\Psi}{\partial t}$ where $k^2 = \frac{2mE}{\hbar^2}$ and $\omega = \frac{E}{\hbar}$)
- This function represents a wave – that is, **a beam of particles with definite momentum, but no definite position**

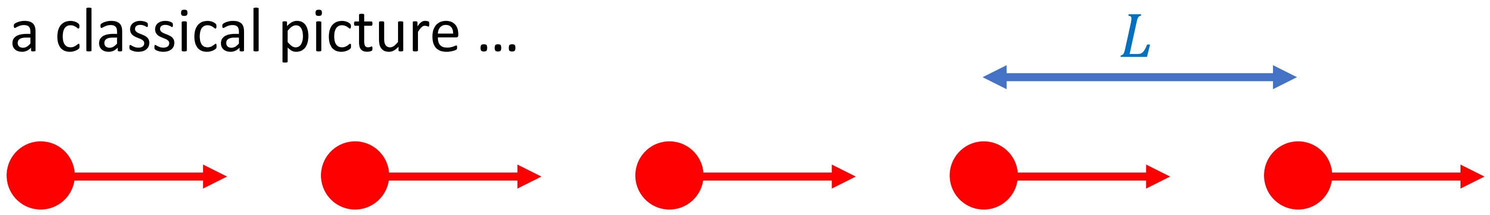
Unbound particles in 1D

Representation of a free particle

- How should we normalise the free-particle wavefunction $\Psi(x,t) = Ne^{i(kx-\omega t)}$? We can see that, $\int_{-\infty}^{\infty} |\Psi|^2 \, dx = \infty$!

- The normalisation N indicates the "average separation of particles in the beam" or the "intensity of the beam"

- In a classical picture …

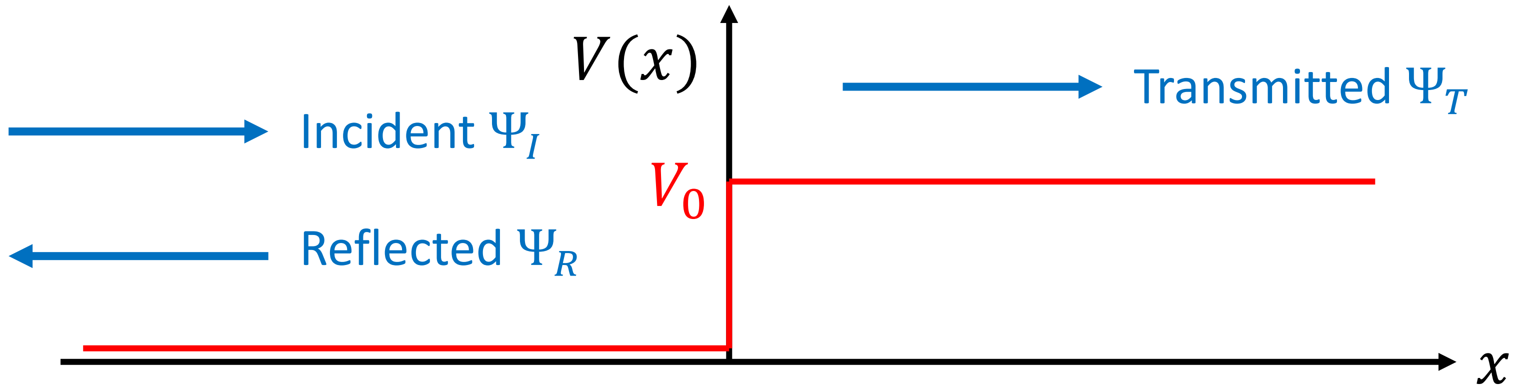


- If $N = \frac{1}{\sqrt{L}}$, then we find 1 particle per distance L. Since the intensity of the beam is $\propto \frac{1}{L}$, then **intensity** $\propto |N|^2$

Unbound particles in 1D

Particles incident on a potential step

- We can use the free particle wavefunction to describe a beam of particles (with energy $E > V_0$) incident on a potential step:



- We can assume the following forms for the solution:

Incident beam: $\Psi_I(x,t) = I\, e^{i(kx-\omega t)}$

Reflected beam: $\Psi_R(x,t) = R\, e^{i(-kx-\omega t)}$

Transmitted beam: $\Psi_T(x,t) = T\, e^{i(lx-\omega t)}$

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

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

Unbound particles in 1D

Particles incident on a potential step

- The general form of the wavefunctions are then,

Region $x < 0$: $\Psi_1(x,t) = \Psi_I + \Psi_R = \left(I\, e^{ikx} + R\, e^{-ikx}\right) e^{-i\omega t}$

Region $x > 0$: $\Psi_2(x,t) = \Psi_T = T\, e^{ilx}\, e^{-i\omega t}$

- We now apply the two boundary conditions at $x = 0$:

Ψ is continuous at $x = 0 \Longrightarrow \Psi_1(0,t) = \Psi_2(0,t) \Longrightarrow I + R = T$

$\frac{\partial\Psi}{\partial x}$ is continuous at $x = 0 \Longrightarrow \frac{\partial\Psi_1}{\partial x}(0,t) = \frac{\partial\Psi_2}{\partial x}(0,t) \Longrightarrow kI - kR = lT$

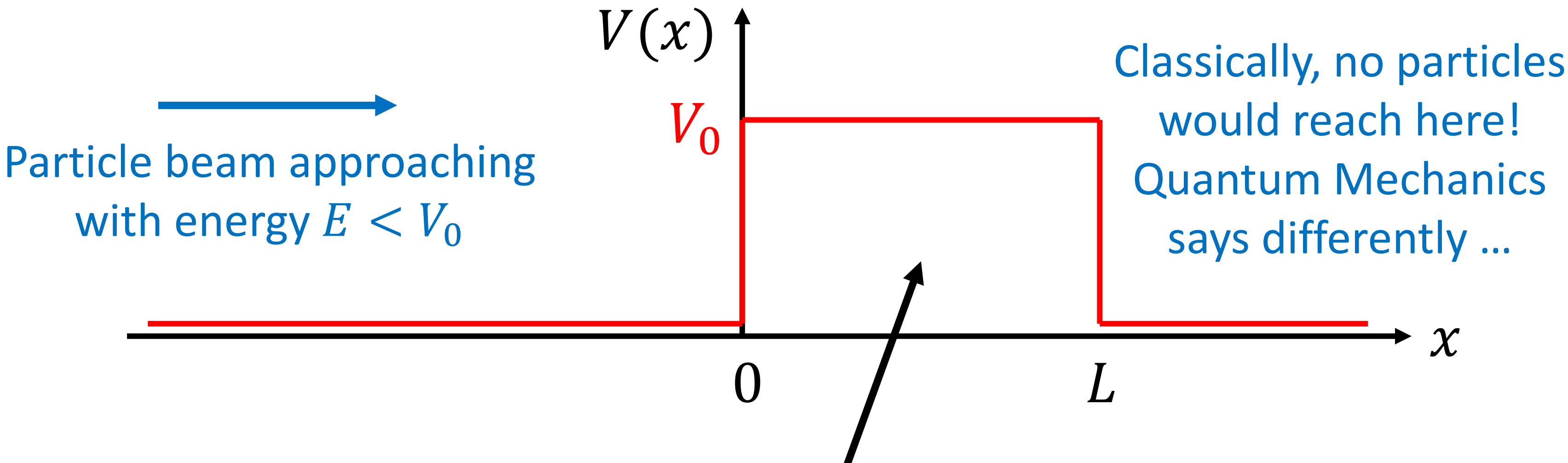
- Re-arranging, we obtain the **reflected/transmitted amplitudes**:

$$\frac{T}{I} = \frac{2}{1 + \sqrt{1 - V_0/E}} \qquad \frac{R}{I} = \frac{1 - \sqrt{1 - V_0/E}}{1 + \sqrt{1 - V_0/E}}$$

Unbound particles in 1D

Quantum tunnelling

- If we apply these methods to a potential barrier ($V_0 > E$) we will find **quantum tunnelling** – some particles reach $x > L$!



Since $E < V_0$, note that the general solution to the Schrödinger equation in the barrier region is $\Psi(x,t) = \left(Ae^{lx} + Be^{-lx}\right)e^{-i\omega t}$, **not** $\Psi(x,t) = \left(Ae^{ilx} + Be^{-ilx}\right)e^{-i\omega t}$ – one way to see that is to notice that $l^2 = \frac{2m(E-V_0)}{\hbar^2}$ (2 slides ago) is **negative** when $E < V_0$

Summary

Square potential wells

- Energy eigenfunctions always satisfy the time-independent Schrödinger equation, $-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x)$
- $\psi(x)$ is continuous everywhere, and $\frac{d\psi}{dx}$ is continuous except where there is an infinite jump in $V(x)$
- Bound solutions for potential wells are $\psi(x) \propto \begin{smallmatrix}\sin\\ \cos\end{smallmatrix}(kx)$
- Particles can be found in classically forbidden regions

The harmonic oscillator

- Solutions for the harmonic oscillator potential $V(x) = \frac{1}{2}kx^2$ are $\psi(x) \propto (\text{polynomial in } x) \cdot e^{-ax^2}$
- Energy levels are quantised as $E_n = \left(n - \frac{1}{2}\right)\hbar\omega$
- Ladder operators $\hat{A}_+$ and $\hat{A}_-$ transform between states

Unbound particles in 1D

- A free particle beam is described by $\Psi(x,t) = Ne^{i(kx-\omega t)}$, where the intensity of the beam is proportional to $|N|^2$
- Continuity conditions can be used to determine reflection and transmission coefficients at potential steps/barriers