Basic Quantum Mechanics

**Probability & the Uncertainty Principle**
In quantum physics, each observable quantity is defined by a probability, which represents the expected value of the observable ("expectation").
This is the underlying basis of the Heisenberg's uncertainty principle.
If one measures the position and momentum of a particle, the best possible measurement will be limited according to
$$\Delta x \Delta p \geq \frac{1}{2}$$

Similarly, the uncertainty in the measurement of energy of a particle is related to the uncertainty in the time instant at which the measurement was made, according to
$$\Delta E \Delta t \geq \frac{1}{2}$$

**Solving the Schrödinger equation**
**Potential Well problem**

\[ V(x) = 0, \quad 0 < x < L \]
\[ V(x) = m, \quad x = 0, L \]

Inside the well,
\[ -\frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2} E\psi(x) = 0, \quad 0 < x < L \]

**Schrödinger Wave Equation**
- Each particle is described by a wave function, \( \psi(x, t) \).
- The probability of finding the particle in between \( x \) and \( x + dx \) is given by
  \[ \rho(x) = |\psi(x, t)|^2 dx \]
This also implies the normalization condition (the particle is somewhere...)
\[ \int_{-\infty}^{\infty} |\psi(x, t)|^2 dx = 1. \]

**Calculating observables**
In quantum mechanics, an operator must " operate " on the wavefunction to calculate the probability of an observable.

The expectation of an observable
\[ \langle S \rangle = \int \psi^*(x) S \psi(x) dx \]

complex conjugate

**Classical Observables**
<table>
<thead>
<tr>
<th>Classical Observables</th>
<th>Quantum Equivalent</th>
</tr>
</thead>
<tbody>
<tr>
<td>Position ( x )</td>
<td>( \psi(x, t) )</td>
</tr>
<tr>
<td>Momentum ( p )</td>
<td>( -i\hbar \frac{d}{dx} \psi(x, t) )</td>
</tr>
<tr>
<td>Energy</td>
<td>( E ) |</td>
</tr>
<tr>
<td>Total Energy (Kinetic + Potential) ( E_{tot} )</td>
<td>( E - \frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi(x, t) )</td>
</tr>
<tr>
<td>Total Energy (Time Dependent) ( E_{tot} )</td>
<td>( \frac{\hbar^2}{2m} \frac{d^2}{dx^2}</td>
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</tbody>
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Probability & the Uncertainty Principle

In quantum physics, each observable quantity is defined by a probability. This represents the expected value of the observable ("expectation").

This is the underlying basis of the Heisenberg's uncertainty principle.

If one measures the position and momentum of a particle, the best possible measurement will be limited according to:

$$\Delta p \Delta x \geq \frac{1}{2} \hbar$$

Similarly, the uncertainty in the measurement of energy of a particle is related to the uncertainty in the time instant at which the measurement was made is according to:

$$\Delta E \Delta t \geq \frac{1}{2} \hbar$$
Schroedinger Wave Equation

- Each particle is described by a wave function, $\Psi(x, t)$.
- The probability of finding the particle in between $x=a$ and $x=b$ is given by

$$P_{a<x<b} = \int_a^b |\Psi(x, t)|^2 \, dx$$

This also implies the normalization condition (the particle is somewhere...)

$$\int_{-\infty}^{\infty} |\Psi(x, t)|^2 \, dx = 1,$$
Standing waves
Schroedinger Wave Equation

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Schroedinger Wave Equation

\[ \text{total energy} = \text{kinetic energy} + \text{potential energy} \]

\[ i\hbar \frac{\partial}{\partial t} \Psi(r, t) = \left[ -\frac{\hbar^2}{2m} \nabla^2 + V(r, t) \right] \Psi(r, t) \]

Using the wave function \[ \Psi(r, t) = \phi(x) \phi(t) \]

Usually, it's easier to solve this equation when we can separate the time and space variables. This is possible if we can write the wave function as \[ \psi(x) \phi(t) \]

Then, we have a time-dependent part

\[ \frac{d\phi(t)}{dt} + \frac{jE}{\hbar} \phi(t) = 0 \]

and a space-dependent part

\[ \frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2} [E - V(x)] \psi(x) = 0 \]

\[ E = \text{energy of the particle} \]
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Solving the Schrodinger equation
Potential Well problem

\[ V(x) = 0, \quad 0 < x < L \]
\[ V(x) = \infty, \quad x = 0, L \]

Inside the well,

\[ \frac{d^2 \psi(x)}{dx^2} + \frac{2m}{\hbar^2} E \psi(x) = 0, \quad 0 < x < L \]

A possible solution is
\[ \psi = A \sin kx, \quad k = \pm \frac{\sqrt{2mE}}{\hbar} \]

The boundary conditions imply that the wave function must go to zero at the boundaries.

\[ k = \frac{n\pi}{L}, \quad n = 1, 2, 3, \ldots \]  Discrete energy levels!

The energy of the particle is then given by
\[ E_n = \frac{n^2 \pi^2 \hbar^2}{2mL^2} \]

The energy is quantized. \( n \) is a quantum number.
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Discrete energy levels!

The energy of the particle is then given by

\[ \frac{\sqrt{2mE_n}}{\hbar} = \frac{n\pi}{L} \]

\[ E_n = \frac{n^2\pi^2\hbar^2}{2mL^2} \]

The energy is quantized. \( n \) is a quantum number.

To calculate the amplitude, \( A \) of the wave-function, we know that the particle must be in the box, so

\[ \int_{-L}^{L} \psi^*\psi \, dx = \int_{-L}^{L} A^2 \left( \sin \frac{n\pi}{L} x \right)^2 \, dx = A^2 \frac{L}{2} = 1 \]

\[ A = \frac{\sqrt{2}}{\sqrt{L}}, \quad \psi_n = \frac{\sqrt{2}}{\sqrt{L}} \sin \frac{n\pi}{L} x \]
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$$

$$
A = \sqrt{\frac{2}{L}}, \quad \psi_n = \sqrt{\frac{2}{L}} \sin \frac{n \pi}{L} x
$$
Exercise: Where are you likely to find the particle? Where will you never find the particle? 

\[ \psi \quad \sqrt{2/L} \quad |\psi_2|^2 \quad 2/L \quad L \quad x \]

probability-density function
Solving the Schrödinger equation
Potential Well problem

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Calculating observables

In quantum mechanics, an operator must "operate" on the wavefunction to calculate the probability of an observable.

The expectation of an observable

\[ \langle \xi \rangle = \int_{-\infty}^{\infty} \Psi^*(x,t) \xi \Psi(x,t) \, dx \]

Operator

complex conjugate

<table>
<thead>
<tr>
<th>Classical Dynamical Variable</th>
<th>QM Operator Representation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Position ( x )</td>
<td>( x )</td>
</tr>
<tr>
<td>Potential Energy ( V(x) )</td>
<td>( V(x) )</td>
</tr>
<tr>
<td>( f(x) )</td>
<td>( f(x) )</td>
</tr>
<tr>
<td>Momentum ( p_x )</td>
<td>( \frac{\hbar}{i} \frac{\partial}{\partial x} )</td>
</tr>
<tr>
<td>Kinetic Energy ( \frac{p_x^2}{2m} )</td>
<td>( -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} )</td>
</tr>
<tr>
<td>( f(p_x) )</td>
<td>( f\left(\frac{\hbar}{i} \frac{\partial}{\partial x}\right) )</td>
</tr>
<tr>
<td>Total Energy (Kinetic + Potential) ( E_{Total} )</td>
<td>( -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) )</td>
</tr>
<tr>
<td>Total Energy (Time Version) ( E_{Total} )</td>
<td>( -\frac{\hbar}{i} \frac{\partial}{\partial t} )</td>
</tr>
</tbody>
</table>
Example Problem:

Given the wave function of a plane wave

\[ \psi = A \exp(jk_x x) \]

What is the expectation value for the x-component of its momentum?

\[
\langle p_x \rangle = \frac{\int_{-\infty}^{\infty} A^* e^{-jk_xx} \left( \frac{\hbar}{j} \frac{\partial}{\partial x} \right) Ae^{jk_xx} \, dx}{\int_{-\infty}^{\infty} |A|^2 e^{-jk_xx} e^{jk_xx} \, dx} = (\hbar k_x)
\]
Quantum Mechanical Tunneling

Purely quantum effect (useful)

When the potential is finite

the wave function & its derivative must be continuous across the boundary

Exponential decrease inside barrier

the particle can "tunnel" through this barrier

Exponential decrease beyond barrier

\[ |\psi|^2 \neq 0 \text{ beyond barrier} \]