Quantum Tunneling

Quantum tunneling is a fundamental phenomenon of quantum mechanics in which a particle has a non-zero probability of crossing a potential energy barrier even when its total energy is less than the height of the barrier. This behavior has no analogue in classical physics and arises directly from the wave nature of quantum particles.

1. Classical Description

In classical mechanics, a particle of total energy E encountering a potential barrier of height V can only cross the barrier if $E \geq V$. If $E < V$, the particle is completely reflected, as the kinetic energy $K = E - V(x)$ would become negative, which is not physically possible.

2. Quantum Mechanical Description

In quantum mechanics, particles are described by a wavefunction $\psi(x, t)$. The evolution and spatial behavior of this wavefunction are governed by the Schrodinger equation. The probability of finding a particle at a given position is given by $|\psi(x)|^2$.

The Schrodinger equation does not forbid solutions in regions where $E < V(x)$. Instead, it predicts exponentially decaying wavefunctions inside such regions, which leads to a finite probability of transmission through the barrier. The Schrodinger equation is:

$$-(\hbar^2 / 2m)\, d^2\psi(x)/dx^2 + V(x)\, \psi(x) = E\psi(x)$$

3. Classically Allowed and Forbidden Regions

When E > V(x): the Schrödinger equation admits oscillatory solutions corresponding to traveling waves. These represent regions where the particle can propagate freely.

When $E > V$, define:

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

The equation becomes:

$$\frac{d^2\psi}{dx^2} + k^2\psi = 0$$

with oscillatory solutions:

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

When E < V(x): the equation yields exponential solutions. These represent evanescent waves that decay inside the barrier. Although these solutions do not represent propagation in the classical sense, they allow the wavefunction to extend into and beyond the barrier.

When $E < V$, define:

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

The equation becomes:

$$\frac{d^2\psi}{dx^2} - \kappa^2\psi = 0$$

with solutions:

$$\psi(x) = Ce^{-\kappa x} + De^{\kappa x}$$

4. Potential Barrier

The tunneling calculator models tunneling using a finite rectangular potential barrier defined as:

V(x) = 0, for x < 0
V(x) = V0, for 0 ≤ x ≤ L
V(x) = 0, for x > L

5. Boundary Conditions

At the boundaries of the barrier, the wavefunction and its first derivative must be continuous. These boundary conditions ensure conservation of probability and uniquely determine the reflected and transmitted components of the wave function.

At each boundary ($x = 0$, $x = L$), the wavefunction must satisfy:

1. Continuity of the wavefunction:

$$\psi_{\text{left}} = \psi_{\text{right}}$$

2. Continuity of the first derivative:

$$\frac{d\psi_{\text{left}}}{dx} = \frac{d\psi_{\text{right}}}{dx}$$

6. Transmission Probability

The transmission coefficient T is defined as the ratio of transmitted probability current to incident probability current. For a finite rectangular barrier with particle energy less than the barrier height, the transmission probability is given by an analytical expression involving the barrier height, width, particle energy, and mass.

The transmission probability decreases exponentially with increasing barrier width and particle mass, and increases as the particle energy approaches the barrier height.

The **transmission coefficient** T is defined as:

$$T = \frac{\text{transmitted probability current}}{\text{incident probability current}}$$

It satisfies:

$$0 \leq T \leq 1$$

For a rectangular barrier of height V_0 and width L, the transmission probability is:

$$T = \left[1 + \frac{V_0^2}{4E(V_0 - E)} \sinh^2(\kappa L)\right]^{-1} \quad \text{where} \quad \kappa = \frac{\sqrt{2m(V_0 - E)}}{\hbar}$$

7. Physical Interpretation

Quantum tunneling does not involve a violation of energy conservation. The particle does not gain extra energy to cross the barrier. Instead, tunneling arises because quantum states are spatially extended and governed by wave equations rather than classical trajectories.

8. Assumptions and Validity

The tunneling model implemented in this project assumes:
- One-dimensional motion
- A single, non-relativistic particle
- A time-independent potential

Within these assumptions, the tunneling calculator provides an accurate description of quantum tunneling phenomena.

Quantum Tunneling Calculator

Explanation

1. Outputs Produced by the Quantum Tunneling Calculator

The quantum tunneling calculator generates numerical, graphical, and physical outputs that demonstrate the wave nature of particles and the breakdown of classical predictions.

1.1 Transmission (Tunneling) Probability

The main numerical output is the transmission probability T, displayed as a percentage. It represents the probability that a particle crosses a potential barrier.

For particle energy E less than barrier height V_0, the transmission probability used in the code is:

$$T = [1 + (V_0^2 \sinh^2 (\kappa L)) / (4E (V_0 - E))]^{-1}$$

Where $\kappa = \sqrt{(2m (V_0 - E))} / \hbar$

1.2 Wave function Output

The calculator plots the real part of the wave function $\psi(x)$. The wave function is oscillatory outside the barrier and exponentially decaying inside it.

The wave function is obtained from the time-independent Schrödinger equation:

$$-(\hbar^2 / 2m)\, d^2\psi/dx^2 + V(x)\, \psi = E\psi$$

1.3 Probability Density $|\psi(x)|^2$

The probability density $|\psi(x)|^2$ is plotted to show the likelihood of finding the particle at a given position. A non-zero probability beyond the barrier confirms tunneling.

1.4 Potential Barrier Visualization

A rectangular potential barrier V(x) is plotted alongside the wave function:

$$V(x) = V_0 \text{ for } 0 \le x \le L, \quad V(x) = 0 \text{ elsewhere}$$

2. Internal Working of the Code

2.1 Input and Unit Conversion

User inputs such as

Energy (eV)

Barrier height (eV) and

Width (nm) are converted into SI units before calculation:

$E (J) = E (eV) \times 1.602 \times 10^{-19}$

2.2 Quantum Engine Solver

The Quantum Engine class solves the Schrödinger equation analytically. The code checks whether $E > V_0$ or $E < V_0$ and applies the corresponding formula.

2.3 Wave Vector and Decay Constant

The following quantities are computed internally:

$k = \sqrt{(2mE)} / \hbar$ (free-particle wave vector)

$\kappa = \sqrt{(2m(V_0 - E))} / \hbar$ (decay constant inside the barrier)

2.4 Piecewise Wave function Construction

The wave function is built in three regions:

Region I ($x < 0$)

Region II ($0 \leq x \leq L$)

Region III ($x > L$): ψ

2.5 Visualization and Output Display

Numerical arrays returned by the solver are passed to plotting functions. Plotly is used to render wave function, probability density, and potential energy graphs.

In a nut shell, we made a calculator to find quantum tunneling in electrons, protons, neutrons and alpha particles. We set the energy (electron volt) in the range 0-2, barrier height (electron volt) in the range 0-30, barrier width (nm) in the range 0.05. We can find the tunneling by varying these parameters, by varying each parameter give different output. Apart from tunneling, we can also the quantum dots, molecular vibrations and Hydrogen 1S orbital.