Quantum Tunnelling Effect in 2D

Benjamin Ocampo

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1 Introduction

The quantum tunnelling effect is a quantum mechanical phenomenon where a particle can pass through a potential barrier even when its energy is lower than the barrier's height. This document explores quantum tunnelling in a 2D setting, where a particle can move both horizontally and vertically.

2 The Schrödinger Equation in 2D

The time-dependent Schrödinger equation for a particle moving in a 2D potential $V(x, y)$ is given by:

$$i\hbar\frac{\partial\Psi(x,y,t)}{\partial t} = \left[-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) + V(x,y)\right]\Psi(x,y,t) \tag{1}$$

2.1 Potential Barrier

Consider a potential barrier defined as:

$$V(x,y) = \begin{cases} 0 & \text{if } (x,y) \text{ is outside the barrier region} \\ V_0 & \text{if } (x,y) \text{ is inside the barrier region} \end{cases} \tag{2}$$

Where V_0 is the height of the potential barrier.

2.2 Wavefunction Initialization

The wavefunction is initialized as a Gaussian wave packet:

$$\Psi(x,y,0) = A\exp\left[-\frac{(x-x_0)^2}{2\sigma_x^2} - \frac{(y-y_0)^2}{2\sigma_y^2} + i(k_x x + k_y y)\right] \tag{3}$$

3 Numerical Method: Pseudospectral Method

The pseudospectral method is a powerful numerical technique used to approximate the solution of partial differential equations, such as the Schrödinger equation, by representing the solution in terms of a series of basis functions.

3.1 Chebyshev Grid and Differentiation Matrices

In the pseudospectral method, the spatial domain is discretized using a non-uniform grid of points known as the Chebyshev grid. The Chebyshev points x_j for $j = 0, 1, \ldots, N$ are defined as:

$$x_j = \cos\left(\frac{j\pi}{N}\right) \tag{4}$$

The differentiation matrices D_x and D_y are used to approximate the spatial derivatives of the wavefunction. These matrices are constructed using the following expressions:

$$(D_x)_{ij} = \begin{cases} \frac{2N^2+1}{6}, & i = j = 0 \\ \frac{-x_j}{2(1-x_j^2)}, & i = j \neq 0 \\ \frac{(-1)^{i+j}}{x_i - x_j}, & i \neq j \end{cases} \tag{5}$$

The second-order spatial derivatives $\frac{\partial^2 \Psi}{\partial x^2}$ and $\frac{\partial^2 \Psi}{\partial y^2}$ are approximated by applying these differentiation matrices:

$$\frac{\partial^2 \Psi}{\partial x^2} \approx D_x \cdot D_x \cdot \Psi \quad \text{and} \quad \frac{\partial^2 \Psi}{\partial y^2} \approx D_y \cdot D_y \cdot \Psi \tag{6}$$

3.2 Constructing the Hamiltonian

The Hamiltonian H governs the dynamics of the wavefunction and is composed of the kinetic energy and potential energy terms. In 2D, the Hamiltonian is constructed as:

$$H = -\frac{\hbar^2}{2m}\left(D_x^T D_x + D_y^T D_y\right) + V(x, y) \tag{7}$$

Where: - $D_x^T D_x$ and $D_y^T D_y$ represent the discretized second derivatives in the x and y directions, respectively. - $V(x, y)$ is the potential energy matrix.

4 Time Evolution: Crank-Nicolson Method

The time evolution of the wavefunction $\Psi(x, y, t)$ is computed using the Crank-Nicolson method, which is an implicit, unconditionally stable numerical scheme for solving time-dependent partial differential equations.

4.1 Crank-Nicolson Discretization

The Crank-Nicolson method is a finite difference method that averages the Schrödinger equation between two successive time steps t and $t + \Delta t$:

$$i\hbar \frac{\Psi(x, y, t + \Delta t) - \Psi(x, y, t)}{\Delta t} = \frac{1}{2} \left[H\Psi(x, y, t + \Delta t) + H\Psi(x, y, t) \right] \tag{8}$$

Rearranging the terms, we obtain the Crank-Nicolson update formula:

$$\left(I - \frac{i\hbar \Delta t}{2} H \right) \Psi(x, y, t + \Delta t) = \left(I + \frac{i\hbar \Delta t}{2} H \right) \Psi(x, y, t) \tag{9}$$

Where I is the identity matrix. This equation can be solved for the updated wavefunction $\Psi(x, y, t + \Delta t)$ by inverting the left-hand side matrix.

4.2 Complex Exponentials in the Wavefunction

The wavefunction contains complex exponentials representing the phase factor due to the initial momentum of the particle:

$$\Psi(x, y, t) = A \exp \left[-\frac{(x - x_0)^2}{2\sigma_x^2} - \frac{(y - y_0)^2}{2\sigma_y^2} \right] \exp \left[i(k_x x + k_y y) \right] \tag{10}$$

The Crank-Nicolson method ensures that the wavefunction's amplitude is preserved while correctly evolving the phase information encoded in these complex exponentials.

5 Boundary Conditions

Boundary conditions play a crucial role in numerical simulations of quantum systems, particularly in determining the behavior of the wavefunction at the edges of the computational domain.

5.1 Dirichlet Boundary Conditions

In this simulation, Dirichlet boundary conditions are applied, where the wavefunction is set to zero at the boundaries of the domain. This condition effectively confines the particle within the domain, preventing it from escaping. Mathematically, this is expressed as:

$$\Psi(x, y, t) = 0 \quad \text{for} \quad x = \text{boundary}, \, y = \text{boundary} \tag{11}$$

This boundary condition ensures that the wavefunction decays to zero at the edges of the grid, which is physically consistent with a particle trapped within a finite potential well.

5.2 Impact on the Wavefunction Evolution

The enforcement of Dirichlet boundary conditions at each time step during the Crank-Nicolson time evolution prevents numerical artifacts, such as the wavefunction artificially growing or reflecting off the domain boundaries. By resetting the wavefunction to zero at the edges, the simulation accurately captures the quantum tunnelling behavior within the central region of the computational domain.

6 Visualization of Quantum Tunnelling via Probability Distribution Function

The quantum tunnelling effect is visualized in this simulation through the square root of the probability distribution function. The probability distribution function is defined as the square of the absolute value of the wavefunction:

$$P(x, y, t) = |\Psi(x, y, t)|^2 \tag{12}$$

However, due to the high amplitude values of the wavefunction, directly visualizing $P(x, y, t)$ can lead to very large and difficult-to-interpret values. To address this, the square root of the probability distribution function is used:

$$P_{\text{sqrt}}(x, y, t) = \sqrt{P(x, y, t)} = |\Psi(x, y, t)| \tag{13}$$

6.1 Reason for Using the Square Root

Taking the square root of the probability distribution function effectively normalizes the amplitude variations, making it easier to visualize and interpret the tunnelling effect. This approach helps highlight regions where the particle is likely to be found while reducing the impact of extreme values that could otherwise dominate the visualization.

7 Comparison Between Finite Difference and Pseudospectral Methods

7.1 Finite Difference Method (FDM)

The Finite Difference Method (FDM) approximates derivatives by using differences between function values at adjacent grid points. While simple to implement, FDM requires a fine grid to achieve high accuracy and can suffer from numerical instability if the grid is too coarse.

7.1.1 Disadvantages of FDM

- Requires very fine grids to achieve high accuracy, leading to increased computational cost.
- Prone to numerical instability if the grid size Δx is not sufficiently small.

7.2 Pseudospectral Method

The Pseudospectral Method, on the other hand, uses global basis functions (e.g., Chebyshev polynomials) to represent the solution. This method approximates derivatives by differentiating the basis functions analytically, resulting in highly accurate approximations even with relatively coarse grids.

7.2.1 Advantages of the Pseudospectral Method

- Extremely accurate for smooth solutions, often requiring fewer grid points than FDM to achieve similar accuracy.
- Handles complex boundary conditions and variable coefficients more naturally.

7.2.2 Disadvantages of the Pseudospectral Method

- More complex to implement, especially in higher dimensions.
- The accuracy can degrade significantly if the solution is not smooth (e.g., at discontinuities).

7.3 Application in the Simulation

In this simulation, the Pseudospectral Method is employed to compute the spatial derivatives of the wavefunction with high accuracy. The Chebyshev grid allows for an efficient representation of the wavefunction's behavior across the domain, capturing the tunnelling effect with fewer grid points than a comparable FDM approach would require.