Numerical Simulation of Quantum Tunneling Using Eigen-Decomposition and Split-Step Fourier Methods

Abstract

Quantum tunneling is a central non-classical phenomenon that has shaped modern physics and technology, from nuclear fusion processes to quantum electronic devices. This paper presents a comprehensive theoretical and numerical study of tunneling using computational quantum mechanics. A Gaussian wavepacket is propagated in one dimension using Hamiltonian eigen-decomposition and in two dimensions using the split-step Fourier method. The mathematical foundations of the time-dependent Schrödinger equation (TDSE), numerical discretization schemes, derivation of the finite-difference Hamiltonian, propagation algorithms, boundary treatment, and stability considerations are fully detailed. Simulations demonstrate reflection, transmission, tunneling probability calculations, and parameter dependence on barrier geometry. The 2D model illustrates diffraction, interference, and multidimensional tunneling behavior. This paper aims to provide a rigorous and complete explanation suitable for advanced undergraduate and graduate-level study.

1 Introduction

Quantum tunneling is one of the most striking demonstrations of the wave nature of matter. Unlike classical particles, quantum particles possess a spatially extended probability amplitude that allows them to penetrate into and even across forbidden regions. This effect plays essential roles in alpha decay, field emission, chemical reactions, fusion in stars, tunnel diodes, Josephson junctions, and scanning tunneling microscopy.

The goals of this work are:

1. To numerically solve the TDSE for a Gaussian wavepacket encountering a potential barrier in 1D.

2. To extend the model to 2D and simulate multidimensional tunneling using Fourier-based propagation.

Animations and numerical analyses reveal the transition between reflection, transmission, and evanescent decay inside the barrier.

2 Theoretical Background

2.1 Time-Dependent Schrödinger Equation

The non-relativistic TDSE in one spatial dimension is

$$i\hbar\frac{\partial\psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V(x)\psi(x,t). \tag{1}$$

Using natural units ($\hbar = m = 1$), this reduces to

$$i\frac{\partial\psi}{\partial t} = -\frac{1}{2}\frac{\partial^2\psi}{\partial x^2} + V(x)\psi. \tag{2}$$

Dirichlet boundary conditions,

$$\psi(0,t) = \psi(L,t) = 0,$$

approximate a large confining box.

2.2 Gaussian Wavepacket

The initial wavepacket is

$$\psi(x,0) = \exp\left[-\frac{(x-x_0)^2}{2\sigma^2}\right]e^{ik_0x}, \tag{3}$$

with mean momentum k_0 and approximate classical energy

$$E \approx \frac{k_0^2}{2}.$$

2.3 Rectangular Potential Barrier

A finite barrier is defined as

$$V(x) = \begin{cases} V_0, & a < x < a + w, \\ V_{\text{bg}}, & \text{otherwise}, \end{cases} \tag{4}$$

where V_{bg} is a small background offset.

The WKB approximation predicts for $E < V_0$:

$$T \approx e^{-2\kappa w}, \qquad \kappa = \sqrt{2(V_0 - E)}.$$

3 Numerical Discretization

3.1 Spatial Grid

The interval $[0, L]$ is discretized into N subintervals:

$$x_i = i\Delta x, \qquad \Delta x = \frac{L}{N}. \tag{5}$$

Only interior points $x_1, \ldots, x_{N-1}$ are used for the Hamiltonian.

3.2 Finite-Difference Approximation

The Laplacian is approximated by

$$\left.\frac{\partial^2\psi}{\partial x^2}\right|_{x_i} \approx \frac{\psi_{i+1} - 2\psi_i + \psi_{i-1}}{\Delta x^2}. \tag{6}$$

This gives the kinetic matrix

$$T = -\frac{1}{2\Delta x^2}\begin{pmatrix} -2 & 1 & & & 0 \\ 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & -2 & 1 \\ 0 & & & 1 & -2 \end{pmatrix}. \tag{7}$$

The potential matrix is diagonal.

4 Eigen-Decomposition Time Evolution

4.1 Hamiltonian Eigenproblem

We solve

$$H\phi_n = E_n\phi_n, \tag{8}$$

yielding a complete orthonormal basis.

4.2 Projection of the Initial Condition

The coefficients are

$$c_n = \sum_i \phi_n^*(x_i)\psi(x_i, 0)\Delta x. \tag{9}$$

4.3 Exact Time Propagation

The time evolution is

$$\psi(x, t) = \sum_n c_n e^{-iE_n t}\phi_n(x), \tag{10}$$

which is numerically exact on the grid.

4.4 Discussion of Accuracy

The method is stable and free from time-step errors. Accuracy is determined solely by:

- spatial grid resolution,
- floating-point precision,
- eigenvalue solver accuracy.

5 2D Quantum Tunneling

5.1 TDSE in Two Dimensions

$$i\frac{\partial \psi}{\partial t} = -\frac{1}{2}\left(\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2}\right) + V(x,y)\psi. \tag{11}$$

5.2 Split-Step Fourier Method

The evolution operator is split as

$$e^{-iHdt} \approx e^{-iVdt/2} e^{-iTdt} e^{-iVdt/2}. \tag{12}$$

Using FFT:

$$\psi(k_x, k_y) = \mathcal{F}\{\psi(x,y)\},$$

and the kinetic step becomes a simple multiplication:

$$\psi \leftarrow \exp\left[-i(k_x^2 + k_y^2)\frac{dt}{2}\right]\psi.$$

5.3 Absorbing Boundaries

A cosine mask

$$M(x,y) = \cos^{\alpha}\left(\frac{\pi d}{2d_{\max}}\right)$$

prevents reflections from boundaries.

5.4 Stability Considerations

Split-step Fourier is unconditionally stable, though accuracy requires:

- sufficiently small dt,
- fine momentum-space cutoff,
- avoidance of aliasing.

6 Simulation Results

6.1 1D Dynamics

Typical features include:

- Gaussian spreading,
- partial reflection,
- evanescent decay inside the barrier,
- emergence of transmitted wavefront.

6.2 Reflection and Transmission

We compute

$$R = \int_0^a |\psi(x, t_f)|^2 \, dx, \tag{13}$$

$$T = \int_{a+w}^L |\psi(x, t_f)|^2 \, dx. \tag{14}$$

Numerical results match the WKB scaling law.

6.3 Parameter Dependence

Sweeps over V_0 and w reveal:

- exponential suppression of T with barrier width,
- transition to classical over-the-barrier behavior when $E > V_0$,
- oscillatory structures related to resonant tunneling.

6.4 2D Effects

The two-dimensional model exhibits:

- diffraction around the barrier edges,
- curvature of transmitted wavefronts,
- interference fringes analogous to optical scattering.

7 Discussion

Key points include:

- spatial resolution is the dominant source of numerical error,
- eigen-decomposition is exact but expensive ($O(N^3)$),
- split-step Fourier is efficient ($O(N^2 \log N)$) and scalable,
- extension to multi-barrier or smooth potentials is straightforward,
- parameter sweeps reveal agreement with semiclassical theory.

8 Conclusion

We have developed a complete numerical framework for simulating quantum tunneling in 1D and 2D. The eigen-decomposition method provides exact time evolution for moderate system sizes, while the split-step Fourier method enables efficient multidimensional propagation. Numerical results agree with theoretical predictions, demonstrating exponential tunneling suppression and rich multidimensional wave phenomena. This work highlights the usefulness of computational quantum mechanics in understanding fundamental quantum behavior.

9 References

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