Simulation of Quantum Wave Transport: Derivations and the Split-Step Fourier Method

High-Performance Computational Physics Analysis

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Abstract

This document details the theoretical and numerical framework for simulating quantum wave packet dynamics in a $3D$ potential landscape. The simulation is founded on solving the **Time-Dependent Schrödinger Equation (TDSE)** using the **Split-Step Fourier Method (SSFM)**. We focus on the mathematical derivations necessary for modeling probability density propagation and quantum interference patterns.

1 The Governing Equation: Time-Dependent Schrödinger Equation (TDSE)

The evolution of a quantum particle, represented by the wave function $\Psi(\mathbf{r}, t)$, is fundamentally dictated by the TDSE. The goal of the simulation is to track this evolution precisely.

1.1 The Hamiltonian Operator

The total energy operator, the **Hamiltonian** ($\hat{H}$), is the sum of the kinetic energy operator ($\hat{T}$) and the potential energy operator ($\hat{V}$):

$$\hat{H} = \hat{T} + \hat{V}$$

In the position representation, in three dimensions, these operators are:

$$\hat{T} = -\frac{\overline{h}^2}{2m}\nabla^2 \quad \text{and} \quad \hat{V} = V(\mathbf{r}, t)$$

where $\overline{h}$ is the reduced Planck constant, m is the mass of the particle, and ∇^2 is the Laplacian operator.

1.2 The TDSE Statement

The fundamental equation defining the time evolution of the wave function is:

$$i\overline{h}\frac{\partial}{\partial t}\Psi(\mathbf{r}, t) = \hat{H}\Psi(\mathbf{r}, t)$$

or, written explicitly with the operators:

$$i\overline{h}\frac{\partial}{\partial t}\Psi(\mathbf{r}, t) = \left(-\frac{\overline{h}^2}{2m}\nabla^2 + V(\mathbf{r}, t)\right)\Psi(\mathbf{r}, t)$$

2 Probability Density and Observables

The physical observable quantity of interest is the **probability density**, $\rho(\mathbf{r}, t)$, which provides the spatial distribution and visualizes the interference effects.

2.1 Probability Density Derivation

The probability density is the square of the magnitude of the complex wave function, $\Psi(\mathbf{r}, t)$:

$$\rho(\mathbf{r}, t) = |\Psi(\mathbf{r}, t)|^2 = \Psi(\mathbf{r}, t)^* \Psi(\mathbf{r}, t)$$

The normalization condition, which states that the particle must be found somewhere in space, is maintained throughout the simulation:

$$\int_{\mathbb{R}^3} \rho(\mathbf{r}, t)\, d\mathbf{r} = \int_{\mathbb{R}^3} |\Psi(\mathbf{r}, t)|^2\, d\mathbf{r} = 1$$

The movement of the wave packet, $\rho(\mathbf{r}, t)$, illustrates physical processes such as quantum tunneling and diffraction, the latter being the source of complex **interference patterns** within the simulation domain.

3 Numerical Solution: The Split-Step Fourier Method (SSFM)

The kinetic and potential operators typically do not commute ($\left[\hat{T}, \hat{V}\right] \neq 0$). This non-commutation prevents a simple closed-form solution. The SSFM overcomes this by breaking the time evolution into short, separable steps.

3.1 Derivation of the Time Evolution Operator Splitting

The formal solution for a small time step Δt is:

$$\Psi(\mathbf{r}, t)(t + \Delta t) = e^{-i\hat{H}\Delta t/\hbar} \Psi(\mathbf{r}, t)(t) = e^{-i(\hat{T}+\hat{V})\Delta t/\hbar} \Psi(\mathbf{r}, t)(t)$$

The SSFM utilizes the first-order approximation (which is more computationally efficient and sufficient for small Δt) or the symmetric second-order Strang splitting. We use the simple, first-order factorization here:

$$\hat{U}(\Delta t) \approx \hat{U}_V(\Delta t)\hat{U}_T(\Delta t) = e^{-i\hat{V}\Delta t/\hbar} e^{-i\hat{T}\Delta t/\hbar}$$

The total evolution is thus an alternating sequence of applying the potential step and the kinetic step.

3.2 Step 1: Potential Energy Propagation (Position Space)

The potential energy operator is local in position space, meaning its action is a direct multiplication:

$$\psi'(\mathbf{r}, t) = e^{-iV(\mathbf{r},t)\Delta t/\hbar} \Psi(\mathbf{r}, t)(t)$$

This step only introduces a position-dependent phase factor to the wave function, which is computationally trivial on a spatial grid.

3.3 Step 2: Kinetic Energy Propagation (Momentum Space)

The kinetic energy operator ($\hat{T} = -\frac{\hbar^2}{2m}\nabla^2$) is non-local in position space, making its direct computation using finite difference methods complex and prone to numerical instability. The key insight of SSFM is that $\hat{T}$ is diagonal in **momentum space** (**p**), where it simplifies to multiplication by the momentum eigenvalue $p^2/(2m)$.

3.3.1 The Forward Fourier Transform Integral

We use the **Fourier Transform** ($\mathcal{F}$) to switch from the position domain (**r**) to the momentum domain (**p**):

$$\tilde{\Psi}(\mathbf{p}, t) = \mathcal{F}\{\Psi(\mathbf{r}, t)\} = \frac{1}{(2\pi\hbar)^{3/2}} \int_{\mathbb{R}^3} \psi'(\mathbf{r}, t) e^{-i\mathbf{p}\cdot\mathbf{r}/\hbar}\, d\mathbf{r}$$

3.3.2 Action of the Kinetic Operator in Momentum Space

In momentum space, the kinetic energy evolution becomes a simple element-wise multiplication:

$$\tilde{\Psi}''(\mathbf{p}, t + \Delta t) = e^{-i\left(\frac{p^2}{2m}\right)\Delta t/\hbar} \tilde{\Psi}(\mathbf{p}, t)$$

where $p^2 = |\mathbf{p}|^2 = p_x^2 + p_y^2 + p_z^2$. The particle's momentum squared is the eigenvalue of the kinetic energy operator.

3.3.3 The Inverse Fourier Transform Integral

Finally, the resulting wave function is transformed back to the position domain to complete the time step:

$$\Psi(\mathbf{r}, t)(t + \Delta t) = \mathcal{F}^{-1}\left\{\tilde{\Psi}''(\mathbf{p}, t + \Delta t)\right\} = \frac{1}{(2\pi\hbar)^{3/2}} \int_{\mathbb{R}^3} \tilde{\Psi}''(\mathbf{p}, t + \Delta t) e^{i\mathbf{p}\cdot\mathbf{r}/\hbar}\, d\mathbf{p}$$

In practice, these continuous integrals are replaced by discrete summations implemented via the **Fast Fourier Transform (FFT)**, which is crucial for the high performance of the SSFM.

4 HPC and Simulation of Interference

The repetitive reliance on 3D FFT/IFFT operations makes this algorithm a prime candidate for HPC, specifically using highly parallel architectures like GPUs.

- **Parallel FFT:** For a $N \times N \times N$ spatial grid, the $O(N^3 \log N)$ complexity of the FFT is handled by distributing the computation across thousands of parallel cores (using CUDA or equivalent), dramatically accelerating the simulation.
- **Interference Visualization:** When the wave packet encounters structures in $V(\mathbf{r}, t)$, such as two adjacent slits, the $\Psi(\mathbf{r}, t)$ splits. When the components overlap again, the phase differences lead to complex constructive and destructive regions in the probability density $\rho(\mathbf{r}, t)$, which are the **interference patterns**. The HPC platform allows these patterns to be computed in real-time, even for complex 3D potentials.

This framework provides a robust and scalable method for visualizing the core principles of quantum mechanics in diverse potential landscapes.