GPU-Accelerated Simulation of Wavepacket Scattering in a Finite Periodic Lattice

Abstract

This document presents the physical model, mathematical formulation, and numerical algorithm underlying a two-dimensional simulation of quantum wavepacket scattering. The system is governed by the time-dependent Schrödinger equation and solved numerically using a split-step Fourier method. A finite periodic lattice potential composed of Gaussian scatterers induces diffraction and interference effects. The simulation is accelerated on a GPU using cuFFT, and the complex-valued wavefunction is visualized in real time using a phase–amplitude color encoding.

Contents

1 Physical Model

We consider the non-relativistic quantum dynamics of a single particle of mass m moving in two spatial dimensions (x, y) under the influence of an external potential $V(x, y)$. The evolution of the wavefunction $\psi(x, y, t)$ is governed by the time-dependent Schrödinger equation (TDSE):

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

where $\nabla^2 = \partial_x^2 + \partial_y^2$ denotes the Laplace operator.

The wavefunction is normalized such that

$$\int_{\mathbb{R}^2} |\psi(x,y,t)|^2\, dx\, dy = 1, \tag{2}$$

and the probability density is given by $|\psi(x, y, t)|^2$.

2 Initial Condition: Gaussian Wavepacket

The initial state is chosen as a Gaussian wavepacket modulated by a plane wave:

$$\psi(x,y,0) = \exp\left(-\frac{(x-x_0)^2 + (y-y_0)^2}{4\sigma^2}\right)\exp(i(k_x x + k_y y))\,, \tag{3}$$

where:

- (x_0, y_0) is the initial center of the wavepacket,
- σ controls the spatial width,
- (k_x, k_y) is the mean wavevector.

The wavepacket has a mean momentum $\boldsymbol{p} = \hbar(k_x, k_y)$ and a finite momentum spread.

3 Finite Periodic Lattice Potential

Scattering is induced by a finite periodic lattice potential composed of Gaussian barriers:

$$V(x,y) = V_0 \sum_{i=1}^{N_x}\sum_{j=1}^{N_y} \exp\left(-\frac{(x-x_i)^2 + (y-y_j)^2}{2\sigma_V^2}\right), \tag{4}$$

where:

- V_0 is the barrier height,
- σ_V determines the spatial extent of each scatterer,
- (x_i, y_j) form a rectangular lattice with spacings (a_x, a_y).

This potential approximates a finite crystal lattice and produces diffraction and interference phenomena.

4 Absorbing Boundary Conditions

To suppress unphysical reflections at the edges of the finite computational domain, a smooth absorbing boundary mask is applied after each time step:

$$\psi(x, y, t) \leftarrow \psi(x, y, t)\, A(x, y), \tag{5}$$

with

$$A(x, y) = \exp\left[-\alpha \left(1 - \frac{d(x, y)}{d_{\max}}\right)^4\right], \tag{6}$$

where $d(x, y)$ is the distance to the nearest boundary and α controls the absorption strength.

5 Operator Splitting

The Hamiltonian operator is decomposed into kinetic and potential parts:

$$\hat{H} = \hat{T} + \hat{V}, \qquad \hat{T} = -\frac{\hbar^2}{2m}\nabla^2, \qquad \hat{V} = V(x, y). \tag{7}$$

Since $\hat{T}$ and $\hat{V}$ do not commute, the time-evolution operator is approximated using second-order Strang splitting:

$$e^{-i\hat{H}\Delta t/\hbar} \approx e^{-i\hat{T}\Delta t/(2\hbar)} e^{-i\hat{V}\Delta t/\hbar} e^{-i\hat{T}\Delta t/(2\hbar)} + \mathcal{O}(\Delta t^3). \tag{8}$$

This scheme is unitary and time-reversible up to second order.

6 Numerical Algorithm: Split-Step Fourier Method

The kinetic operator is diagonal in momentum space, while the potential operator is diagonal in real space. The numerical propagation alternates between these representations using fast Fourier transforms.

Algorithm 1 Split-Step Fourier Method for the 2D TDSE

Require: Initial wavefunction $\psi(x, y, 0)$, potential $V(x, y)$, time step Δt, number of time steps N_t

Ensure: Wavefunction $\psi(x, y, t_n)$ for $n = 1, \ldots, N_t$

for $n = 0$ **to** $N_t - 1$ **do**
  $\tilde{\psi}(\boldsymbol{k}) \leftarrow \mathcal{F}\{\psi(x, y, t_n)\}$
  $\tilde{\psi}(\boldsymbol{k}) \leftarrow \tilde{\psi}(\boldsymbol{k}) \exp\left(-i\frac{\hbar|\boldsymbol{k}|^2}{2m}\frac{\Delta t}{2}\right)$
  $\psi(x, y) \leftarrow \mathcal{F}^{-1}\{\tilde{\psi}(\boldsymbol{k})\}$
  $\psi(x, y) \leftarrow \psi(x, y) \exp\left(-i\frac{V(x,y)\Delta t}{\hbar}\right)$
  $\tilde{\psi}(\boldsymbol{k}) \leftarrow \mathcal{F}\{\psi(x, y)\}$
  $\tilde{\psi}(\boldsymbol{k}) \leftarrow \tilde{\psi}(\boldsymbol{k}) \exp\left(-i\frac{\hbar|\boldsymbol{k}|^2}{2m}\frac{\Delta t}{2}\right)$
  $\psi(x, y, t_{n+1}) \leftarrow \mathcal{F}^{-1}\{\tilde{\psi}(\boldsymbol{k})\}$
  $\psi(x, y, t_{n+1}) \leftarrow \psi(x, y, t_{n+1}) \cdot A(x, y)$
end for

7 Visualization of the Wavefunction

The complex-valued wavefunction is visualized using an HSV color mapping:

$$\text{Hue} = \frac{\arg(\psi) + \pi}{2\pi}, \tag{9}$$

$$\text{Value} = \left(\frac{|\psi|^2}{\max(|\psi|^2)} \right)^{\gamma}, \tag{10}$$

$$\text{Saturation} = 1, \tag{11}$$

where $\gamma < 1$ enhances low-intensity interference fringes.

This representation simultaneously reveals phase singularities, interference patterns, and diffraction features.

8 Physical Interpretation

The simulation captures fundamental quantum phenomena:

- free-space wavepacket dispersion,
- diffraction from a finite periodic lattice,
- interference and phase dislocations,
- partial reflection and transmission.

The finite lattice bridges the regimes of free propagation and crystalline scattering.

9 Conclusion

A split-step Fourier method combined with GPU acceleration provides an efficient and physically faithful approach to simulating time-dependent quantum dynamics. The use of absorbing boundaries and phase-resolved visualization enables real-time exploration of complex scattering phenomena in structured potentials.