

GPU-Accelerated Simulation of Wavepacket Scattering in a Periodic Lattice

Abstract

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

Contents

1	Physical Model	2
2	Initial Condition: Gaussian Wavepacket	2
3	Periodic Lattice Potential	2
4	Absorbing Boundary Conditions	3
5	Operator Splitting Formulation	3
6	Fourier-Space Kinetic Propagation	3
7	Numerical Algorithm: Split-Step Fourier Propagation	4
8	Visualization: Phase–Amplitude Encoding	5
9	Physical Interpretation	5
10	Conclusion	5

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 system is governed by the time-dependent Schrödinger equation (TDSE):

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

where $\psi(x, y, t) \in \mathbb{C}$ is the quantum wavefunction and $\nabla^2 = \partial_x^2 + \partial_y^2$ is the Laplacian.

The wavefunction is normalized such that

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

and $|\psi|^2$ represents the probability density.

2 Initial Condition: Gaussian Wavepacket

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

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

where:

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

This choice produces a localized packet with mean momentum $\mathbf{p} = \hbar(k_x, k_y)$ and finite momentum spread.

3 Periodic Lattice Potential

To model scattering and diffraction, a finite periodic lattice of Gaussian scatterers is introduced:

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

where:

- V_0 is the lattice amplitude (barrier height),
- σ_V controls the size of each scatterer,
- (x_i, y_j) form a rectangular lattice with spacing (a_x, a_y) .

This potential approximates a finite crystal or optical lattice and induces diffraction, interference, and multiple scattering effects.

4 Absorbing Boundary Conditions

To suppress unphysical reflections from the finite simulation domain, a smooth absorbing boundary mask is applied after each time step:

$$\psi(x, y, t) \leftarrow \psi(x, y, t) A(x, y), \quad (5)$$

with

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

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

This technique mimics an open domain and prevents artificial wave reflection.

5 Operator Splitting Formulation

The Hamiltonian operator is decomposed as

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

Since \hat{T} and \hat{V} do not commute, the exact propagator $\exp(-i\hat{H}\Delta t/\hbar)$ is approximated using a second-order Strang splitting:

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

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

6 Fourier-Space Kinetic Propagation

In Fourier space, the kinetic operator is diagonal. Let $\tilde{\psi}(\mathbf{k}, t)$ denote the Fourier transform of $\psi(x, y, t)$. Then:

$$\tilde{\psi}(\mathbf{k}, t + \frac{\Delta t}{2}) = \exp \left(-i \frac{\hbar |\mathbf{k}|^2}{2m} \frac{\Delta t}{2} \right) \tilde{\psi}(\mathbf{k}, t). \quad (9)$$

The simulation alternates between:

1. FFT to momentum space,
2. pointwise multiplication by the kinetic phase,
3. inverse FFT back to real space.

This is the computational bottleneck and is accelerated using cuFFT on the GPU.

7 Numerical Algorithm: Split-Step Fourier Propagation

The time-dependent Schrödinger equation is solved numerically using a second-order Strang splitting scheme combined with Fourier spectral methods. The algorithm advances the wavefunction $\psi(x, y, t)$ in time by alternating between real space and momentum space representations.

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

Require: Initial wavefunction $\psi(x, y, 0)$, potential $V(x, y)$, time step Δt , grid size (N_x, N_y) , total steps N_t

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

1: **for** $n = 0$ **to** $N_t - 1$ **do**

2: **Fourier transform to momentum space**

$$\tilde{\psi}(\mathbf{k}, t_n) \leftarrow \mathcal{F}\{\psi(x, y, t_n)\}$$

3: **Apply half kinetic propagation**

$$\tilde{\psi}(\mathbf{k}) \leftarrow \tilde{\psi}(\mathbf{k}) \cdot \exp\left(-i \frac{\hbar |\mathbf{k}|^2}{2m} \frac{\Delta t}{2}\right)$$

4: **Inverse Fourier transform to real space**

$$\psi(x, y) \leftarrow \mathcal{F}^{-1}\{\tilde{\psi}(\mathbf{k})\}$$

5: **Apply potential propagation**

$$\psi(x, y) \leftarrow \psi(x, y) \cdot \exp\left(-i \frac{V(x, y) \Delta t}{\hbar}\right)$$

6: **Fourier transform to momentum space**

$$\tilde{\psi}(\mathbf{k}) \leftarrow \mathcal{F}\{\psi(x, y)\}$$

7: **Apply second half kinetic propagation**

$$\tilde{\psi}(\mathbf{k}) \leftarrow \tilde{\psi}(\mathbf{k}) \cdot \exp\left(-i \frac{\hbar |\mathbf{k}|^2}{2m} \frac{\Delta t}{2}\right)$$

8: **Inverse Fourier transform to real space**

$$\psi(x, y, t_{n+1}) \leftarrow \mathcal{F}^{-1}\{\tilde{\psi}(\mathbf{k})\}$$

9: **Apply absorbing boundary mask**

$$\psi(x, y, t_{n+1}) \leftarrow \psi(x, y, t_{n+1}) \cdot A(x, y)$$

10: **end for**

8 Visualization: Phase–Amplitude Encoding

The complex wavefunction is visualized using an HSV color mapping:

$$\text{Hue} = \frac{\arg(\psi) + \pi}{2\pi}, \quad (10)$$

$$\text{Value} = \left(\frac{|\psi|^2}{\max(|\psi|^2)} \right)^\gamma, \quad (11)$$

$$\text{Saturation} = 1, \quad (12)$$

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

This mapping reveals:

- phase singularities,
- interference patterns,
- diffraction cones and scattering paths.

The resulting RGB image is rendered in real time using OpenGL.

9 Physical Interpretation

The simulation reproduces key quantum phenomena:

- wavepacket dispersion,
- Bragg-like diffraction from a periodic structure,
- phase dislocations and interference fringes,
- tunneling and partial reflection.

The finite lattice produces rich transient behavior that bridges free-space propagation and crystal scattering physics.

10 Conclusion

A GPU-accelerated split-step Fourier solver provides an efficient and physically faithful method for simulating quantum wavepacket scattering in structured potentials. The combination of FFT-based propagation, absorbing boundaries, and phase-aware visualization enables real-time exploration of quantum dynamics at high spatial resolution.