From Local Rules to Global Waves: Simulating Quantum Mechanics as a Coupled Map Lattice

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Contents

Abstract

This project explores the emergence of quantum mechanical phenomena through the lens of Complex Systems theory. By discretizing the Time-Dependent Schrödinger Equation (TDSE), we construct a **Coupled Map Lattice (CML)** where global wave behavior emerges solely from nearest-neighbor interactions on a grid. We systematically build the simulation from a 1D free particle verification to complex 2D interference patterns (Double Slit) and finally extend the architecture to 3D. The results demonstrate that complex quantum behavior can be simulated efficiently using localized tensor operations, bridging the gap between computational physics and lattice dynamics.

1 Introduction

Standard approaches to Quantum Mechanics typically involve global operators (Hamiltonians) acting on abstract Hilbert spaces. However, in the context of Complex Systems, we ask: can these behaviors emerge from a grid of locally interacting cells?

This project implements a **Coupled Map Lattice (CML)**. Unlike Cellular Automata (CA), which use discrete states, a CML utilizes continuous state variables (complex amplitudes) evolving in discrete time and space. This allows us to preserve the phase information necessary for interference while maintaining the local connectivity characteristic of lattice models.

2 Mathematical Formulation: The Update Rule

We start from the Time-Dependent Schrödinger Equation (TDSE) in natural units ($\hbar = 1, m = 1$):

$$i\frac{\partial \psi}{\partial t} = -\frac{1}{2}\nabla^2\psi + V(\mathbf{r})\psi \tag{1}$$

Rearranging for time evolution:

$$\frac{\partial \psi}{\partial t} = i\left(\frac{1}{2}\nabla^2\psi - V(\mathbf{r})\psi\right) \tag{2}$$

To implement this on a lattice, we must discretize the Laplacian operator ∇^2.

2.1 Discrete Laplacian Stencil

In 1D, the second derivative is approximated by the central difference:

$$\nabla^2\psi_i \approx \frac{\psi_{i+1} - 2\psi_i + \psi_{i-1}}{\Delta x^2} \tag{3}$$

In 2D, this extends to the 5-point stencil (Von Neumann Neighborhood):

$$\nabla^2\psi_{i,j} \approx \frac{\psi_{i+1,j} + \psi_{i-1,j} + \psi_{i,j+1} + \psi_{i,j-1} - 4\psi_{i,j}}{\Delta x^2} \tag{4}$$

In 3D, this extends to:

$$\nabla^2\psi_{i,j,k} \approx \frac{\psi_{i+1,j,k} + \psi_{i-1,j,k} + \psi_{i,j+1,k} + \psi_{i,j-1,k} + \psi_{i,j,k+1} + \psi_{i,j,k-1} - 6\psi_{i,j,k}}{\Delta x^2} \tag{5}$$

This derivation reveals that the "Kinetic Energy" of a quantum system is effectively a **local diffusion process** with a complex phase factor.

2.2 The Time-Step (Euler Integration)

The final update rule for cell (i, j, k) at time $t + 1$ is:

$$\psi_{i,j,k}^{(t+1)} = \psi_{i,j,k}^{(t)} + \Delta t \cdot \mathcal{F}(\psi_{neighbors}, V_{i,j,k}) \tag{6}$$

where $\mathcal{F}$ is the computed rate of change.

2.3 Statistical Measures

To analyze the emergent behavior of the system from a Complex Systems perspective, we monitor two key global observables: the total probability norm and the information entropy.

1. Normalization and Probability Density The wavefunction $\psi_{i,j}$ represents a complex amplitude. The probability density at a lattice site is given by the Born rule:

$$\rho_{i,j}(t) = |\psi_{i,j}(t)|^2 \tag{7}$$

To ensure physical validity, the system must conserve the total probability (Unitary evolution). We calculate the global norm $N(t)$ at each time step (where ΔV is the cell volume):

$$N(t) = \sum_{i,j} \rho_{i,j}(t)\Delta V \tag{8}$$

2. Shannon Entropy (Information Delocalization) We utilize Shannon Entropy as a measure of the wavefunction's spatial delocalization (or "spread") across the lattice. In the context of quantum lattices, this quantifies the information content of the position distribution:

$$S(t) = -\sum_{i,j} \rho_{i,j}(t) \ln(\rho_{i,j}(t) + \epsilon)\Delta V \tag{9}$$

where ϵ is a small constant (10^{-15}) added for numerical stability to avoid $\ln(0)$ errors. A low $S(t)$ indicates a highly localized particle, while a high $S(t)$ indicates a dispersed, delocalized wave.

3 Experiment I: 1D Free Particle (Calibration)

To validate the CML logic, I first implemented a 1D system with zero potential ($V = 0$).

- **Setup:** 1D Grid of size $N = 200$.
- **Initial Condition:** Gaussian Wave Packet with initial momentum.
- **Dynamics:** Free propagation.

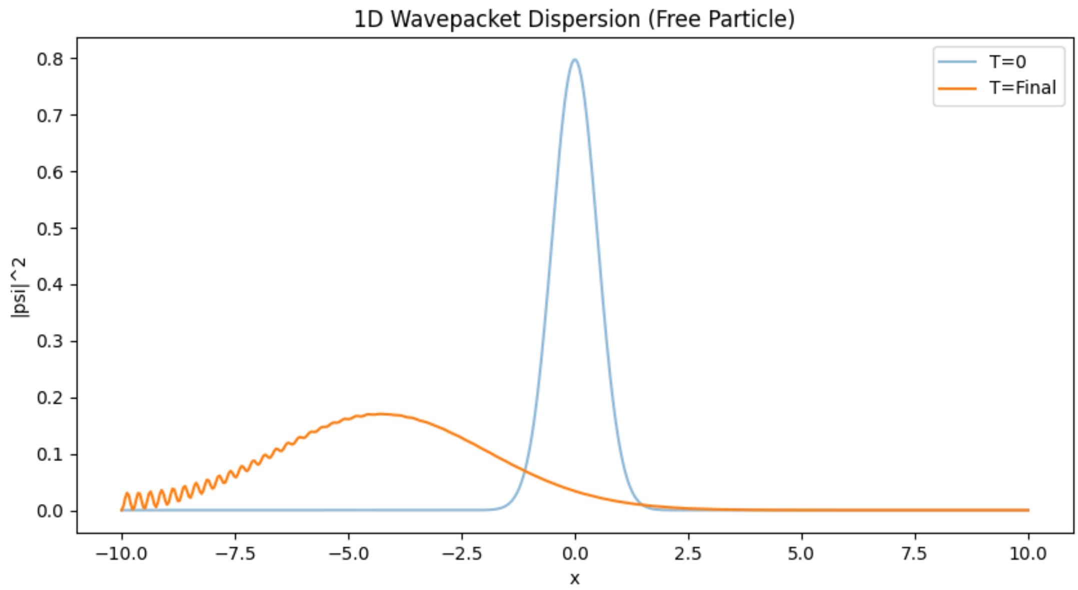
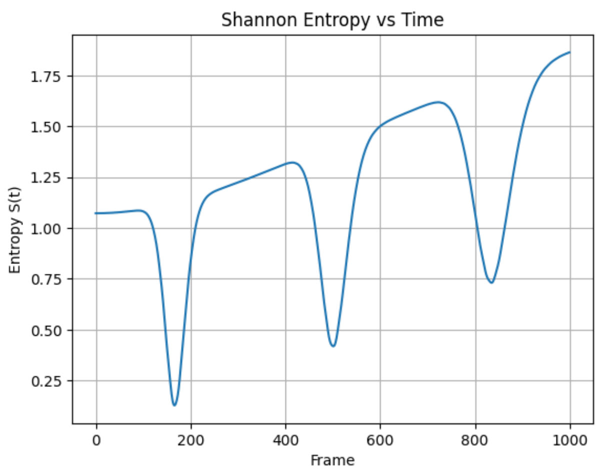


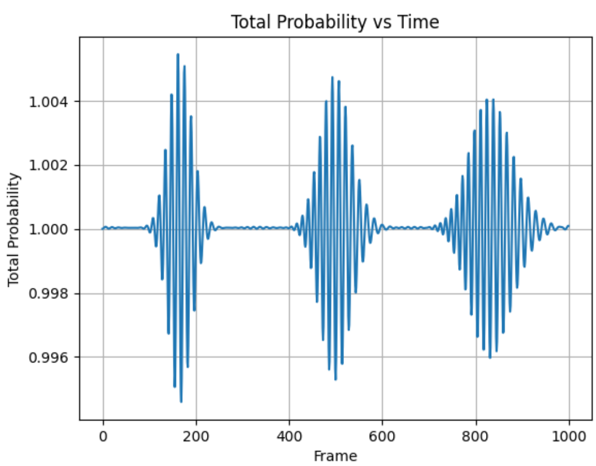
Figure 1: Evolution of a 1D Gaussian wave packet. The wave spreads (disperses) and moves side to side over time as expected from quantum theory.

Observation: The packet maintains its Gaussian shape while spreading. This confirms that our discrete Laplacian kernel correctly approximates the kinetic energy operator. Stability issues were observed for large Δt, necessitating a strict CFL condition ($\Delta t < \Delta x^2/2$).

3.1 Numerical Validation and Stability Analysis



(a) Entropy of the System over Time



(b) Total Probability over Time

Plotting the Total Probability over Time, and the Entropy over time, we observe the following:

- **Norm Conservation:** The total probability does not drift linearly but exhibits bounded oscillations within a margin of $< 0.5\%$. This confirms the stability of the semi-implicit (symplectic) update rule.

- **Boundary Dynamics:** The Shannon Entropy generally increases due to wavepacket dispersion. However, periodic sharp dips are observed. These correspond to **boundary-induced compression**, where the wavefunction squeezes against the infinite potential wall during reflection, temporarily reducing the spatial uncertainty (and thus entropy) of the system.

4 Experiment II: 2D Interference (The Core)

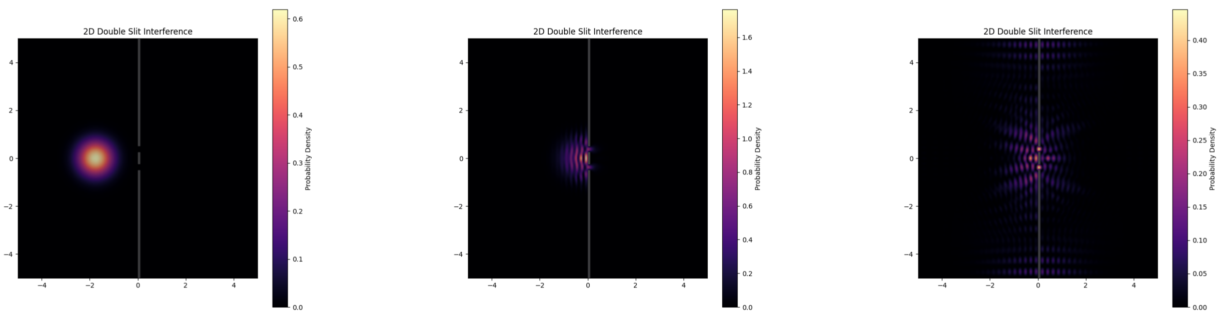
Moving to 2D, we introduce a potential barrier to observe interaction and emergence.

4.1 The Double Slit Setup

- **Grid:** 100×100.
- **Potential $V(x, y)$:** A wall of infinite potential (represented by high V) bisecting the grid, with two slit gaps.
- **Initial Condition:** Gaussian packet with momentum k_y aimed at the slits.

4.2 Results

The simulation clearly shows the emergence of interference fringes.

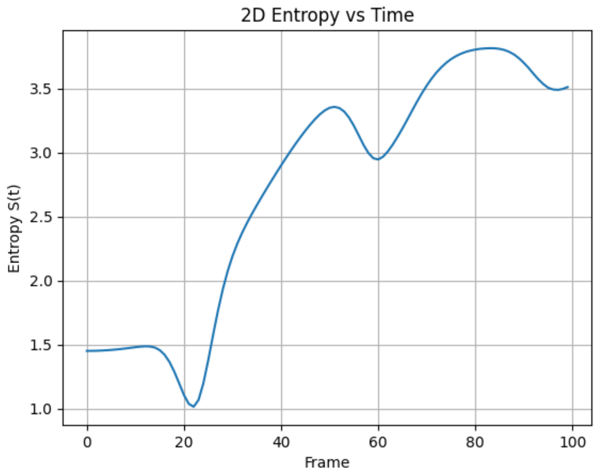


(a) Initial Approach (b) Initial Interference (c) Interference after reflection

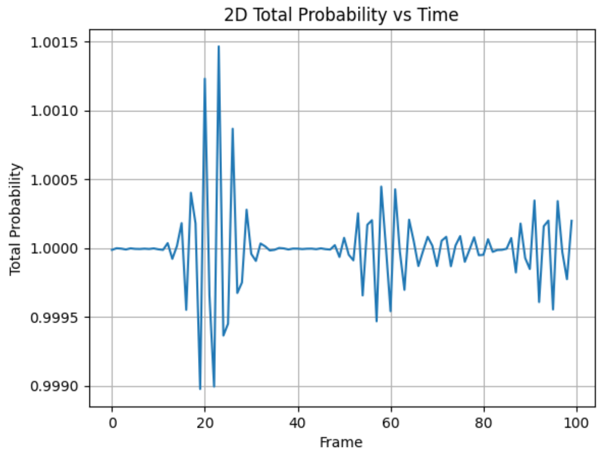
Figure 3: Evolution of $|\psi|^2$ through a double slit.

Crucially, no "wave physics" was hard-coded. Each cell simply followed the local update rule. The interference pattern is an emergent global property of the lattice.

4.3 Numerical Validation and Stability Analysis



(a) Entropy of the System over Time



(b) Total Probability over Time

Plotting the Total Probability over Time, and the Entropy over time, we observe the following:

- **Stability:** The probability error remains negligible ($< 0.15\%$), validating the solver even in the presence of complex scattering geometry.
- **Spatial Filtering:** The sharp dip in entropy at $t \approx 22$ marks the passage of the wavepacket through the slits. The potential barrier effectively acts as a **spatial filter**, forcing the system into a highly localized (low entropy) state. The subsequent rapid rise in entropy corresponds to the diffractive expansion and the formation of interference fringes on the other side.

5 Experiment III: High-Dimensional Extension (3D)

5.1 The Setup

To test the scalability of the CML approach, I extended the framework to 3D using PyTorch tensors.

- **Grid:** $64 \times 64 \times 64$ (125k cells).
- **Kernel:** 7-point 3D Laplacian stencil.
- **Visualization:** Volumetric slices.

5.2 Results

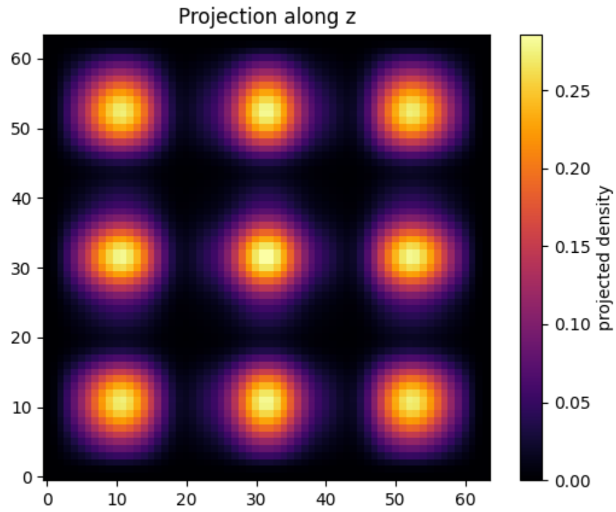


Figure 5: Slice of a 3D Gaussian wave packet evolving in a cubic domain.

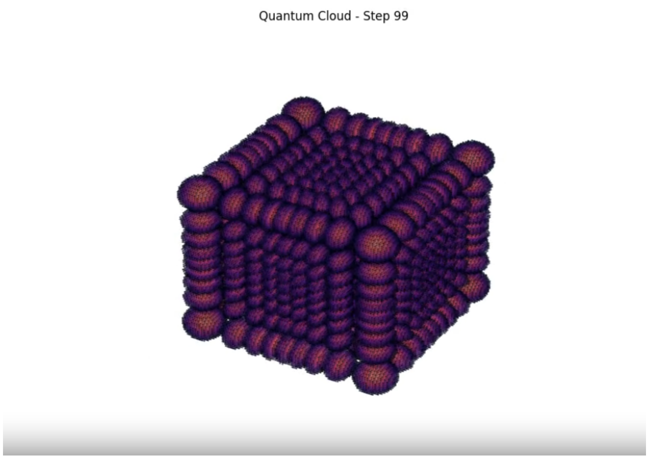
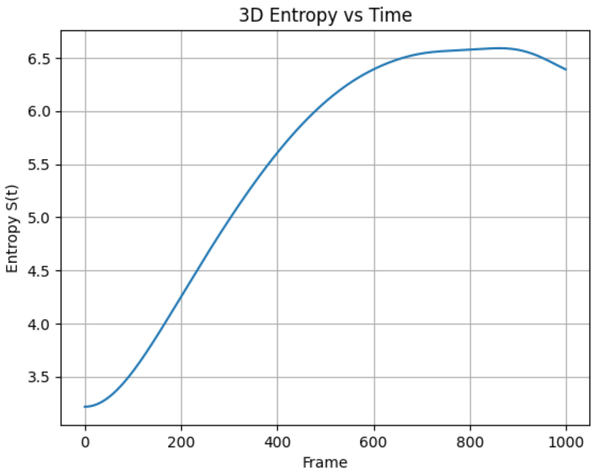


Figure 6: Full 3d View of a Gaussian wave packet evolving in a cubic domain

This demonstrates that the logic naturally extends to higher dimensions, limited only by VRAM.

5.3 Numerical Validation and Stability Analysis



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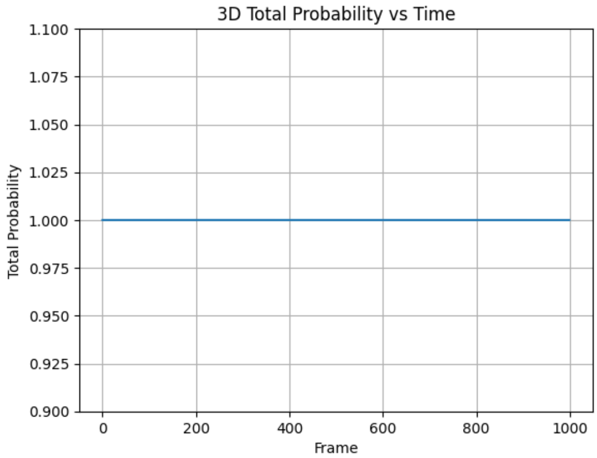

(b) Total Probability over Time

Plotting the Total Probability over Time, and the Entropy over time, we observe the following:

- **Scalability:** The 3D tensor implementation maintains norm conservation with $< 0.5\%$ error, demonstrating that the symplectic CML approach scales robustly to higher dimensions.
- **Interference Patterning:** The entropy initially rises due to diffusion. Towards the end of the simulation, the decrease in entropy signifies the formation of a standing wave pattern (interference). The wavefunction redistributes into distinct, localized lobes (as seen in the 9-packet structure in Figure 5), effectively reducing the randomness of the spatial distribution.

6 Conclusion

This project successfully models Quantum Mechanics as a Complex System. By reducing the global Schrödinger equation to a set of local update rules on a Coupled Map Lattice, we demonstrated:

1. **Validation:** The 1D case reproduces standard dispersion.
2. **Emergence:** The 2D case reproduces interference fringes without explicit wave equations.
3. **Scalability:** The logic extends trivially to 3D.

The code for this simulation, implemented in Python/PyTorch for GPU acceleration, is available at: https://github.com/Jedop/QuantumCML