A Discrete-Lattice Numerical Simulation of Near-Field Electron Diffraction and Environmental Decoherence

D. G. Elliman
Neuro-Symbolic Ltd, United Kingdom
dave@neusym.ai

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Abstract

We present a highly efficient discrete-lattice numerical method for simulating electron wavepacket propagation, diffraction, and environmental decoherence without relying on continuum approximations. By executing an exact unitary quantum walk on a finite truncated square (4.8.8) lattice, the model natively bridges the near-field (Fresnel) and far-field (Fraunhofer) regimes. The approach avoids the numerical sign problem typical of Monte Carlo path sampling and naturally accounts for waveguide collimation effects from finite-thickness physical slits. The simulation yields double-slit interference profiles in close quantitative agreement with empirical nanoscale data. Furthermore, by introducing an orthogonal ancillary lattice dimension, we provide a computationally lightweight method for simulating exact environmental decoherence, generating classical Born rule statistics directly from unitary evolution.

Contents

1 Introduction

The double-slit experiment remains the fundamental touchstone for wave-particle duality and quantum interference [1]. Despite its ubiquity, the exact analytical calculation of double-slit diffraction for realistic physical geometries remains exceptionally difficult in closed form. Standard treatments rely heavily on the Fraunhofer approximation, while addressing the near-field Fresnel regime requires evaluating the Kirchhoff-Fresnel integral, which rapidly becomes intractable for slits of finite width and depth. The deeper mathematical issue lies in the boundary conditions: as established by Sommerfeld's half-plane solution [2], electromagnetic and matter-wave field equations in continuous space become singular at perfectly sharp edges.

While Feynman's path integral formulation is conceptually elegant, direct numerical evaluations face severe computational bottlenecks. Evaluating the uncountably infinite sum over all continuous paths through a physical slit geometry is notoriously difficult. Monte Carlo path sampling approaches are inherently plagued by the numerical sign problem, where oscillating complex phases lead to exponential cancellation errors [3].

This paper presents an exact computational solution by framing the propagation space fundamentally as a discrete lattice. In this regime, the path integral ceases to be an uncountably infinite sum. A slit edge is no longer a mathematical singularity; it is simply a topological boundary where propagation routing terminates. We demonstrate that this straightforward discrete kinematic model natively reproduces exact macroscopic wave optics and quantum decoherence without requiring continuum approximations.

2 A Discrete Kinematic Lattice Model

We briefly review the kinematic substrate required for this simulation. The spatial domain is modelled as a discrete 2D 4.8.8 (truncated square) tiling. The state of a particle is described by a 4-component complex spinor residing on the octagonal sites, representing the physical combinations of spatial routing (Left/Right, Up/Down).

The quantum walk is driven entirely by spatial shifting and chirality mixing. The local unitary "coin" operator that applies this mixing is:

$$U(m) = \cos(m)I - i\sin(m)\sigma_x \tag{1}$$

where m is a dimensionless mass parameter defining the mixing angle (in radians) per simulation tick, and σ_x couples counter-propagating spatial channels. This continuous unitary toggling imparts inertia and subluminal group velocity, natively generating dispersive behavior characteristic of the Dirac equation's *Zitterbewegung*.

3 Wavepacket Propagation on the Lattice

To avoid the exponential scaling and numerical sign problems inherent in Monte Carlo path sampling, we compute the direct unitary evolution of the entire lattice simultaneously via explicit finite-difference steps. Because quantum evolution is strictly linear, propagating the full amplitude field for T steps automatically and exactly computes the coherent sum over all lattice paths of length T, without requiring explicit path enumeration.

The wavepacket is initialised as a finite Gaussian distribution. Evolution consists of two steps per lattice tick: shifting amplitudes to adjacent sites, and applying the local coin operator $U(m)$. To prevent unphysical boundary reflections, the extreme edges of the lattice act as a Perfectly Matched Layer (PML), applying a $\sin^2$ attenuation envelope. The physical slits are defined simply by a boolean routing mask.

4 Single-Slit Diffraction

Initial validation of the discrete kinematics was performed using a single slit. As the wavepacket passes through the aperture, the discrete lattice natively bridges the near-field and far-field regimes, seamlessly demonstrating the Fresnel-to-Fraunhofer transition as propagation distance increases (see Figure 1).

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Figure 1: Near-field (Fresnel) single-slit electron diffraction on the discrete computational lattice. Left: Propagation heatmap of the wavepacket interacting with the barrier. Right: The characteristic asymmetric near-field intensity ringing and amplitude creeping into the geometric shadow, natively generated by discrete unitary operations without evaluating continuous Fresnel integrals.

Crucially, the discrete lattice model captures a physical reality often omitted by textbook analytical equations, which typically assume slits are punched into an infinitely thin 2D plane. In our simulation, the mask possesses a physical thickness. This thickness acts as a waveguide, naturally collimating the forward beam and suppressing wide-angle transverse scattering. This correctly reduces the amplitude of the outer diffraction lobes—a physical feature that the lattice model natively reproduces without ad hoc corrections.

5 Double-Slit Interference

To test the model against physical reality, we recreated the nanoscale geometry of the 2013 double-slit experiment by Bach *et al.* [6]. Because wave diffraction is scale-invariant, we aligned our discrete lattice to preserve the experimental physical ratios.

In the physical experiment, the slits were 62 nm wide and separated by 272 nm. On our computational lattice, we set the slit width to $w = 6$ sites, the separation to $d = 26$ sites, and injected a wavepacket with a wavelength of $\lambda \approx 6.0$ sites. The detector screen was placed at $L = 1190$ sites from the slit exit plane. This yields a computational Fresnel number of $\mathcal{F} = w^2/(L\lambda) \approx 0.005$, ensuring the simulation is rigorously evaluated in the far-field (Fraunhofer) regime, precisely mirroring the empirical data capture conditions.

fig_doubleslit.pdf

Figure 2: Left: Probability density of the discrete lattice wavepacket undergoing diffraction. Right: Overlay of the theoretical continuum Fraunhofer envelope (gold dotted), the discrete lattice intensity (cyan), and the empirical single-electron detection data from Bach *et al.* 2013 (white dots). The lattice natively captures the waveguide suppression of the outer fringes.

The spatial probability distribution is shown in Figure 2. The simulation reveals that the discrete lattice provides close quantitative agreement with the empirical single-electron hits, organically reproducing the suppressed outer fringes caused by the waveguide collimation of the physical mask. The discrete dispersion relation introduces expected computational finite-size effects (slightly widening the fringe spacing), but effectively captures the core continuous wave mechanics without integration singularities.

6 Simulating Environmental Decoherence

When a detector interacts with a particle at the slit, the interference pattern vanishes. In standard computational formulations, modelling this process can be mathematically cumbersome. Using the explicit discrete kinematics of the lattice, we can simulate this environmental decoherence deterministically.

To model measurement, we expand the lattice state space to include a single orthogonal environmental dimension (an Ancilla dimension): $D = 0$ (environment unperturbed) and $D = 1$ (environment triggered). We place a single-site unitary SWAP gate at the exit plane of Slit 1. Any amplitude traversing this slit is deterministically swapped from the $D = 0$ sub-lattice into the $D = 1$ sub-lattice.

Because the two sub-lattices are mathematically orthogonal, these two spatial waves can no longer interfere. When the simulated photographic plate accumulates the total probability density, it traces out the environment:

$$I(y) = \int \left(|\psi_{D=0}(y,t)|^2 + |\psi_{D=1}(y,t)|^2\right) dt \tag{2}$$

The interference cross-terms strictly vanish. The result (plotted as the red curve in Figure 2) is a perfectly smooth, classical probability distribution representing the Born rule statistics. The transition from quantum interference to classical statistics emerges naturally and efficiently from unitary evolution on the expanded finite lattice. A weaker unitary coupling would transfer only partial amplitude to $D = 1$, leaving residual cross-terms and yielding partial decoherence with reduced fringe visibility—a regime heavily explored in asymmetric slit experiments [7].

7 Discussion

The computational results presented here provide a practical, highly efficient numerical bridge between wave mechanics and environmental decoherence theory [4, 5].

A natural question arises regarding numerical lattice artefacts: how can one be certain that the observed fringes are genuine physical interference rather than Moiré-type artefacts of a discrete grid? The 4.8.8 truncated square tiling exhibits reduced dispersion anisotropy compared to a simple Cartesian square grid, owing to its octagonal vertex coordination. This strongly mitigates anisotropic propagation errors. Furthermore, convergence tests at increasing grid resolutions confirm that lattice-scale discrete effects successfully wash out in the macroscopic continuum limit.

By routing phase information into orthogonal environmental channels, the local capacity to sustain spatial coherence is saturated, and the interference mathematically resolves into a classical distribution. The orthogonal $D = 0$ and $D = 1$ sub-lattices operate equivalently to branches in the Everettian universal wavefunction [8], providing a computationally lightweight mechanism for studying decoherence dynamics.

8 Conclusion

By executing a discrete quantum walk on a 2D grid, we have demonstrated a numerical methodology where:

1. Exact wave optics, including waveguide collimation, emerge directly from local discrete operations, successfully avoiding continuum singularities and the Monte Carlo sign problem.
2. The double-slit interference profile closely matches the empirical nanoscale data of Bach *et al.* (2013).
3. The transition from quantum superposition to the classical Born rule emerges directly from deterministic unitary entanglement into an orthogonal simulated environment.

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A Numerical Details

The simulations were performed using vectorised arrays. The domain was a 2048×4096 grid. The boundary PML utilised a $\sin^2$ taper over 200 pixels. Evolution time was $2,200$ steps. Execution time was approximately 90 seconds, demonstrating the extreme efficiency of direct unitary evolution compared to path sampling.

B Computational Implementation and Source Code

The complete, executable Python codebase—along with the empirical dataset extracted from Bach *et al.* (2013) required to reproduce the numerical results—has been made freely available in a public repository at:

`https://github.com/dgedge/circlette-doubleslit.git`

To demonstrate the algorithmic simplicity of the discrete approach, the core kinematic engine is reproduced below. The entire physical universe of the simulation, including exact finite-difference propagation, dispersive mass, waveguide collimation, and unitary decoherence, is executed natively in fewer than 40 lines of local array operations:

```python
# Core Lattice Evolution (2 Universes, 4 Spinor Components)
# psi.shape = (2, 4, HEIGHT, WIDTH)

c, s = np.cos(m), np.sin(m)

for t in range(STEPS):
    # 1. Spatial Shift (Propagation along routing channels)
    in0[:, :, 1:] = psi[:, 0, :, :-1]
    in0[:, :, 0] = 0
    in1[:, :, :-1] = psi[:, 1, :, 1:]
    in1[:, :, -1] = 0
    in2[:, 1:, :] = psi[:, 2, :-1, :]
    in2[:, 0, :] = 0
    in3[:, :-1, :] = psi[:, 3, 1:, :]
    in3[:, -1, :] = 0

    # 2. Vertex Summation
    sum_in = (in0 + in1 + in2 + in3) * 0.5
    v0, v1 = sum_in - in0, sum_in - in1
    v2, v3 = sum_in - in2, sum_in - in3

    # 3. Apply Chirality Coin U(m)
```

```
    psi[:, 0] = c * v0 - 1j * s * v1
    psi[:, 1] = c * v1 - 1j * s * v0
    psi[:, 2] = c * v2 - 1j * s * v3
    psi[:, 3] = c * v3 - 1j * s * v2

    # 4. Apply Physical Boundary Mask (Slits and Absorbing Sponge)
    psi[:, 0] *= mask
    psi[:, 1] *= mask
    psi[:, 2] *= mask
    psi[:, 3] *= mask

    # 5. Deterministic Unitary Decoherence (Measurement)
    if measured:
        # True unitary SWAP between universes at Slit 1
        temp = psi[0, :, s1_slice, exit_x].copy()
        psi[0, :, s1_slice, exit_x] = psi[1, :, s1_slice, exit_x]
        psi[1, :, s1_slice, exit_x] = temp

    # Accumulate photographic plate exposure
    screen_exposure += np.sum(np.abs(psi[:, :, :, detector_x])**2, axis=(0, 1))
```

References

[1] R. P. Feynman, R. B. Leighton, and M. Sands, *The Feynman Lectures on Physics, Vol. 3*, Addison-Wesley (1965).

[2] A. Sommerfeld, *Mathematische Theorie der Diffraction*, Math. Ann. **47**, 317 (1896).

[3] M. Gondran and A. Gondran, *Numerical simulation of the double-slit interference with ultracold atoms*, Am. J. Phys. **73**, 507 (2005).

[4] H. D. Zeh, *On the interpretation of measurement in quantum theory*, Foundations of Physics **1**, 69 (1970).

[5] W. H. Zurek, *Quantum Darwinism*, Nature Physics **5**, 181-188 (2009).

[6] R. Bach, D. Pope, S.-H. Liou, and H. Batelaan, *Controlled double-slit electron diffraction*, New Journal of Physics **15**, 033018 (2013).

[7] K. Harada *et al.*, *Interference experiment with asymmetric double slit by using 1.2-MV field emission transmission electron microscope*, Scientific Reports **8**, 1008 (2018).

[8] H. Everett, *Relative State Formulation of Quantum Mechanics*, Rev. Mod. Phys. **29**, 454 (1957).