



Quantum vs. Classical

Simulations of the Schrödinger Equation

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Physical System



GOVERNING EQUATION

Time-Dependent Schrödinger Equation

$$i\hbar \frac{\partial \psi(x, t)}{\partial t} = \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right) \psi(x, t)$$

INITIAL STATE

Gaussian wavepacket with μ , σ , k_0 (natural units: $m = \hbar = 1$):

$$\psi(x, 0) = \frac{1}{(2\pi\sigma^2)^{1/4}} \exp \left(-\frac{(x - \mu)^2}{4\sigma^2} + ik_0x \right)$$

POTENTIALS

Free Particle: $V(x) = 0$

Harmonic Oscillator: $V(x) = \frac{1}{2}m\omega^2x^2$

PARAMETERS

Center position	μ
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Wavepacket width	σ
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Initial momentum	k_0
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Particle mass	$m = 1$
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Reduced Planck const.	$\hbar = 1$
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Qubits range	$2 - 12$
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System Evolution

Formal Solution:

$$\psi(x, t + \Delta t) = e^{-i\hat{H}\Delta t/\hbar}\psi(x, t)$$

Hamiltonian:

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

Trotterization:

$$e^{-i\hat{H}\Delta t} \approx e^{-i\hat{V}\Delta t/2} e^{-i\hat{T}\Delta t} e^{-i\hat{V}\Delta t/2}$$

Coordinate Space:

$$\hat{V} = V(x) - \text{diagonal}$$

Momentum Space:

$$\hat{T} = \frac{p^2}{2m}$$

$$\psi(x, t + \Delta t) = e^{\frac{-iV(x)\Delta t}{2}} \mathcal{F}^{-1} \left[e^{-i\frac{p^2}{2m}\Delta t} \mathcal{F}[\psi(x, t)] \right] e^{\frac{-iV(x)\Delta t}{2}} \psi(x, t)$$

Classical Simulation: Split-Operator Method

$$x \in (x_{\min}, x_{\max}), \quad N = 2^n \text{ points}$$
$$x_j = x_{\min} + j \cdot \Delta x, \quad j = 0, 1, \dots, N-1$$

The wavefunction becomes a vector:

$$\psi(x, t) \rightarrow \vec{\psi}(t) = \begin{bmatrix} \psi(x_0, t) \\ \psi(x_1, t) \\ \vdots \\ \psi(x_{N-1}, t) \end{bmatrix}$$

Normalization:

$$\sum_{j=0}^{N-1} |\psi(x_j)|^2 \Delta x = 1$$

Impulse Grid:

$$k_n = \frac{2\pi}{L} \cdot \tilde{n} \quad \tilde{n} = \begin{cases} n, & n < \frac{N}{2} \\ n - N, & n \geq \frac{N}{2} \end{cases}$$

Discrete Fourier Transform:

$$\tilde{\psi}_n = \frac{1}{\sqrt{N}} \sum_{j=0}^{N-1} \psi_j e^{-i2\pi jn/N}$$

Inverse Fourier Transform:

$$\psi_j = \frac{1}{\sqrt{N}} \sum_{n=0}^{N-1} \tilde{\psi}_n e^{i2\pi jn/N}$$

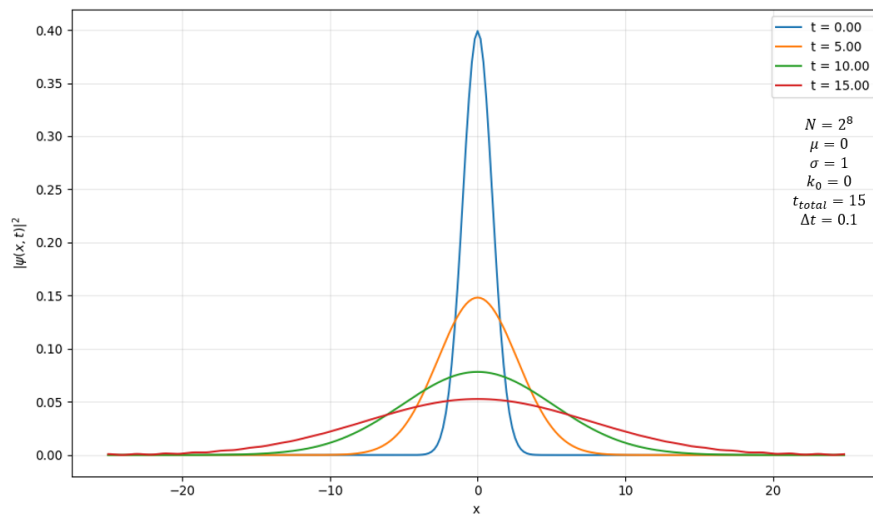
Classical Simulation Results



Free Particle ($V = 0$)

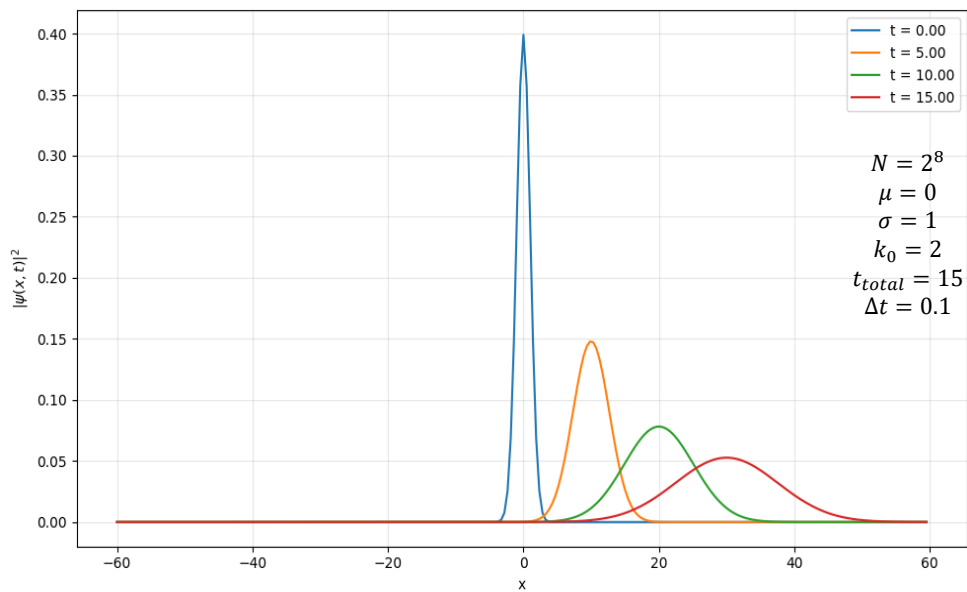
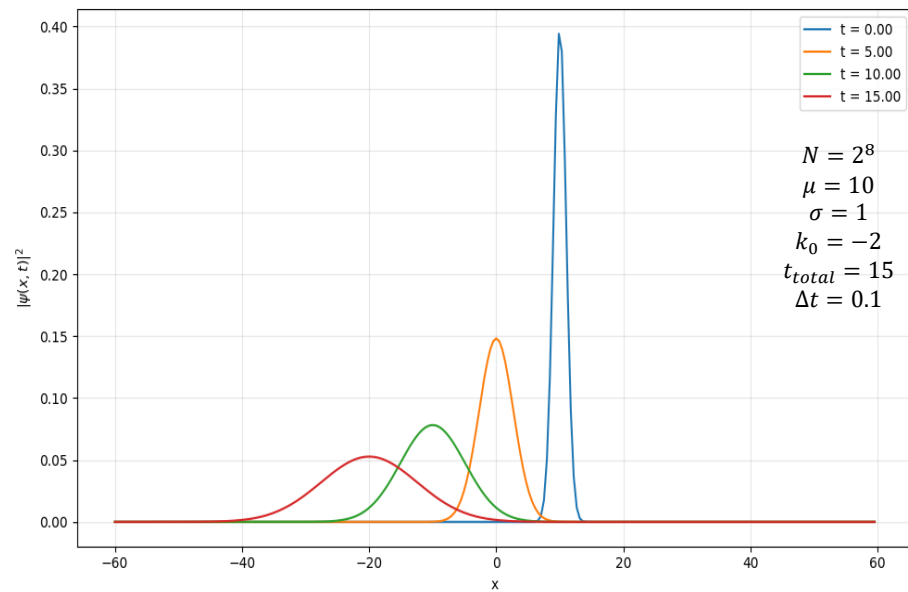
Wavepacket undergoes coherent free propagation. The probability density $|\psi|^2$ spreads and translates with momentum $k_0 = 0$.

- ▶ Analytic solution: Gaussian spread in time
- ▶ Norm conservation verified at each step



The split-operator FFT method provides a highly accurate reference solution — used as the ground truth for benchmarking the quantum approach.

Free Particle ($V = 0$)

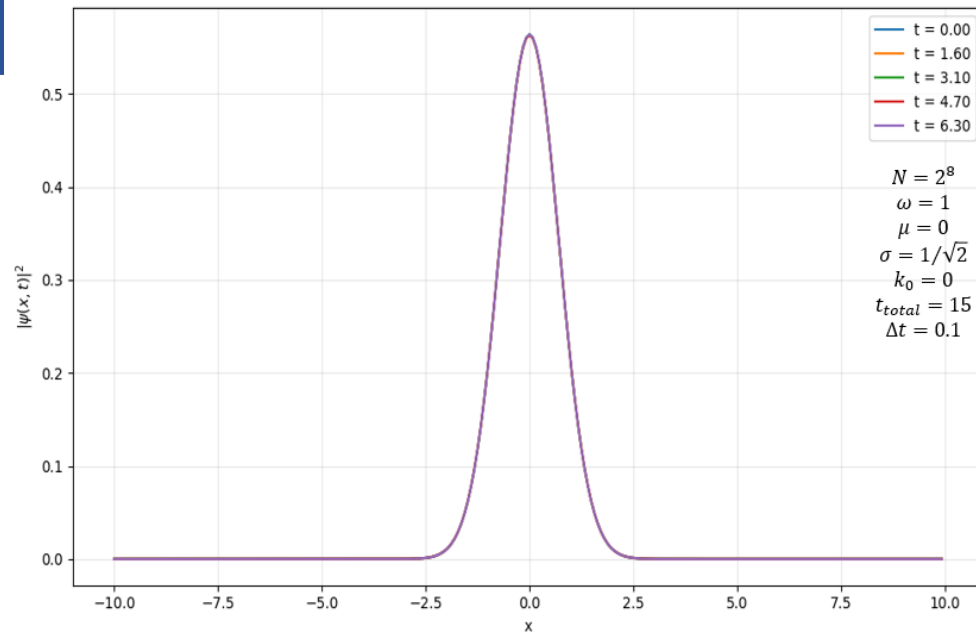


Classical Simulation Results

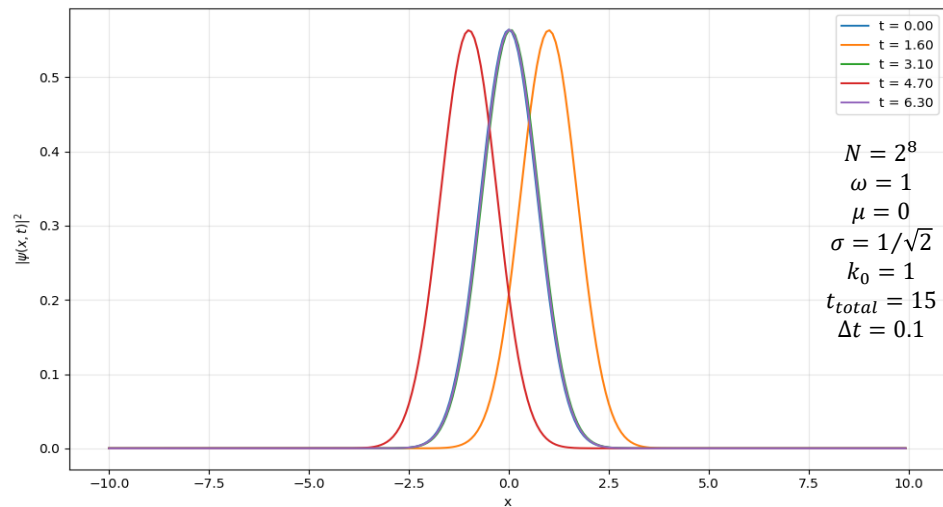
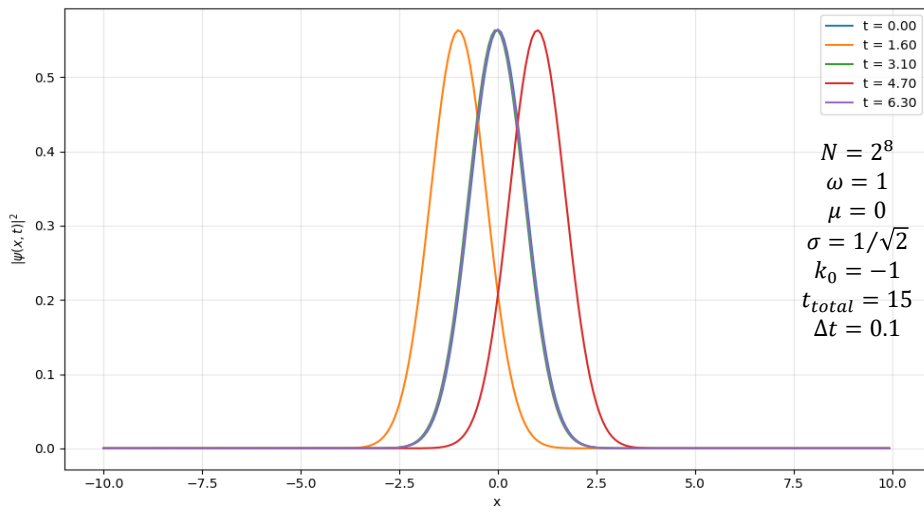
Harmonic Oscillator ($V = \frac{1}{2}x^2$)

Wavepacket oscillates in the parabolic potential. With $\omega = 1$, the coherent state undergoes periodic revival.

- ▶ Classical turning points define oscillation range
- ▶ Norm conservation verified at each step



Harmonic Oscillator ($V = \frac{1}{2}x^2$)



Quantum evolution of the system using the Qiskit library

Discretization of Space:

$$N = 2^{\#qubits}$$

$$x_j = x_{min} + j \cdot \Delta x, \quad j = 0, 1, \dots, N-1$$

$$|j\rangle \leftrightarrow x_j$$

Representation of the quantum state:

$$|\psi\rangle = \sum_{j=0}^{N-1} a_j |j\rangle$$

Determining amplitude:

$$a_j = \psi(x_j) \sqrt{\Delta x}$$

Normalization

$$\sum_{j=0}^{N-1} |\psi(x_j)|^2 \Delta x = 1 \Rightarrow \sum_{j=0}^{N-1} |a_j|^2 = 1$$

Quantum Fourier Transform (QFT)



DEFINITION

The QFT replaces the classical FFT in the quantum circuit:

$$\text{QFT}_N |x\rangle = \frac{1}{\sqrt{N}} \sum_{k=0}^{N-1} e^{2\pi i x k / N} |k\rangle$$

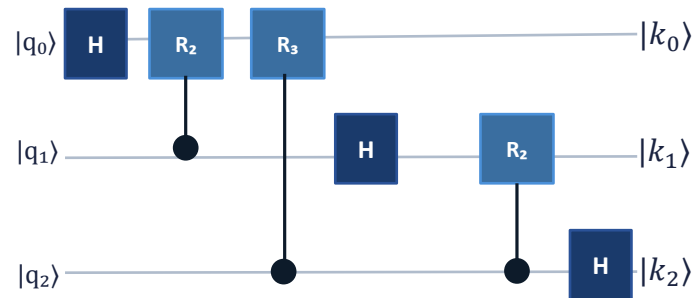
EXPONENTIAL SPEEDUP

Algorithm	Gate Complexity
Classical FFT	$O(N \log N)$
Quantum QFT	$O(n^2) = O(\log^2 N)$

CIRCUIT STRUCTURE

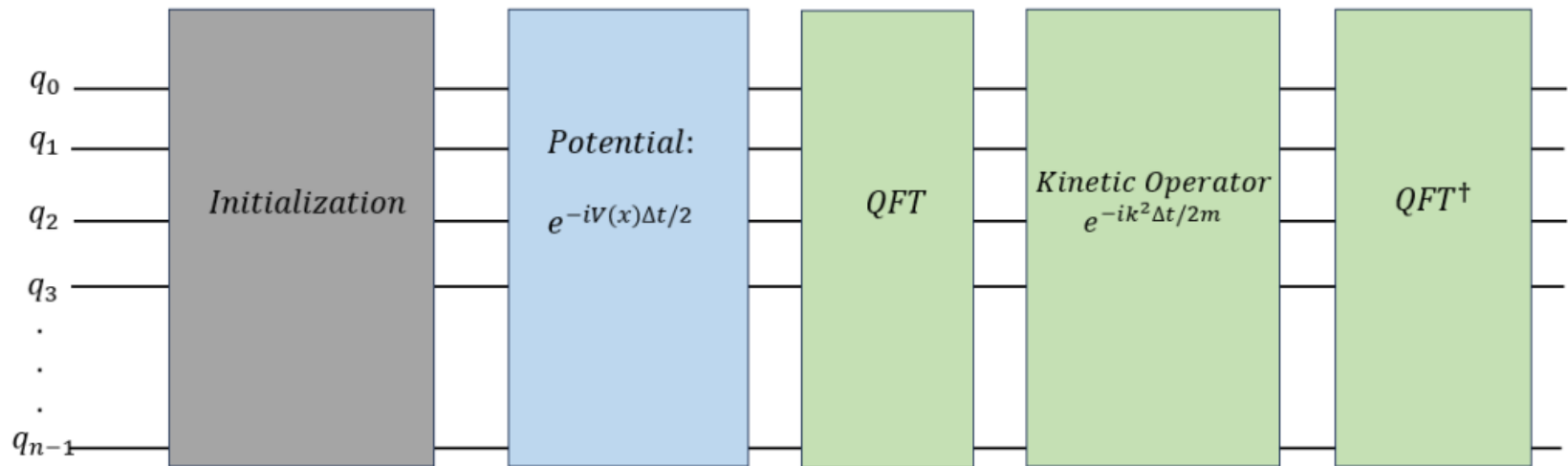
Implemented via Hadamard gates and controlled R_k phase rotations, with bit-reversal permutation.

QFT CIRCUIT (3 QUBITS)



The QFT achieves exponential compression: an n -qubit circuit achieves what the FFT does on $N = 2^n$ classical points.

Quantum Circuit Architecture

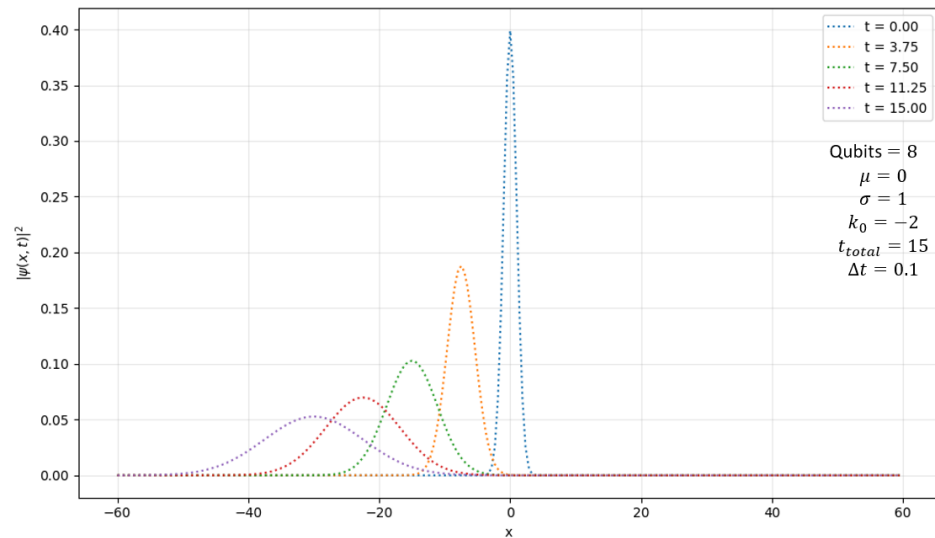
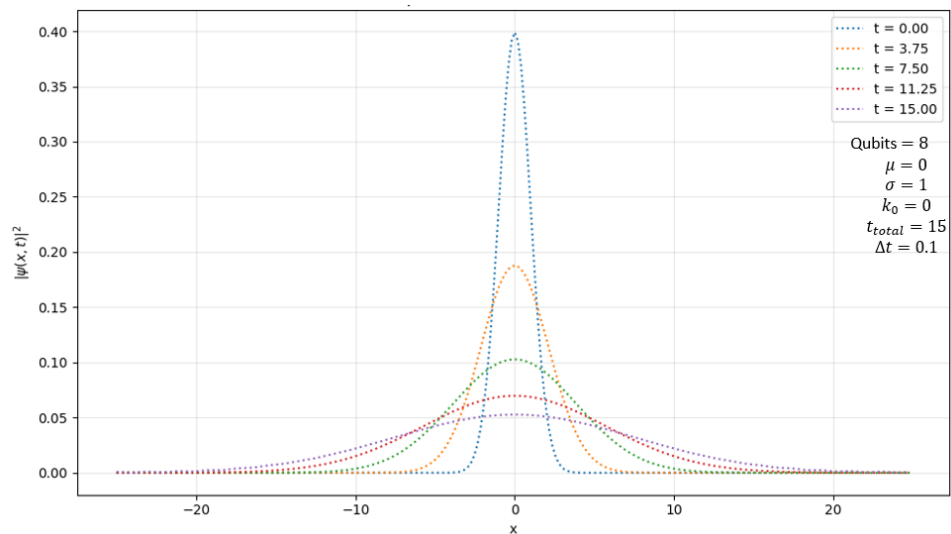


The n -qubit register encodes $N = 2^n$ spatial grid points: $|j\rangle \leftrightarrow x_j$. State amplitudes satisfy quantum normalization: $a_j = \psi(x_j)\sqrt{\Delta x}$.

Quantum Simulation Results (Qiskit)



Free Particle — Qiskit Circuit

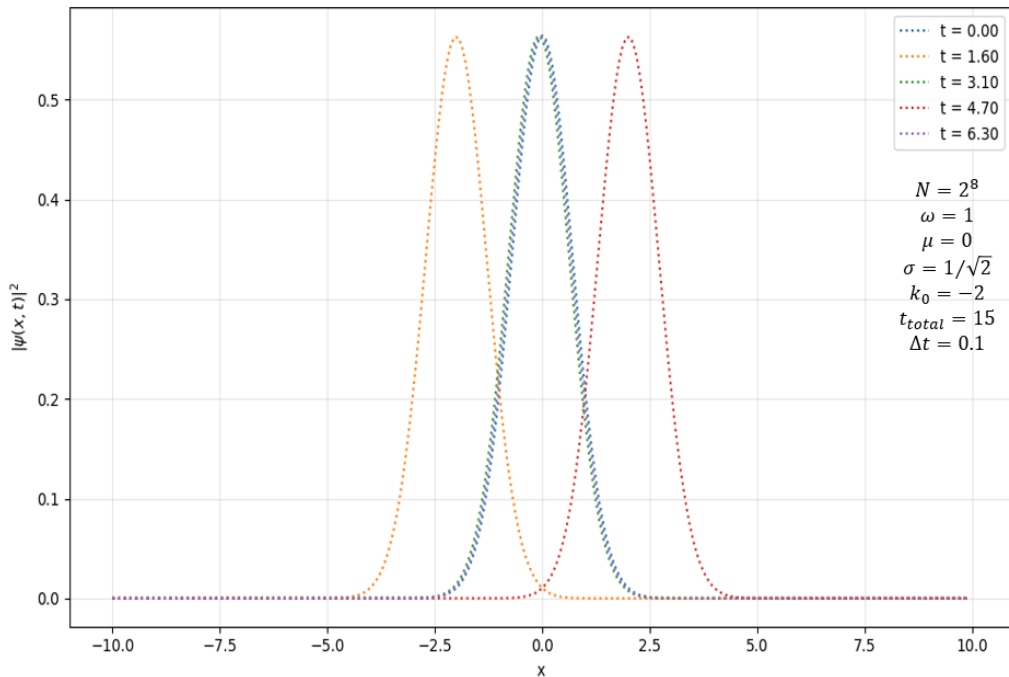


Both cases implemented as Qiskit statevector simulations with no hardware noise — pure algorithmic comparison.

Quantum Simulation Results (Qiskit)



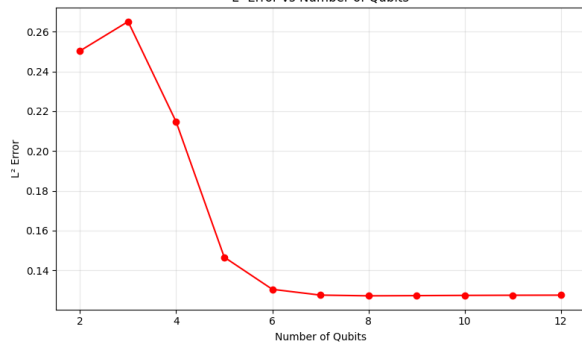
Harmonic Oscillator — Qiskit Circuit



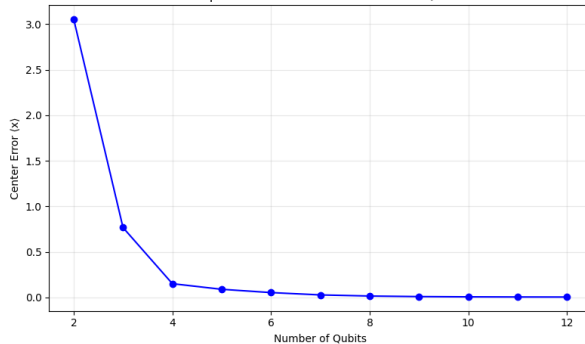
Accuracy vs. Qubit Count



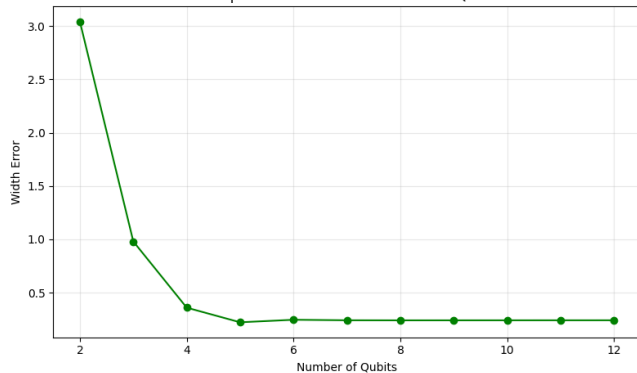
L² Error vs Number of Qubits



Wavepacket Center Error vs Number of Qubits



Wavepacket Width Error vs Number of Qubits



Convergence

Error drops sharply from 2→8 qubits, then plateaus — dominated by Trotter discretization error, not spatial resolution.

Center Error $\langle x \rangle$

Position expectation value error also rapidly decays with additional qubits — confirming spatial discretization is the bottleneck at low qubit counts.

Width Error $\sigma(t)$

Wavepacket width variance error similarly converges, validating correct time-dependent spreading dynamics.

Fidelity & Error Analysis



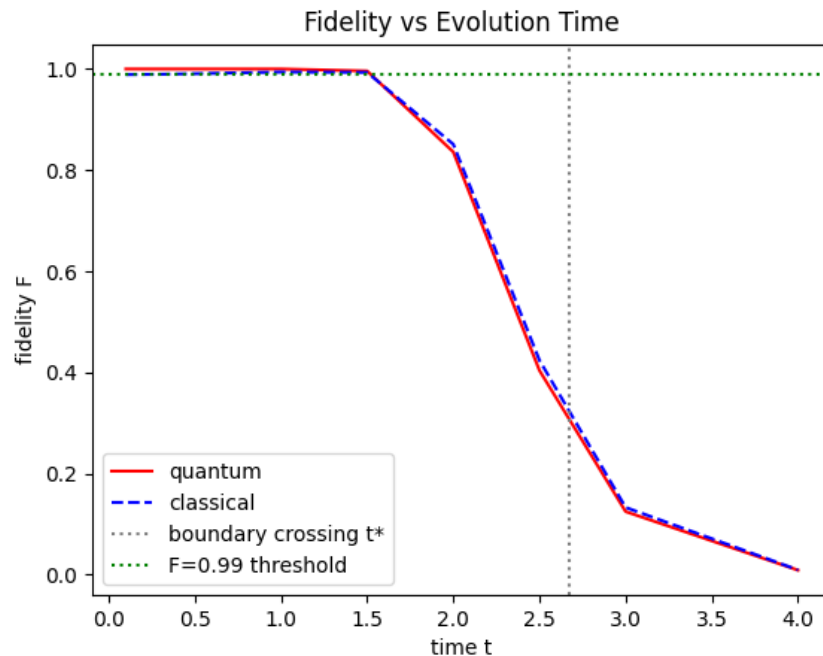
STATE FIDELITY OVER TIME

Fidelity F measures overlap between quantum and classical states:

$$F(t) = |\langle \psi_{\text{classical}} | \psi_{\text{quantum}} \rangle|^2$$

Key observations:

- ▶ $F \approx 1.0$ maintained up to boundary crossing time t^*
- ▶ Both quantum and classical curves overlap almost exactly
- ▶ Fidelity falls below 0.99 threshold near $t^* \approx 2.0$
- ▶ Degradation is due to boundary leakage, not quantum error



Boundary Effects & Momentum Analysis



BOUNDARY LEAKAGE

The periodic domain introduces wrap-around: when the wavepacket reaches the boundary, probability density 'leaks' to the opposite side.

Leakage timeline:

$$t < t^*$$

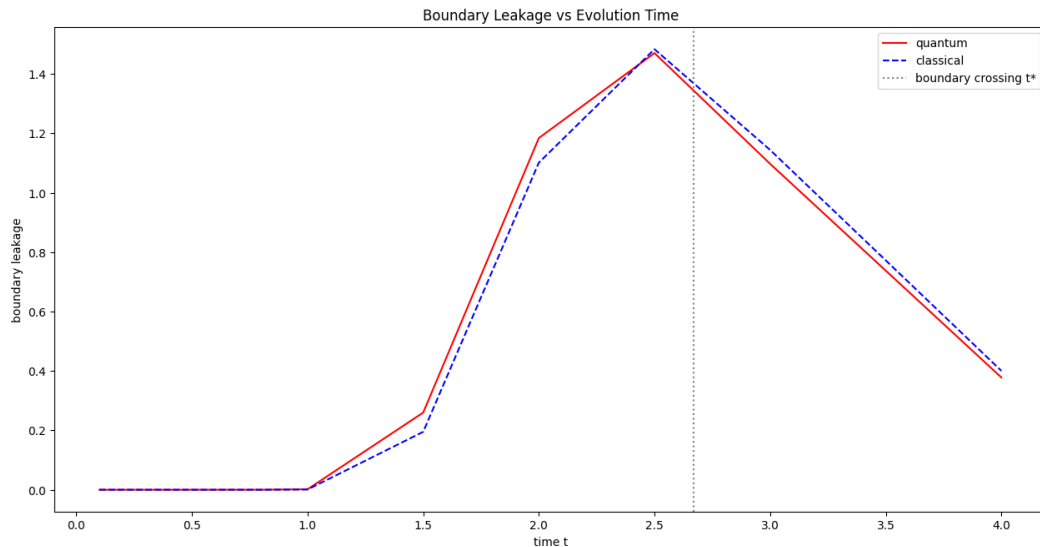
Leakage minimal — wavepacket fully within domain

$$t = t^*$$

Boundary crossing — leakage spikes dramatically

$$t > t^*$$

Spurious wrap-around artifacts degrade accuracy



Boundary Effects & Momentum Analysis

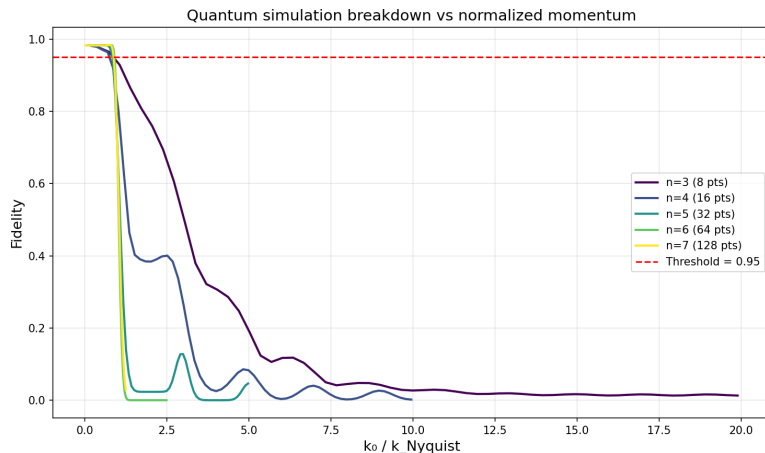
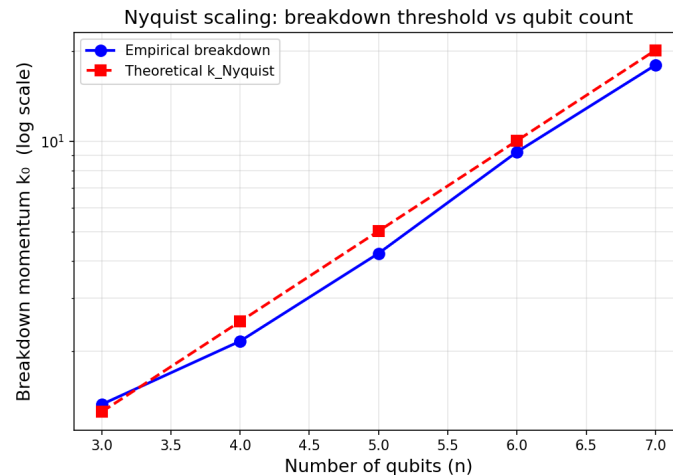


NYQUIST & MOMENTUM CONSTRAINTS

The discrete spatial grid imposes a fundamental momentum limit:

$$k_{max} = \frac{\pi}{\Delta x}; x = \frac{\pi N}{L}$$

With $k_0 = 3$: the initial momentum must satisfy $k_0 < k_{max}$. For $n = 2$ qubits and a typical domain, this Nyquist constraint is violated — causing aliasing and large errors.



Practical implication:

At least 6–8 qubits are required to faithfully represent the initial wavepacket with $k_0 = 3$ without aliasing. This explains the sharp accuracy improvement visible between 5 and 8 qubits.

Conclusions

01

Quantum Algorithm Validated

The QFT-based Trotter circuit accurately reproduces classical Schrödinger dynamics for both free-particle and harmonic-oscillator potentials.

02

Qubit Scaling is Critical

Accuracy improves sharply from 2 to 8 qubits and then plateaus. At ≥ 8 qubits, the quantum simulation matches the classical reference to high fidelity.

03

Boundary & Nyquist Constraints

Identical leakage in both approaches confirms that accuracy limitations are domain geometry effects — not quantum circuit errors.

04

Path to Quantum Advantage

This work demonstrates a concrete methodology for quantum simulation of PDEs, laying the groundwork for scaling to larger, classically intractable systems.



Thank You

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