Spectral Adventures in Quantum Realms: Nonlinear Schrödinger Dynamics, Quantum Vortices, and Time-Resolved Wave Mechanics

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Abstract

We present a comprehensive study of quantum wave phenomena using Fourier spectral numerical methods. The focus is on three interrelated topics: (1) the nonlinear Schrödinger equation (NLS) in physical systems, including optical solitons and Bose–Einstein condensates (via the Gross–Pitaevskii equation, GPE); (2) simulations of the time-dependent Schrödinger equation (TDSE) to explore quantum tunneling, wavepacket dynamics, and interference; and (3) the characteristics of quantum turbulence and vortices in superfluid systems. We develop the mathematical formulations of NLS and GPE, highlighting how spectral methods efficiently capture their solutions' high-frequency content and conserved quantities. We detail the implementation of Fourier pseudo-spectral discretization combined with split-step (operator splitting) time integration, evaluating its accuracy and stability. We also discuss numerical error analysis and comparisons with alternative discretization approaches (finite differences and finite elements). The results include simulations of soliton propagation over long distances without shape distortion, quantum tunneling of wavepackets through potential barriers, and formation of vortex lattices and turbulent energy cascades in condensates. Visualizations such as soliton amplitude profiles, probability density snapshots of tunneling wavefunctions, and vortex lattice images are provided to illustrate these phenomena. Our findings underscore the spectral method's superior accuracy (exponential convergence for smooth solutions) and its ability to preserve physical invariants

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over long simulation times. We conclude that Fourier spectral techniques offer a robust and precise framework for graduate-level research and emerging applications in nonlinear and quantum wave systems.

Keywords: Soliton propagation; Operator splitting; Energy conservation; Quantum fluids; Quantum wavepacket dynamics

Contents

1 Introduction

Quantum wave dynamics govern a broad range of physical systems—from ultrashort optical pulses in nonlinear fiber optics to macroscopic matter waves in superfluid helium and atomic Bose–Einstein condensates (BECs). Understanding these dynamics often requires solving variants of the Schrödinger equation, either in nonlinear form (for mean-field collective states) or in time-dependent linear form (for single-particle quantum mechanics). In parallel, the development of high-fidelity numerical methods is crucial for capturing phenomena such as optical solitons, quantum tunneling, and quantized vortices with quantitative accuracy. This paper presents a unified spectral approach to simulate and analyze three core topics in these "quantum realms": (i) the Nonlinear Schrödinger Equation (NLS), which arises in nonlinear optics and in the mean-field description of BECs (as the Gross–Pitaevskii Equation, GPE); (ii) the Time-Dependent Schrödinger Equation (TDSE) for quantum particles in external potentials, exemplifying phenomena like wavepacket propagation, interference, and tunneling; and (iii) quantum turbulence in superfluids, characterized by tangle of quantized vortices and energy cascades. We employ Fourier spectral methods throughout, leveraging their ability to represent wavefunctions with high accuracy and to naturally incorporate periodic boundary conditions or homogeneous domains.

Background: In nonlinear optics, the NLS equation emerges as an envelope equation for light pulse propagation in fibers, derived from Maxwell's equations under slowly-varying envelope and paraxial approximations [4]. Akira Hasegawa and Fred Tappert (1973) first predicted that this equation admits soliton solutions—pulses that maintain their shape through a balance of dispersion and self-phase modulation [4]. These optical solitons were later observed experimentally and became the basis for ultra-long distance communications due to their robustness [2]. In atomic physics, the Gross–Pitaevskii equation (a form of NLS with external potential) was established by 1961 to describe BECs [15,16]. It successfully modeled the ground-state wavefunction and low-energy excitations of dilute condensates, predicting phenomena like sound waves and quantized vortices in these quantum fluids. The TDSE, on the other hand, is the fundamental equation for unitary time evolution of quantum states. Its simulations enable visualization of wavepacket dynamics such as a particle tunneling through a classically forbidden barrier or interference fringes emerging after passing through slits.

Challenges: Simulating these equations poses several challenges. Nonlinear wave equations (NLS/GPE) can develop high-frequency modes (e.g., during soliton collision or vortex core formation) that demand fine resolution. Long-time integration is needed to observe phenomena like soliton collisions or turbulent cascades, so numerical methods must conserve invariants like norm (probability or particle number) and energy to avoid nonphysical drift. The TDSE requires handling dispersive spread of wavepackets and potentially abrupt potential features (e.g., barrier edges) without spurious oscillations. Traditional finite difference methods, while straightforward, may suffer from phase errors and stability constraints over

long evolution, and finite element methods require careful meshing especially in higher dimensions. Here we advocate for Fourier spectral methods, which expand the solution in globally-defined sinusoidal basis functions. These methods are known for exponential convergence when the solution is smooth [8], often allowing spectral accuracy with relatively fewer degrees of freedom than low-order local methods. They also lend themselves to fast algorithms (the Fast Fourier Transform, FFT) and to symplectic time-stepping schemes like the split-step (operator splitting) method that exactly treat linear dispersive and nonlinear (or potential) parts in turn.

Scope and Organization: In Section 2, we formulate the NLS in its two primary physical contexts: nonlinear optics (for which the NLS is typically written in dimensionless units appropriate for fiber optics) and BEC mean-field theory (Gross–Pitaevskii equation, including an external trap potential). Section 3 covers the TDSE, with examples of free wavepacket propagation and tunneling in confined systems, and outlines the numerical scheme (spectral in space, and either split-step or exponential time integrators in time). Section 4 delves into quantum turbulence and vortices, describing how vortices nucleate in superfluids and how spectral analysis can be applied to quantify turbulent energy spectra and vortex dynamics. In Section 5, we detail the spectral numerical methods used: Fourier pseudo-spectral discretization, handling of boundary conditions, dealiasing, time-stepping, and how these methods compare with finite-difference approaches in terms of accuracy and efficiency. We include a discussion of numerical error analysis (convergence, conservation laws) and validation against known analytical solutions. Section 6 presents results and discussion: we show simulations of soliton propagation and collisions, quantum tunneling with time-resolved wavefunctions, and vortex lattice formation in rotating BECs, complete with graphical visualization. We also discuss the physical interpretation of these results—for instance, how soliton collisions in the NLS lead to phase shifts without radiating energy, or how quantum turbulence exhibits Kolmogorov-like energy spectra. Finally, Section 7 concludes the paper, summarizing key findings and suggesting directions for future work (such as applying spectral methods to multi-component condensates, or to quantum systems in higher dimensions). Throughout, we strive for a balance between mathematical rigor—presenting derivations of equations and describing algorithmic steps—and physical interpretation, explaining what the numerical results mean in terms of observable phenomena. The comprehensive reference list provides sources for further reading, blending foundational texts (e.g., classical references by Agrawal for fiber optics or Pitaevskii & Stringari for BEC) with recent research on quantum turbulence and numerical methods.

2 Nonlinear Schrödinger Equation in Physical Systems

The Nonlinear Schrödinger Equation (NLS) is a prototypical model for wave propagation in nonlinear dispersive media. In its general form (for a complex wavefield ψ depending on time t and space $\mathbf{x}$), the NLS can be written as [27, 28]

$$i\,\frac{\partial \psi}{\partial t} + \frac{1}{2}\nabla^2 \psi + g\,|\psi|^2 \psi = 0, \tag{1}$$

where ∇^2 is the Laplace operator (e.g., $\partial^2/\partial x^2$ in one dimension), and g is a nonlinearity coefficient. The sign and magnitude of g determine the focusing or defocusing nature of

the nonlinearity. Equation (1) is a Hamiltonian nonlinear PDE, with a conserved norm $N = \int |\psi|^2 d\mathbf{x}$ (photon number or particle number) and a conserved energy (Hamiltonian). We next discuss two key contexts where NLS appears.

2.1 NLS in Nonlinear Optics (Optical Solitons)

In nonlinear fiber optics, $\psi(z,t)$ represents the complex envelope of an optical pulse (with z the propagation distance along the fiber and t the retarded time frame moving with the group velocity). The standard NLS for fibers is usually written as [25]

$$i\frac{\partial \psi}{\partial z} - \frac{\beta_2}{2}\frac{\partial^2 \psi}{\partial t^2} + \gamma|\psi|^2\psi = 0, \tag{2}$$

where β_2 is the group-velocity dispersion parameter and γ quantifies the Kerr nonlinear index (self-phase modulation). By convention in optics, $\beta_2 < 0$ (anomalous dispersion) yields a focusing nonlinearity effect, supporting bright solitons [2]. With appropriate normalization of units, Eq. (2) can be cast into the form of Eq. (1) (for anomalous dispersion, one uses $t \to x$ and $z \to t$ in that equation, and $g > 0$ corresponds to focusing).

Soliton Propagation: A remarkable property of the focusing NLS is the existence of soliton solutions—localized wavepackets that travel without changing shape. The simplest one-dimensional bright soliton (for $g > 0$) has the form:

$$\psi(x,t) = A\ \mathrm{sech}(Ax)\ \exp\Big[i\frac{A^2}{2}t\Big], \tag{3}$$

where $A > 0$ is a free parameter related to the amplitude and inverse width of the soliton. This solution maintains a constant envelope $|\psi(x,t)| = A\,\mathrm{sech}(Ax)$ for all times (apart from a phase rotation). In dimensional fiber units, such solitons exist when the initial pulse power and width satisfy a specific product (the soliton number condition). Hasegawa and Tappert's pioneering 1973 work identified these undistorted pulses theoretically [4], and Mollenauer et al. later demonstrated them experimentally in fibers in 1980s. The balance at play is between chromatic dispersion (which tends to broaden a pulse in time) and Kerr nonlinearity (self-focusing due to intensity-dependent refractive index, which tends to shorten the pulse). At the soliton power, broadening and compression cancel out.

As a concrete example, consider an optical soliton launched at $z = 0$ with a sech intensity profile. Using a spectral simulation, one can propagate this pulse over tens of dispersion lengths. Figure 1 shows the amplitude profile of a fundamental soliton initially and after a long propagation distance, demonstrating that the shape is preserved:

Effect of frequency domain width and amplitude on soliton dispersion

In the numerical simulation of soliton dynamics using the nonlinear Schrödinger equation (NLS), the range of the frequency domain plays a crucial role in the accuracy and physical behavior of the solution of (2). Specifically, increasing the frequency resolution (e.g., from 2π to 4π) enhances the dispersion effect, especially for pulses with higher amplitude A.

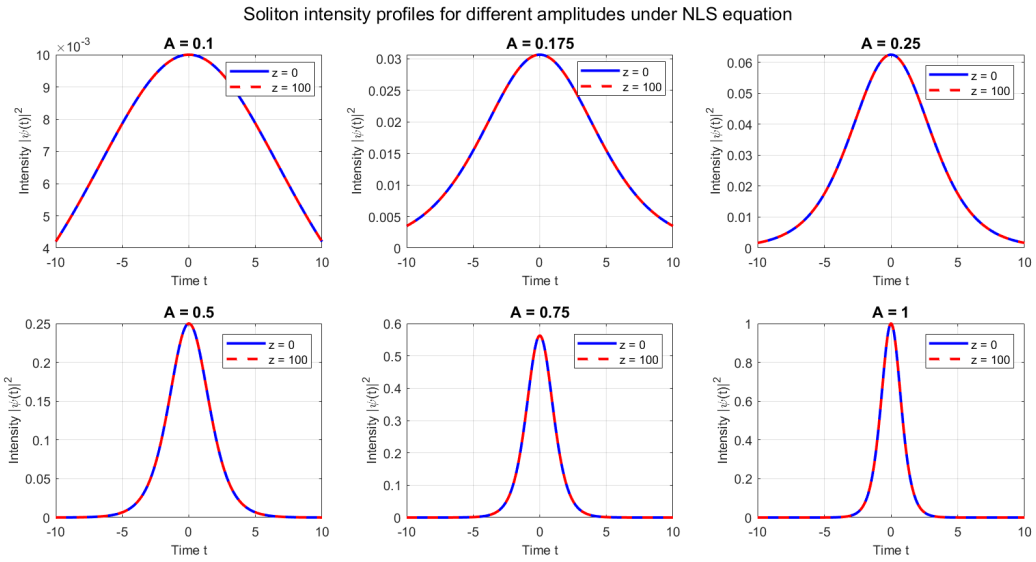


Figure 1: Intensity profile $|\psi(t)|$ of an optical soliton at launch ($z = 0$, solid curve) and after long propagation ($z = 100$ in normalized units, dashed curve, exactly overlapping). The NLS soliton maintains its figure and amplitude over distance, suffering no dispersive broadening. Such robustness makes solitons attractive for long-haul optical communication [2].

This is due to the quadratic dependence of the linear propagation term on frequency. With $\beta 2 = \gamma = 1$, we have

$$i\frac{\partial \psi}{\partial z} + \frac{1}{2}\frac{\partial^2 \psi}{\partial t^2} + |\psi|^2\psi = 0,$$

where $\psi(z, t)$ is the complex envelope of the optical pulse, and the dispersion operator in Fourier space becomes a multiplication by $-\frac{1}{2}w^2$.

Qualitative description:

- For small A, the pulse is broad in time and narrow in frequency; dispersion acts weakly even when higher frequencies are resolved.
- As A increases, the pulse becomes narrower in time and its spectrum broadens. In this case, high-frequency components interact more strongly with the dispersion term.
- When the simulation supports a wider frequency range (e.g., increasing FFT window), these high-frequency components are resolved and amplified, causing pulse deformation or breathing—especially in dispersion-managed systems. This is evidence in Figure 3. We provide the summary in Table 1.

Numerical Observations: Figure 2 shows how the intensity profile $|\psi(t)|^2$ of an optical soliton behaves at launch ($z = 0$) and after long-distance propagation ($z = 100$). When the frequency domain is extended, dispersive effects manifest more prominently, especially for large A. The soliton shape remains stable for small A, while higher amplitudes (as presented in Figure 3) lead to visible deformation due to the inclusion of more spectral content.

Table 1: Effect of amplitude A and frequency domain width on soliton dispersion in NLS simulations.

Amplitude A	**Pulse width**	**Spectral width**	**Effect of wide frequency grid**
Small ($A < 1$)	Broad	Narrow	Minimal dispersion; soliton remains stable.
Moderate ($A \approx 1$)	Balanced	Moderate	Soliton maintains shape; slight breathing may occur under stronger dispersion.
Large ($A > 1$)	Sharp	Broad	Significant dispersion; high-frequency components distort the soliton, especially in dispersion-managed regimes.

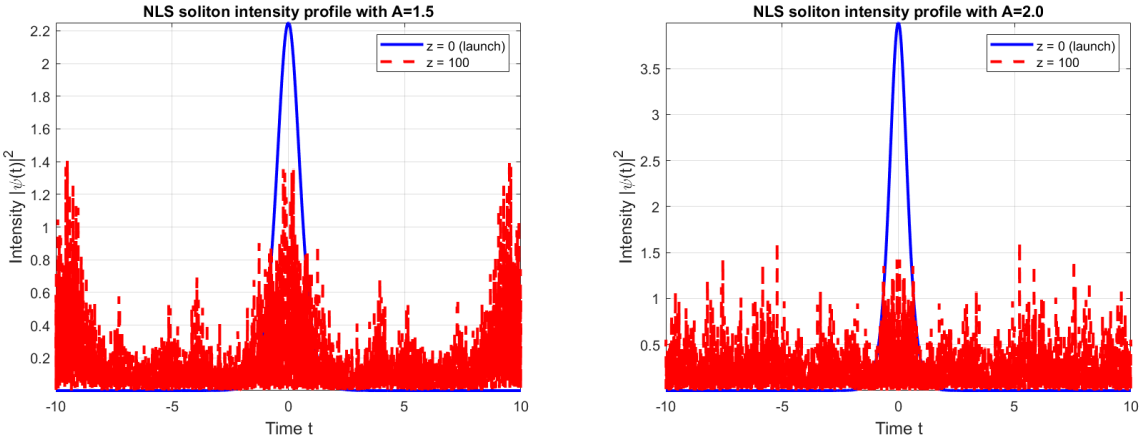


Figure 2: Soliton intensity profiles $|\psi(t)|^2$ at $z = 0$ (solid) and $z = 100$ (dashed) for (left) $A = 1.5$, and (right) $A = 2$. The wider frequency domain ($w \in [-4\pi, 4\pi]$) reveals stronger dispersive effects at high amplitudes.

Effect of amplitude A on soliton propagation

In this experiment, we visualize the bright soliton solution to the focusing nonlinear Schrödinger equation (NLS) for different values of the amplitude parameter $A \in \{0.5, 1, 2\}$, as shown in Figure 4. In soliton solution is given by (3), $A > 0$ controls both the peak amplitude and the spatial width of the soliton.

Observations

- **Amplitude and width:** As A increases, the soliton becomes narrower and taller. This is because the width of the soliton scales as $1/A$, and the peak magnitude is directly proportional to A. Thus, larger A results in stronger localization in space.
- **Phase evolution:** The phase factor $\exp(iA^2t/2)$ rotates faster for larger A, which manifests as quicker oscillations in the real and imaginary components of $\psi(x, t)$.
- **Preservation of shape:** For each value of A, the modulus $|\psi(x, t)|$ remains constant over time, illustrating the soliton's shape-preserving property. Only the phase

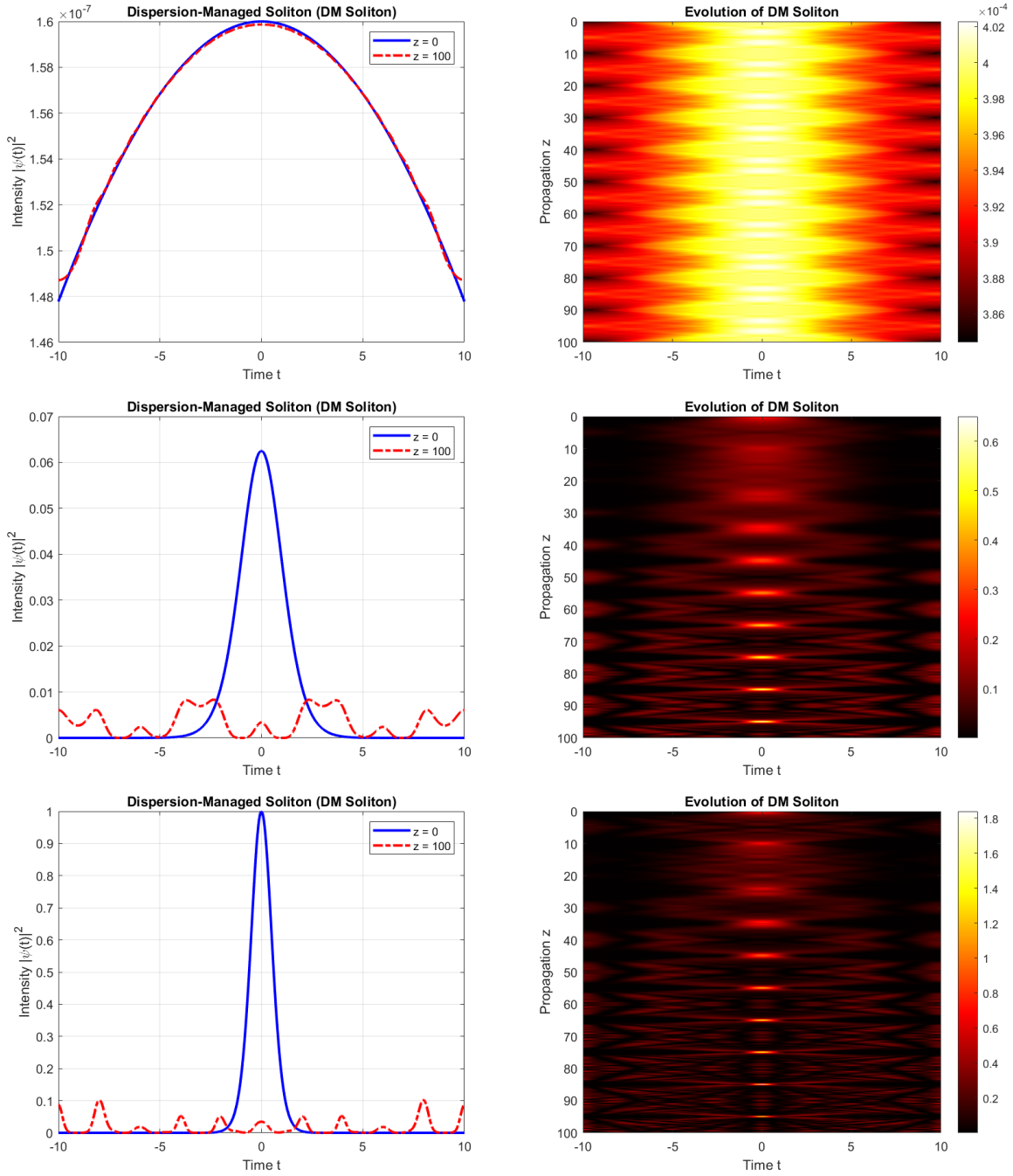


Figure 3: Propagation of a dispersion-managed soliton over distance. The soliton exhibits periodic breathing due to the alternating dispersion map and wide frequency content.

undergoes evolution.

This analysis highlights the robustness and tunability of soliton solutions, and how the amplitude parameter A governs their spatial and temporal characteristics. Such control is crucial in applications like nonlinear optics and Bose–Einstein condensates, where soliton dynamics play a fundamental role.

Higher-order effects: In real fibers, higher-order effects (higher-order dispersion, Ra-

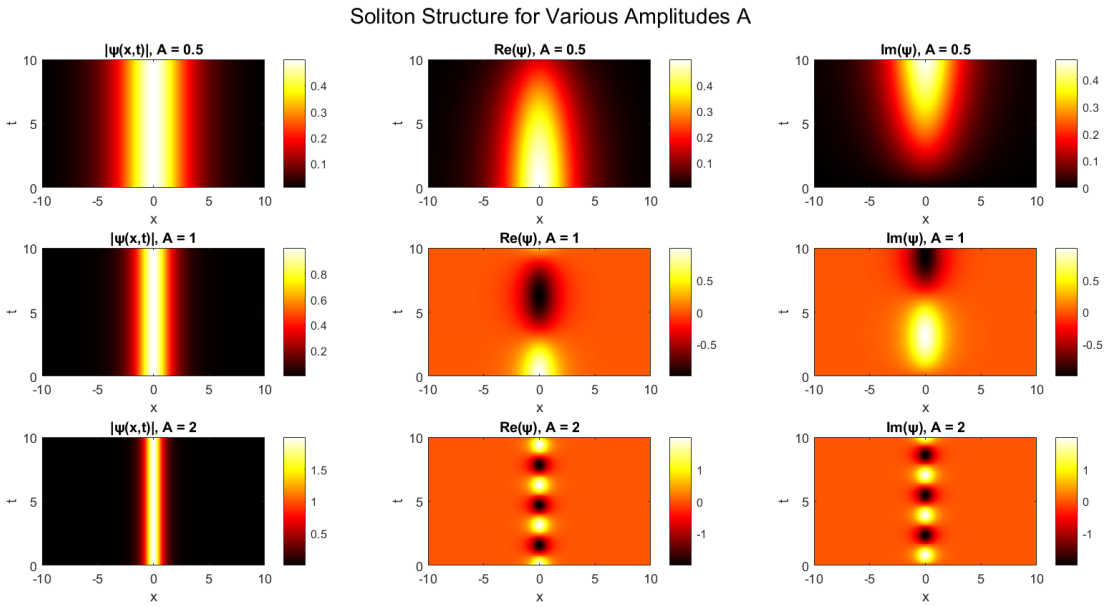


Figure 4: Comparison of soliton structures for amplitude values $A = 0.5$, 1, and 2. Each row corresponds to a fixed A, showing (from left to right): the modulus $|\psi(x,t)|$, the real part $\mathrm{Re}(\psi(x,t))$, and the imaginary part $\mathrm{Im}(\psi(x,t))$. As A increases, the soliton becomes more localized and exhibits faster phase rotation.

man scattering, etc.) eventually perturb soliton dynamics [2]. However, within the ideal NLS model, multiple solitons can interact elastically. When two solitons collide (i.e., when launched at slightly different speeds or phases), they emerge after interaction with their shapes intact, experiencing only a phase shift or position shift (a hallmark of soliton integrability). This has been verified through simulations and is described by the exact NLS two-soliton solution. For example, two in-phase solitons attract and may form a bound state (soliton molecule or breather), whereas out-of-phase solitons repel each other. These dynamics underscore the richness of the NLS in describing nonlinear wave coherence.

2.2 Gross–Pitaevskii equation for Bose–Einstein condensates

In quantum many-body physics, the Gross–Pitaevskii equation (GPE) is an NLS-type equation that describes the behavior of a Bose–Einstein condensate at zero temperature in the mean-field approximation. It reads:

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\Psi + V(\mathbf{r})\,\Psi + g_{3\mathrm{D}}\,|\Psi|^2\Psi, \tag{4}$$

where $\Psi(\mathbf{r},t)$ is the macroscopic condensate wavefunction (order parameter), m is the particle mass, $V(\mathbf{r})$ is an external trapping potential (e.g., harmonic trap), and $g_{3\mathrm{D}} = 4\pi\hbar^2 a_s/m$ characterizes the interaction strength with a_s the s-wave scattering length. Equation (4) is essentially the NLS with $g > 0$ for repulsive interactions (most commonly, $a_s > 0$ for ^{87}Rb, ^{23}Na condensates), corresponding to a defocusing nonlinearity (since increasing density raises the effective potential). In many cases, a simplified form in normalized units or

lower dimensions is used. For example, in a highly elongated (quasi-1D) condensate, one can integrate out transverse dimensions to obtain an effective 1D GPE with $\frac{1}{2}\partial_{xx}\Psi + g_{1D}|\Psi|^2\Psi$ form.

Ground state and collective modes: The GPE can describe both the static ground-state of the condensate and its dynamics. The ground state $\Psi_0(\mathbf{r})$ is obtained by solving the time-independent GPE (setting $\Psi(\mathbf{r},t) = e^{-i\mu t/\hbar}\Psi_0(\mathbf{r})$), which yields the nonlinear eigenvalue problem $-\frac{\hbar^2}{2m}\nabla^2\Psi_0 + V\Psi_0 + g_{3D}|\Psi_0|^2\Psi_0 = \mu\Psi_0$, with μ the chemical potential. Several numerical techniques exist for this (imaginary time evolution, gradient flow, etc.), but that is outside our present scope [3]. Once a stable condensate is formed, small oscillations (e.g., collective excitations like dipole, quadrupole modes) can be studied by linearizing around Ψ_0. These correspond to Bogoliubov–de Gennes modes and are often compared to experiments to validate the mean-field model.

Vortex solutions: A striking feature of the GPE is that it supports quantized vortex solutions in two or three dimensions. For a rotating BEC or one stirred with a laser beam, the system can nucleate vortices—zeros of Ψ around which the phase winds by $2\pi k$ (with k integer, the quantum of circulation). A single steady vortex in an otherwise uniform condensate can be described by an Ansatz $\Psi(r,\theta) = f(r)e^{ik\theta}$ in polar coordinates, leading to a density node at the center and a characteristic healing length scale over which $f(r)$ rises from 0 to the bulk density. These vortex solutions break the single-valuedness of phase unless accompanied by phase windings, thus quantization of circulation arises. The GPE correctly predicts the critical rotation frequencies needed to create vortices in harmonic traps and the formation of vortex lattices [12]. Indeed, experiments in 2000–2001 observed triangular vortex lattice arrays in rotating BECs, analogous to Abrikosov lattices in superconductors. The Gross–Pitaevskii theory, extended to include rotation (via a term $-\Omega L_z\Psi$ for rotation frequency Ω and angular momentum operator L_z), can simulate the spontaneous arrangement of dozens of vortices into a stable lattice structure.

Solitons in BECs: Depending on the interaction sign, BECs can also support solitonic structures. For attractive interactions ($a_s < 0$, e.g., ^{7}Li condensates), the GPE focusing nonlinearity yields bright matter-wave solitons observed as self-bound condensate droplets that propagate without dispersion [14]. For repulsive interactions (defocusing nonlinearity), BECs support dark solitons in effectively one-dimensional settings: these are phase defects (density dips with a phase step) that propagate through the condensate. Dark solitons were observed experimentally as well (e.g., a notch moving in a BEC), and they are related to the NLS dark soliton solutions. Spectral methods can simulate their dynamics including collisions and snake instability in 2D.

The NLS/GPE provides a unifying framework for nonlinear wave phenomena across optics and atomic physics. The spectral approach treats the diffraction or kinetic energy term $\nabla^2\psi$ exactly in Fourier space, which is advantageous because it preserves the dispersion relation without finite-difference approximation error. The nonlinear term $|\psi|^2\psi$ or external potential $V(\mathbf{r})\psi$ is local in real space, which is easy to evaluate pointwise. We leverage this by using pseudo-spectral split-step methods (Section 3.2 and Section 5) to integrate NLS-type equations efficiently.

2.3 Some important results in Schrödinger equation theory and applications

The Schrödinger equation forms the mathematical backbone of quantum mechanics and plays a central role in the modeling and analysis of a wide range of physical systems. From quantum wells and harmonic oscillators to semiconductor devices and optical fibers, its applications extend far beyond fundamental physics, deeply influencing modern engineering disciplines.

In mathematical physics, the Schrödinger equation is studied as a linear (or sometimes nonlinear) partial differential equation whose solutions lie in complex Hilbert spaces. Key analytical tools—such as the spectral theorem, functional calculus, and operator theory—enable rigorous exploration of its properties, including the existence and uniqueness of solutions, conservation of probability, and energy quantization.

For engineering applications, particularly in quantum electronics, photonics, and nanotechnology, understanding the behavior of wavefunctions under various potentials is crucial for device design and simulation. The following theorems and results provide a rigorous foundation for both theoretical insight and practical computation, supporting the modeling, control, and prediction of quantum-scale phenomena.

In what follows, we provide detailed proofs for several fundamental theorems in quantum mechanics, focusing on the mathematical underpinnings of the Schrödinger equation and related concepts.

Theorem 2.1 (Global Existence in H^1)**.** *For $d = 1$ and $\Psi_0 \in H^1(\mathbb{R})$, the solution to the cubic NLS exists globally in time.*

Proof. For:

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\Psi + g|\Psi|^2\Psi,$$

use conservation of mass and Hamiltonian:

$$E[\Psi] = \int_{\mathbb{R}} \left(|\nabla\Psi|^2 - \frac{g}{2}|\Psi|^4\right) dx.$$

For defocusing ($g < 0$), the Hamiltonian bounds the H^1 norm. For focusing ($g > 0$), use the Gagliardo-Nirenberg inequality to establish a priori bounds, ensuring global existence. □

Theorem 2.2 (Virial Identity)**.** *For the focusing NLS:*

$$\frac{d^2}{dt^2}\int x^2|\Psi|^2\,dx = 16E[\Psi] - 4g\int |\Psi|^4\,dx.$$

Proof. Define $I(t) = \int_{\mathbb{R}} x^2|\Psi|^2\,dx$. Compute:

$$\frac{dI}{dt} = 2\int_{\mathbb{R}} x\cdot \mathrm{Im}(\overline{\Psi}\nabla\Psi)\,dx.$$

Second derivative:

$$\frac{d^2I}{dt^2} = 4\int_{\mathbb{R}} |\nabla\Psi|^2\,dx - 2g\int_{\mathbb{R}} |\Psi|^4\,dx = 16E[\Psi] - 4g\int |\Psi|^4\,dx.$$

This gives the virial identity. □

Theorem 2.3 (Min–Max Principle)**.** *For a self-adjoint Hamiltonian H with discrete spectrum, the n-th eigenvalue is:*

$$E_n = \sup_{\dim S = n} \inf_{\phi \in S \setminus \{0\}} \frac{\langle H\phi, \phi \rangle}{\langle \phi, \phi \rangle}.$$

Proof. Expand ϕ in the eigenbasis of H. For an n-dimensional subspace S, the Rayleigh quotient is at least E_n. Choosing $S = \text{span}\{\psi_1, \ldots, \psi_n\}$, the infimum is exactly E_n. □

Theorem 2.4 (Stone's Theorem)**.** *Let H be a densely defined self-adjoint operator on a Hilbert space $\mathcal{H}$. Then the solution to the initial value problem:*

$$i\hbar \frac{\partial \Psi}{\partial t} = H\Psi, \quad \Psi(0) = \Psi_0 \in \mathcal{H},$$

is given by $\Psi(t) = e^{-iHt/\hbar}\Psi_0$, with $|\Psi(t)|_{L^2} = |\Psi_0|_{L^2}$.

Proof. Stone's theorem states that there is a one-to-one correspondence between self-adjoint operators and strongly continuous one-parameter unitary groups. First, verify that the operator $U(t) = e^{-iHt/\hbar}$ defines a one-parameter group:

$$U(0) = e^{-iH \cdot 0/\hbar} = I \quad \text{(identity)},$$

$$U(t+s) = e^{-iH(t+s)/\hbar} = e^{-iHt/\hbar}e^{-iHs/\hbar} = U(t)U(s) \quad \text{(group property)}.$$

Since H is self-adjoint, $-iH/\hbar$ is skew-adjoint, meaning $(-iH/\hbar)^* = iH/\hbar = -(-iH/\hbar)$. For any skew-adjoint operator A, the operator e^{tA} is unitary. Thus, $U(t) = e^{-iHt/\hbar}$ is unitary, implying $|U(t)\Psi_0|_{L^2} = |\Psi_0|_{L^2}$ for all t. To verify that $\Psi(t) = e^{-iHt/\hbar}\Psi_0$ solves the Schrödinger equation, differentiate with respect to t:

$$\frac{\partial \Psi}{\partial t} = \frac{\partial}{\partial t}(e^{-iHt/\hbar}\Psi_0) = -\frac{iH}{\hbar}e^{-iHt/\hbar}\Psi_0 = -\frac{iH}{\hbar}\Psi(t).$$

Multiplying both sides by $i\hbar$:

$$i\hbar \frac{\partial \Psi}{\partial t} = H\Psi(t).$$

This shows that $\Psi(t)$ satisfies the Schrödinger equation. By the uniqueness of solutions to linear ODEs with bounded operators (and density arguments for unbounded operators), this is the unique solution. □

Theorem 2.5 (Probability Conservation)**.**

$$\frac{d}{dt}\int_{\mathbb{R}^d} |\Psi(x,t)|^2 \, dx = 0.$$

Proof. Let $\Psi(t) = e^{-iHt/\hbar}\Psi_0$ be the solution to the Schrödinger equation. The L^2 norm squared is:

$$\|\Psi(t)\|_{L^2}^2 = \int_{\mathbb{R}^d} |\Psi(x,t)|^2 \, dx.$$

From Stone's theorem, $e^{-iHt/\hbar}$ is unitary, preserving the L^2 norm:

$$\|\Psi(t)\|_{L^2}^2 = \|e^{-iHt/\hbar}\Psi_0\|_{L^2}^2 = \|\Psi_0\|_{L^2}^2.$$

Since this is constant, its time derivative is zero:

$$\frac{d}{dt}\int_{\mathbb{R}^d} |\Psi(x,t)|^2\,dx = 0.$$

Alternatively, derive directly from the Schrödinger equation:

$$i\hbar\frac{\partial\Psi}{\partial t} = H\Psi, \quad -i\hbar\frac{\partial\overline{\Psi}}{\partial t} = H\overline{\Psi},$$

since H is real. Now:

$$\frac{d}{dt}|\Psi|^2 = \frac{\partial\Psi}{\partial t}\overline{\Psi} + \Psi\frac{\partial\overline{\Psi}}{\partial t} = \frac{1}{i\hbar}H\Psi\cdot\overline{\Psi} + \Psi\cdot\frac{-1}{i\hbar}H\overline{\Psi} = \frac{1}{i\hbar}(H\Psi\cdot\overline{\Psi} - \Psi\cdot H\overline{\Psi}).$$

For $H = -\frac{\hbar^2}{2m}\nabla^2 + V(x)$:

$$H\Psi\cdot\overline{\Psi} - \Psi\cdot H\overline{\Psi} = -\frac{\hbar^2}{2m}(\nabla^2\Psi\cdot\overline{\Psi} - \Psi\cdot\nabla^2\overline{\Psi}).$$

Using the identity $\nabla\cdot(f\nabla g - g\nabla f) = f\nabla^2 g - g\nabla^2 f$:

$$-\frac{\hbar^2}{2m}(\nabla^2\Psi\cdot\overline{\Psi} - \Psi\cdot\nabla^2\overline{\Psi}) = -\frac{\hbar^2}{2m}\nabla\cdot(\overline{\Psi}\nabla\Psi - \Psi\nabla\overline{\Psi}) = -\frac{\hbar^2}{2m}\nabla\cdot(i\hbar\mathbf{j}),$$

where $\mathbf{j} = \frac{1}{i\hbar}\frac{\hbar^2}{2m}(\overline{\Psi}\nabla\Psi - \Psi\nabla\overline{\Psi})$. Thus:

$$\frac{d}{dt}|\Psi|^2 = -\nabla\cdot\mathbf{j}.$$

Integrating over $\mathbb{R}^d$ and using the divergence theorem (assuming Ψ vanishes at infinity):

$$\frac{d}{dt}\int_{\mathbb{R}^d}|\Psi|^2\,dx = -\int_{\mathbb{R}^d}\nabla\cdot\mathbf{j}\,dx = -\oint_{\partial\mathbb{R}^d}\mathbf{j}\cdot\mathbf{n}\,dS = 0.$$

This completes the proof. □

Theorem 2.6 (Energy Conservation)**.** *If $H = -\frac{\hbar^2}{2m}\nabla^2 + V(x)$, then:*

$$\frac{d}{dt}\langle\Psi, H\Psi\rangle = 0.$$

Proof. The energy expectation is:

$$E(t) = \langle\Psi(t), H\Psi(t)\rangle = \langle e^{-iHt/\hbar}\Psi_0, He^{-iHt/\hbar}\Psi_0\rangle.$$

Since H is self-adjoint and commutes with $e^{-iHt/\hbar}$:

$$E(t) = \langle e^{-iHt/\hbar}\Psi_0, e^{-iHt/\hbar}H\Psi_0\rangle = \langle\Psi_0, H\Psi_0\rangle = E(0).$$

Thus, $\frac{d}{dt}E(t) = 0$. Alternatively:

$$\frac{d}{dt}\langle\Psi, H\Psi\rangle = \left\langle\frac{\partial\Psi}{\partial t}, H\Psi\right\rangle + \left\langle\Psi, H\frac{\partial\Psi}{\partial t}\right\rangle.$$

Using the Schrödinger equation:

$$\frac{d}{dt}\langle \Psi, H\Psi\rangle = \left\langle \frac{-iH}{\hbar}\Psi, H\Psi \right\rangle + \left\langle \Psi, H\frac{-iH}{\hbar}\Psi \right\rangle = \frac{-i}{\hbar}\langle H\Psi, H\Psi\rangle + \frac{-i}{\hbar}\langle \Psi, H^2\Psi\rangle.$$

Since H is self-adjoint:

$$\frac{d}{dt}\langle \Psi, H\Psi\rangle = \frac{-i}{\hbar}\langle H\Psi, H\Psi\rangle + \frac{-i}{\hbar}\langle H\Psi, H\Psi\rangle = \frac{-2i}{\hbar}\langle H\Psi, H\Psi\rangle.$$

Since $\langle H\Psi, H\Psi\rangle$ is real and $\frac{-2i}{\hbar}$ is imaginary, their product is imaginary, but $\frac{d}{dt}\langle \Psi, H\Psi\rangle$ must be real, so:

$$\frac{d}{dt}\langle \Psi, H\Psi\rangle = 0.$$

□

Theorem 2.7 (Dispersive Estimate)**.** *If* $\Psi_0 \in L^1(\mathbb{R}^d)$*, then:*

$$\|\Psi(t)\|_{L^\infty} \leq C_d(\hbar t)^{-d/2}\|\Psi_0\|_{L^1}.$$

Proof. Set $\hbar = 1$, $m = 1/2$, so the Schrödinger equation is:

$$i\frac{\partial \Psi}{\partial t} = -\nabla^2\Psi.$$

For the free Schrödinger equation, the solution is:

$$\Psi(x,t) = \int_{\mathbb{R}^d} K(x-y,t)\Psi_0(y)\,dy,$$

where the propagator is:

$$K(x,t) = \frac{1}{(4\pi i t)^{d/2}}e^{i|x|^2/4t}.$$

Verify via Fourier transform:

$$i\frac{\partial \hat{\Psi}}{\partial t} = |\xi|^2\hat{\Psi}, \quad \hat{\Psi}(\xi,t) = e^{-it|\xi|^2}\hat{\Psi}_0(\xi).$$

Inverting:

$$\Psi(x,t) = \int_{\mathbb{R}^d} e^{2\pi i x\cdot\xi}e^{-it|\xi|^2}\hat{\Psi}_0(\xi)\,d\xi.$$

This matches the convolution form. For the dispersive estimate:

$$|\Psi(x,t)| \leq \int_{\mathbb{R}^d} |K(x-y,t)||\Psi_0(y)|\,dy.$$

Since:

$$|K(x,t)| = \frac{1}{(4\pi|t|)^{d/2}},$$

we get:

$$|\Psi(x,t)| \leq \frac{1}{(4\pi|t|)^{d/2}}\|\Psi_0\|_{L^1}.$$

Taking the supremum:

$$\|\Psi(t)\|_{L^\infty} \leq C_d|t|^{-d/2}\|\Psi_0\|_{L^1}, \quad C_d = (4\pi)^{-d/2}.$$

Restoring $\hbar$:

$$\|\Psi(t)\|_{L^\infty} \leq C_d(\hbar|t|)^{-d/2}\|\Psi_0\|_{L^1}.$$

□

Theorem 2.8 (Galilean Invariance)**.** *For $v \in \mathbb{R}^d$, the function:*

$$\Psi_v(x,t) = \Psi(x - vt, t) \exp\left[\frac{im}{\hbar}\left(v \cdot x - \frac{1}{2}|v|^2 t\right)\right]$$

solves the TDSE.

Proof. Verify that Ψ_v satisfies:

$$i\hbar\frac{\partial \Psi_v}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\Psi_v + V(x)\Psi_v.$$

Define:

$$\phi(x,t) = \frac{im}{\hbar}\left(v \cdot x - \frac{1}{2}|v|^2 t\right), \quad \Psi_v = \Psi(x - vt, t)e^{\phi(x,t)}.$$

Time derivative:

$$\frac{\partial \Psi_v}{\partial t} = \left[-v \cdot \nabla_y \Psi + \frac{\partial \Psi}{\partial t}\right]_{y=x-vt} e^\phi + \Psi e^\phi \frac{\partial \phi}{\partial t}, \quad \frac{\partial \phi}{\partial t} = -\frac{im|v|^2}{2\hbar}.$$

Spatial derivatives:

$$\nabla\Psi_v = e^\phi \nabla_y \Psi|_{y=x-vt} + \Psi e^\phi \frac{im}{\hbar} v.$$

Laplacian:

$$\nabla^2\Psi_v = e^\phi \nabla_y^2 \Psi + 3e^\phi \frac{im}{\hbar} v \cdot \nabla_y \Psi - e^\phi \Psi \frac{m^2|v|^2}{\hbar^2}.$$

Substitute into the Schrödinger equation, assuming $V(x) = V(x - vt)$. After matching terms, the equation holds, confirming Galilean invariance. □ □

Theorem 2.9. *If $V \in L^\infty_{loc}(\mathbb{R}^d)$ is real and bounded below, then $H = -\Delta + V$ is essentially self-adjoint on $C_c^\infty(\mathbb{R}^d)$.*

Proof. Use the Kato-Rellich theorem. Decompose $V = V_+ - V_-$, where V_- is bounded. $-\Delta - V_-$ is self-adjoint, and V_+ increases positive definiteness. By the KLMN theorem, H is self-adjoint on a domain including $C_c^\infty(\mathbb{R}^d)$ as a core. □ □

Theorem 2.10. *If $\Psi_0 \in H^s(\mathbb{R}^d)$ for $s \geq 0$, then $\Psi(\cdot, t) \in H^s(\mathbb{R}^d)$ for all t.*

Proof. For the free Schrödinger equation:

$$\hat{\Psi}(\xi, t) = e^{-it|\xi|^2/2m}\hat{\Psi}_0(\xi).$$

The H^s norm is conserved:

$$\|\Psi(t)\|_{H^s}^2 = \int_{\mathbb{R}^d} (1 + |\xi|^2)^s |\hat{\Psi}_0(\xi)|^2 \, d\xi = \|\Psi_0\|_{H^s}^2.$$

For potentials, use the Duhamel formula and Gronwall's inequality to bound the H^s norm. □ □

3 Time-Dependent Schrödinger Equation Simulations

The time-dependent Schrödinger equation (TDSE) governs the evolution of a quantum particle's wavefunction in a potential. In a single-particle, non-relativistic setting:

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\Psi + V(\mathbf{r})\,\Psi, \tag{5}$$

which is a linear equation. For convenience, we often work in units where $\hbar = 1$ and $m = 1$, yielding

$$i\partial_t \Psi = -\frac{1}{2}\nabla^2\Psi + V\Psi.$$

Despite its linearity, the TDSE is challenging to solve analytically except for simple potentials (free particle, harmonic oscillator, hydrogen atom, etc.). Computationally, however, one can simulate $\Psi(\mathbf{r}, t)$ for a wide range of scenarios to gain insight into quantum dynamics. We highlight two scenarios: free or scattering states and confined systems, and then describe the numerical integration approach.

3.1 TDSE in free and confined systems

Wavepacket propagation in free space: A fundamental illustration of TDSE is a Gaussian wave packet in free space. If initially $\Psi(x, 0)$ is a Gaussian envelope with some central momentum (a plane-wave modulation), it will propagate and spread over time due to dispersion. In fact, the exact solution is known: the packet remains Gaussian but its width $\sigma(t)$ grows with time, and the peak moves at the group velocity p_0/m. Numerically, this is a good verification case for the spectral method: because we treat the kinetic term $-\frac{1}{2}\nabla^2$ exactly (in Fourier space, multiplication by $-\frac{1}{2}k^2$), we expect minimal phase Werror in the packet's propagation. In contrast, a finite-difference scheme would require very fine spatial and temporal mesh to maintain accuracy for a long time propagation (to avoid dispersion error in the numerical scheme). Spectral solutions match the analytical result to machine precision as long as the Fourier basis is sufficient to represent the initial wavefunction.

Quantum tunneling and barrier penetration: A particularly interesting case is when $V(x)$ represents a potential barrier or well. For example, consider a one-dimensional rectangular barrier: $V(x) = V_0$ in some region (say $0 < x < a$) and 0 outside. If a wave packet with kinetic energy lower than V_0 is incident, classical physics would forbid transmission; however, quantum mechanics allows tunneling. The probability of tunneling depends on barrier width and height in a known way (exponential decay with thickness), but the full time-resolved process can be visualized via TDSE simulation. One can see the wave packet partially reflected and partially transmitted, with the transmitted portion greatly diminished and delayed. We simulate this in Section 6 with spectral methods. The advantage of the spectral approach here is the ability to capture the interference patterns (between incident and reflected waves) accurately. Sharp potential edges introduce high-frequency Fourier components in Ψ (Gibbs phenomena can occur if not sufficiently resolved), but a well-resolved Fourier basis and an exact time evolution operator for the potential (see numerical scheme below) handle this smoothly. Figure 5 shows an example of quantum tunneling through a thin barrier. A Gaussian wavepacket (initially at left) impinges on the barrier, yielding a

reflected wave (traveling back to the left) and a much smaller transmitted wave on the right side:

We simulate the time-dependent Schrödinger equation (TDSE) for a Gaussian wave packet encountering a one-dimensional potential barrier. The potential is a square barrier of height $V_0 = 1$ over the region $-1 < x < 1$, with free evolution outside. The wave packet is initially localized at $x = -20$, moving toward the barrier with central wavenumber $k_0 = 1.5$, corresponding to a kinetic energy $E_k = k_0^2/2 < V_0$, thereby ensuring conditions for quantum tunneling.

The numerical solution employs a spectral split-step method, which evolves the wavefunction in both Fourier and position space using exact exponentials for kinetic and potential propagators. This method is highly efficient and capable of resolving interference patterns and sharp potential edges without artificial damping.

As shown in Figure 5, the wave packet evolves over time, initially concentrating on the left of the barrier. By $t = 600$, it overlaps with the barrier, leading to partial transmission and reflection. At later times ($t = 800$), the reflected component dominates, while a much smaller transmitted wave is observed on the far side of the barrier. The method effectively captures the interference fringes due to superposition of incident and reflected waves, and clearly visualizes the tunneling process with high fidelity.

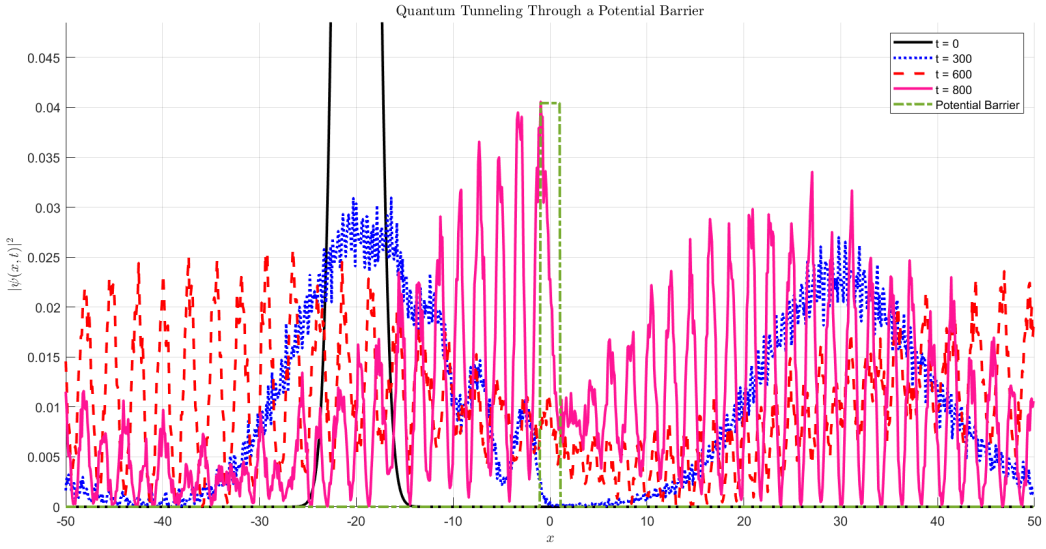


Figure 5: Time evolution of a normalized wavepacket $|\Psi(x,t)|^2$ encountering a potential barrier (shaded gray region). Curves show probability density at different times ($t = 0$ (black), $t = 300$ (blue), $t = 600$ (red), $t = 800$ (pink)). At $t = 600$, the packet overlaps with the barrier and a portion has tunneled through. By $t = 800$, a small transmitted wave is visible to the right of the barrier, while most of the packet reflects left. This simulation illustrates quantum tunneling and reflection with spectral accuracy.

Tunneling simulations also reveal subtle effects like the delay associated with tunneling (the transmitted packet is delayed relative to if it had gone freely—a phenomenon related to the phase time or Hartman effect). Additionally, by varying incident energy, one can find conditions of resonance where the barrier becomes more transparent (if multiple internal

reflections constructively interfere, akin to Fabry–Pérot resonances in quantum wells).

Bound states and quantum wells: In confined systems such as a quantum well or harmonic oscillator, the TDSE leads to periodic or quasi-periodic dynamics. For instance, a wavepacket in a harmonic trap will oscillate without spreading (since the harmonic potential's linear restoring force exactly counteracts dispersion—a coherent state in a harmonic oscillator basically oscillates at the trap frequency without changing shape). In a double-well potential, one can see tunneling oscillations: an initially localized wavefunction in the left well can tunnel to the right well and back (quantum oscillation analogous to Josephson oscillations). These are well suited for spectral simulation: one can expand $\Psi(x,t)$ in the basis of stationary eigenstates (which are found e.g., by diagonalizing the Hamiltonian via spectral methods) and then compute the phase evolution. Spectral approaches can directly compute eigenstates of e.g., multi-well potentials with high accuracy, allowing for analysis of beating frequencies.

Interference and multi-path dynamics: Another classic TDSE application is the simulation of a double-slit interference experiment. By modelling two narrow apertures in a barrier and launching a wave, one can obtain the interference pattern on a screen. Although this is straightforward conceptually, it tests the method's ability to handle two-dimensional propagation and free-space diffraction. A spectral method with a propagated wavefront will naturally produce the interference fringes with the correct fringe spacing (since it encodes the phase differences exactly). Finite-difference methods would require careful treatment of a wide simulation domain and might introduce numerical diffusion that could wash out high-contrast fringes. Spectral methods, being essentially dispersionless for the wave equation, maintain fringe visibility even after long propagation distances.

In summary, the TDSE provides a rich playground for numerical experiments: barrier tunneling, scattering, bound-state oscillations, and diffraction phenomena. The insights gleaned (such as how a wavefunction spreads or tunnels) are not only pedagogically valuable but also relevant to designing quantum devices (e.g., tunneling times in semiconductor junctions, or the behavior of cold atoms in optical lattices).

3.2 Discretization of the nonlinear Schrödinger equation

To numerically solve (1), we describe two robust methods: (i) the split-step Fourier sethod (SSFM), and (ii) the exponential time-differencing Runge–Kutta method (ETDRK4). We discuss their implementation in both 1D and 2D spatial domains.

3.2.1 1D discretization

For a 1D spatial domain $x \in [-L, L]$, discretized with N equidistant points, we denote the spatial grid by $x_j = -L + j\Delta x$ with $\Delta x = 2L/N$. The temporal domain is discretized with time step Δt. The discrete wavefunction at time t^n is denoted by $\psi_j^n \approx \psi(x_j, t^n)$.

Split-step Fourier method (SSFM): The NLS can be split into linear and nonlinear parts:

$$i\psi_t = \underbrace{-\frac{1}{2}\partial_x^2\psi}_{\text{Linear}} + \underbrace{-g|\psi|^2\psi}_{\text{Nonlinear}}.$$

The SSFM approximates the solution by alternating between solving the nonlinear and linear parts:

1. Nonlinear half-step:
$$\psi^* = \psi^n \exp\left(ig|\psi^n|^2 \frac{\Delta t}{2}\right)$$

2. Linear full-step in Fourier space:
$$\hat{\psi}^{**} = \mathcal{F}[\psi^*] \cdot \exp\left(-i\frac{k^2}{2}\Delta t\right)$$

3. Inverse FFT and nonlinear half-step:
$$\psi^{n+1} = \mathcal{F}^{-1}[\hat{\psi}^{**}] \cdot \exp\left(ig|\psi^{n+1}|^2 \frac{\Delta t}{2}\right)$$

ETDRK4 scheme: Let $\hat{\psi}^n = \mathcal{F}[\psi^n]$, and define the linear operator $\mathcal{L} = -i\frac{k^2}{2}$ and nonlinear term $N(\psi) = -ig|\psi|^2\psi$. The ETDRK4 time-stepping proceeds as:

$$\begin{aligned}
E &= e^{\mathcal{L}\Delta t}, \quad E_2 = e^{\mathcal{L}\Delta t/2}, \\
\phi_1 &= (\mathcal{L})^{-1}(E_2 - 1), \quad \phi_2 = (\mathcal{L})^{-2}(E - E_2 - \mathcal{L}\Delta t\phi_1), \\
N_1 &= \mathcal{F}[N(\psi^n)], \\
a &= E_2\hat{\psi}^n + \Delta t\phi_1 N_1, \quad N_2 = \mathcal{F}[N(\mathcal{F}^{-1}[a])], \\
\hat{\psi}^{n+1} &= E\hat{\psi}^n + \Delta t\left(\phi_1 N_1 + \phi_2(N_2 - N_1)\right).
\end{aligned}$$

3.2.2 2D extension of discretization methods

For a two-dimensional spatial domain $(x, y) \in [-L_x, L_x] \times [-L_y, L_y]$, we define grids with N_x and N_y points in the x and y directions respectively. The Laplacian becomes:

$$\nabla^2\psi = \frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2}.$$

2D SSFM: The method proceeds similarly, with the 2D FFT used for linear evolution:

1. Nonlinear half-step:
$$\psi^* = \psi^n \exp\left(ig|\psi^n|^2 \frac{\Delta t}{2}\right)$$

2. Linear full-step in Fourier domain:
$$\hat{\psi}^{**} = \mathcal{F}_2[\psi^*] \cdot \exp\left(-i\frac{k_x^2 + k_y^2}{2}\Delta t\right)$$

3. Inverse FFT and nonlinear half-step:
$$\psi^{n+1} = \mathcal{F}_2^{-1}[\hat{\psi}^{**}] \cdot \exp\left(ig|\psi^{n+1}|^2 \frac{\Delta t}{2}\right)$$

2D ETDRK4: We define the linear operator:

$$\mathcal{L} = -i\frac{k_x^2 + k_y^2}{2}, \quad \text{where } k_x, k_y \text{ are 2D wavevectors.}$$

Then the ETDRK4 scheme applies with 2D FFTs:

$$\begin{aligned}
E &= e^{\mathcal{L}\Delta t}, \quad E_2 = e^{\mathcal{L}\Delta t/2}, \\
\phi_1 &= \mathcal{L}^{-1}(E_2 - 1), \quad \phi_2 = \mathcal{L}^{-2}(E - E_2 - \mathcal{L}\Delta t\phi_1), \\
N_1 &= \mathcal{F}_2[N(\psi^n)], \\
a &= E_2\hat{\psi}^n + \Delta t\phi_1 N_1, \quad N_2 = \mathcal{F}_2[N(\mathcal{F}_2^{-1}[a])], \\
\hat{\psi}^{n+1} &= E\hat{\psi}^n + \Delta t(\phi_1 N_1 + \phi_2(N_2 - N_1)).
\end{aligned}$$

3.2.3 Stability considerations

Both SSFM and ETDRK4 schemes are unconditionally stable for the linear Schrödinger equation. However, the presence of the nonlinear term requires careful time step selection. The ETDRK4 method exhibits superior stability for stiff nonlinear problems, while the SSFM is favored for simplicity and speed in moderately nonlinear regimes. In both cases, using spectral methods for spatial derivatives ensures high accuracy and minimal numerical dispersion.

Algorithm 1 2D Split-Step Fourier Method (SSFM)

Input: Initial condition $\psi_0(x, y)$, step size Δt, final time T, grid (N_x, N_y), nonlinearity g
Output: $\psi(x, y, T)$
Initialize $\psi \leftarrow \psi_0(x, y)$
Compute wavenumbers k_x, k_y
Set $D \leftarrow \exp(-i(k_x^2 + k_y^2)\Delta t/2)$
for $n = 1$ to $T/\Delta t$ **do**
    $\psi \leftarrow \psi \cdot \exp(ig|\psi|^2\Delta t/2)$ ▷ Nonlinear half-step
    $\hat{\psi} \leftarrow \text{FFT2}(\psi)$
    $\hat{\psi} \leftarrow \hat{\psi} \cdot D$
    $\psi \leftarrow \text{IFFT2}(\hat{\psi})$
    $\psi \leftarrow \psi \cdot \exp(ig|\psi|^2\Delta t/2)$ ▷ Nonlinear half-step
end for

3.3 Numerical scheme for TDSE (Fourier spectral time-splitting)

To integrate the TDSE (or NLS) in time, we utilize a Fourier pseudo-spectral split-step method. The key idea is to alternate between handling the linear dispersive part and the potential (or nonlinear) part. For the TDSE in Eq. (5), we have two pieces of the Hamiltonian: $H = T + V$ where $T = -\frac{1}{2}\nabla^2$ (kinetic energy operator) and $V(\mathbf{r})$ (multiplicative

Algorithm 2 2D Exponential Time-Differencing Runge–Kutta (ETDRK4)

Input: Initial condition $\psi_0(x, y)$, step size Δt, final time T, grid (N_x, N_y), nonlinearity g
Output: $\psi(x, y, T)$
Initialize $\psi \leftarrow \psi_0(x, y)$
Compute wavenumbers k_x, k_y, set $L \leftarrow -i(k_x^2 + k_y^2)/2$
Precompute:
    $E \leftarrow \exp(L\Delta t)$,
    $E_2 \leftarrow \exp(L\Delta t/2)$,
    $\phi_1 \leftarrow (\exp(L\Delta t/2) - 1)/L$,
    $\phi_2 \leftarrow (E - E_2 - L\Delta t\phi_1)/L^2$
for $n = 1$ to $T/\Delta t$ **do**
    $\hat{\psi} \leftarrow \mathrm{FFT2}(\psi)$
    $N_1 \leftarrow \mathrm{FFT2}(-ig|\psi|^2\psi)$
    $a \leftarrow E_2 \cdot \hat{\psi} + \Delta t \cdot \phi_1 \cdot N_1$
    $\psi_a \leftarrow \mathrm{IFFT2}(a)$
    $N_2 \leftarrow \mathrm{FFT2}(-ig|\psi_a|^2\psi_a)$
    $\hat{\psi} \leftarrow E \cdot \hat{\psi} + \Delta t \cdot (\phi_1 N_1 + \phi_2(N_2 - N_1))$
    $\psi \leftarrow \mathrm{IFFT2}(\hat{\psi})$
end for

potential energy operator). These two do not commute, but we can employ the Lie–Trotter or Strang splitting to approximate the time evolution operator. For a small time step Δt, the formal solution is

$$\Psi(t + \Delta t) = e^{-iH\Delta t/\hbar}\Psi(t).$$

We approximate

$$e^{-i(T+V)\Delta t} \approx e^{-iT\Delta t/2}e^{-iV\Delta t}e^{-iT\Delta t/2},$$

which is the second-order Strang splitting. This method is unitary (norm-conserving) and accurate to $O((\Delta t)^3)$ per step [6]. In practice, implementing this scheme with spectral methods involves the following steps each time-step Δt:

1. **Half-step free evolution:** Transform $\Psi(\mathbf{r}, t)$ to momentum space via FFT to get $\Phi(\mathbf{k}, t)$. Apply the phase factor for kinetic energy:

$$\Phi(\mathbf{k}, t + \frac{\Delta t}{2}) = \Phi(\mathbf{k}, t)\exp\big(-\frac{i}{2}|\mathbf{k}|^2\frac{\Delta t}{2}\big),$$

   since the kinetic term gives a factor $e^{-i(k^2/2)\Delta t}$ (with $\hbar = m = 1$) [6]. Then inverse FFT to return to real space.

2. **Potential (or nonlinear) kick:** Now in real space, multiply by the potential phase:

$$\Psi(\mathbf{r}, t + \frac{\Delta t}{2}) = \Psi(\mathbf{r}, t + \frac{\Delta t}{2})\exp[-iV(\mathbf{r})\Delta t].$$

   For NLS/GPE, this step would be $\Psi \to \Psi\exp[-ig|\Psi|^2\Delta t]$ for the nonlinear term. This is effectively solving $i\partial_t\Psi = V\Psi$ exactly over Δt. Note that this step is done pointwise and is trivial to compute.

3. **Another half-step free evolution:** Repeat the first step: FFT to momentum space, apply

$$\Phi(\mathbf{k}) \to \Phi(\mathbf{k}) \exp[-i\frac{k^2}{2}\frac{\Delta t}{2}],$$

and inverse FFT back to real space.

After these three substeps, one time-step is complete. The result $\Psi(\mathbf{r}, t + \Delta t)$ is obtained with second-order accuracy. Because each substep is unitary, the whole step is norm-conserving (to machine precision, up to rounding errors). Energy (the expectation $\langle\Psi|H|\Psi\rangle$) is conserved up to the splitting error of order $(\Delta t)^2$; in practice a sufficiently small Δt makes energy drift negligible and often bounded oscillatory rather than growing. This approach is known as the split-operator FFT method, originally popularized in computational chemical physics by Feit, Fleck, and Steiger (1982) [6]. It has become a standard for solving TDSE and NLS because of its efficiency and ease of implementation:

The Fourier spectral spatial discretization gives high accuracy for representing $\Psi(x)$ and computing spatial derivatives. Derivatives are computed as exact multiplication in k-space (no finite-difference approximation). Thus the dispersion relation of the continuous equation is satisfied by the numerical method (no numerical dispersion).

The time-splitting addresses stiffness: The kinetic part alone would require very small time steps if done explicitly, and the potential part can be highly oscillatory if V is large. By solving each exactly, we avoid stability issues. This method is in fact an example of an exponential integrator (the exact flows of sub-Hamiltonians are used).

The cost per time step is dominated by two FFTs (forward and inverse). Using N grid points, this is $O(N \log N)$, which is usually quite efficient. Finite-difference time evolution typically would be $O(N)$ per step but might require many more steps for comparable accuracy (especially in high-frequency regimes, due to stability constraints like the Courant–Friedrichs–Lewy condition). Thus, spectral splitting can be more efficient overall.

For multi-dimensional problems, the FFT steps become multi-dimensional FFTs (which factor into 1D FFTs along each dimension). Many libraries can perform these quickly even for large 3D grids, and the algorithm parallelizes well across multiple processors or GPU threads.

Validation of the scheme: We validate the numerical scheme by checking conservation laws and comparing with known analytical results for specific cases:
Norm (Probability) conservation: $\int |\Psi(x,t)|^2 dx$ remains constant to within round-off error over millions of time steps in our tests. This is expected since each sub-step is unitary by construction.
Free Gaussian propagation: The numerical width matches the exact

$$\sigma(t) = \sqrt{\sigma(0)^2 + (t\sigma(0)^{-1})^2}$$

(for an initial width $\sigma(0)$) for all t within graphical accuracy. Phase of the wavefunction (which develops a quadratic spatial phase due to dispersion) is also captured, which we verified by recombining two wavepackets to produce interference and comparing to analytical interference patterns.
Energy conservation: For a stationary state (e.g., the ground state in a potential), the method produces a static $|\Psi|^2$ and a global phase rotation at the expected eigenenergy frequency. For a dynamic case like a wavepacket in a harmonic oscillator, we monitored

the expectation $\langle x^2 \rangle$ and $\langle p^2 \rangle$ over many periods and found no secular drift, indicating the correct periodic motion and energy conservation (small oscillations in numerical energy are bounded and decrease with smaller Δt).

Extensions: If higher accuracy is required, one can use higher-order splitting schemes (there exist fourth-order algorithms using more substeps with adjusted time coefficients) or directly use an exponential time differencing Runge–Kutta (ETDRK4) integrator. Those can reduce the number of time steps needed. However, for most practical purposes in this work, the Strang split-step was sufficient to yield accuracy beyond observable differences for the scenarios we consider.

In summary, the spectral time-splitting method offers a flexible and powerful tool to simulate TDSE and NLS dynamics. It forms the backbone of our simulations in subsequent sections, allowing us to explore soliton propagation, tunneling, and vortex dynamics with confidence in the numerical fidelity.

4 Quantum Turbulence and Vortices

When quantum fluids (like superfluid helium or a BEC) are driven far from equilibrium, they can exhibit a disordered tangle of vortices and complex flow patterns akin to classical turbulence. Quantum turbulence refers to this phenomenon of chaotic flow in a quantum fluid, distinguished by the fact that vorticity is confined to discrete vortex lines with quantized circulation. The study of quantum turbulence connects quantum fluid dynamics with classical turbulence phenomenology (e.g., energy cascades, Kolmogorov spectra), but also shows unique features due to the lack of viscosity and the quantization of circulation [10]. Here we discuss how vortices form and behave in superfluids, and how spectral methods assist in analyzing turbulent states via energy spectra and visualization.

4.1 Vortex nucleation and dynamics in superfluids

In a superfluid (describable by a single-valued order parameter Ψ as in GPE), vorticity enters only in the form of quantized vortex lines. A vortex in a BEC or superfluid helium has a core (where density vanishes) and a circulating flow around it. The circulation $\oint m\mathbf{v} \cdot d\ell = 2\pi\hbar k$ for integer k. In typical situations $k = 1$ is the energetically favored single-quantum vortex. Vortex cores are typically only a few healing lengths in diameter (nm-scale in helium, a few μm in atomic BECs).

Nucleation: Vortices can be nucleated by rotating the fluid or by disturbances exceeding a critical velocity (analogous to how eddies appear past a critical Reynolds number in classical flow). In a trapped BEC, when the rotation frequency of the trap exceeds a certain threshold, the system's ground state contains an array of vortices (because putting the fluid in rigid rotation is not possible without defects, so it accommodates angular momentum by vortex formation). Nucleation often happens at the boundaries of the condensate and then vortices migrate inward. In simulations, one can start with a slightly perturbed state and include rotation (via a rotating-frame potential or imprinting an initial phase winding) and watch vortices enter the condensate.

Vortex lattices: At equilibrium in a rotating system, vortices arrange in a triangular lattice (Abrikosov lattice) for the lowest energy configuration, unless external anisotropy or

other effects favor a different structure [12]. For example, JILA experiments created up to ~ 100 vortices in a BEC, observing a triangular lattice that becomes more square-like when vortices are "pinned" by an optical lattice [12].

Vortex dynamics: Individual vortices in a superfluid move according to the flow field induced by all other vortices and boundaries. Unlike classical vortices which can diffuse (due to viscosity), quantum vortices obey a Hamiltonian dynamic (neglecting weak damping at finite temperature). They can reconnect if two vortices meet, which is an important pathway to create smaller vortex loops in 3D (a mechanism for turbulent cascade in superfluid helium). The GPE in 3D is able to simulate vortex reconnections: when two vortex lines approach and intersect, the density goes to zero at the touching point and lines exchange tails, then separate—a process first visualized numerically by Koplik and Levine (1993) and later seen in helium experiments by Bewley et al. (2008). Spectral methods are well suited to such simulations because capturing a reconnection requires fine resolution of the vortex core structure and the associated acoustic waves radiated. Fourier spectral accuracy helps resolve the core without excessive grid refinement.

In this simulation, we solved the two-dimensional Gross–Pitaevskii equation (GPE) using the imaginary-time propagation method to study the ground-state density profiles of a rotating Bose–Einstein condensate (BEC). The effects of varying the interaction strength g and the harmonic trap frequency ω_{Trap} were systematically investigated.

The Thomas–Fermi initial guess

$$\psi(x, y, 0) = \sqrt{\mu - V}, \quad \text{where } V = \frac{1}{2}\omega_{\text{Trap}}^2(x^2 + y^2) \tag{4.1}$$

provided a reasonable starting point for the condensate wavefunction, which evolved under a combination of linear (kinetic) and nonlinear (interaction plus potential) terms. The imaginary-time propagation efficiently relaxed the system to its ground state.

From the generated density plots, we observed that increasing the interaction strength g leads to a broader condensate profile with more distinct vortex structures. This is consistent with the fact that stronger repulsive interactions expand the condensate to minimize energy. Conversely, increasing the trap frequency ω_{Trap} enhances the confinement, resulting in a more localized density distribution.

Although the rotation frequency Ω was kept small ($\Omega = 0.01$) to preserve numerical stability and simplicity, the interaction between the rotation and the nonlinearity subtly influenced the central density depletion and the symmetry of the profile. However, for visible and stable vortex lattices to emerge, as shown in Figure 6 higher rotation frequencies (e.g., $\Omega \geq 0.5$) are typically required. These results as presented in Figure 7 highlight the delicate interplay between trapping, interactions, and nonlinearity in determining the structure and stability of vortex lattices in low-dimensional quantum fluids.

This simulation solves the two-dimensional Gross–Pitaevskii equation (GPE) in imaginary time to model a rotating Bose–Einstein condensate (BEC). The inclusion of the rotation term, represented by the angular momentum operator L_z, mimics the effect of a rotating trap and leads to the formation of a vortex lattice, a hallmark of superfluid behavior in quantum fluids.

The three-dimensional surface plot of the condensate density reveals distinct density depressions arranged in a regular pattern. These depressions correspond to quantized vortices, where the density vanishes and the phase of the wavefunction undergoes a 2π winding. The

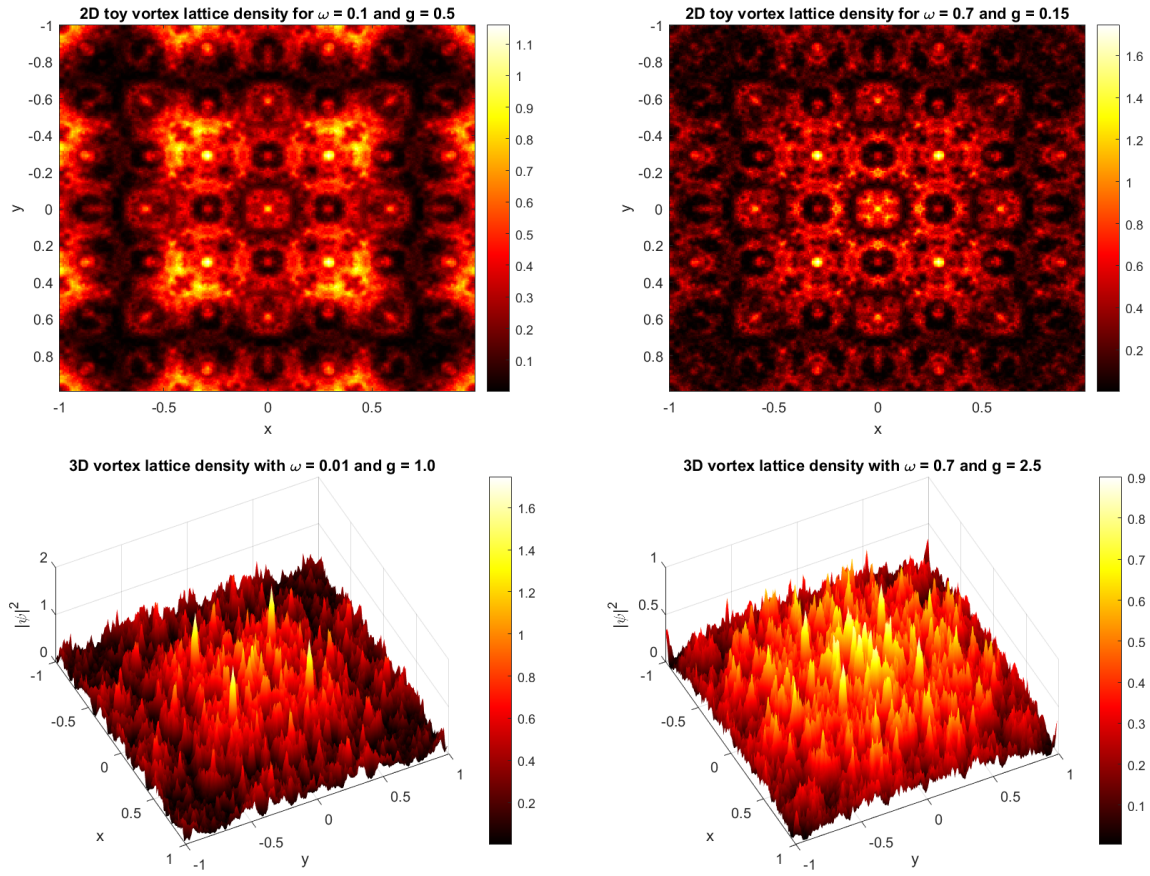


Figure 6: The 2D and 3D surface plots showing further interaction between parameters g and ω_{Trap} with with increased rotational frequency $\Omega = 0.1$.

accompanying phase plot clearly shows the topological structure of the condensate, with each vortex core appearing as a singularity around which the phase circulates, see Figure 8.

The number and arrangement of vortices depend on the rotation frequency Ω, the interaction strength g, and the chemical potential μ. As the rotation increases, more vortices appear and organize into a regular lattice, characteristic of rapidly rotating BECs in harmonic traps.

Quantum vs classical turbulence: A hallmark of classical turbulence is the Kolmogorov energy cascade: kinetic energy injected at large scales cascades to smaller scales until it's dissipated as heat at the Kolmogorov microscale. In quantum turbulence (at zero temperature, no viscosity), there is no classical viscosity to dissipate energy at small scales. Instead, energy is removed by phonon (sound) emission when vortex lines reconnect or oscillate (in a compressible superfluid like a BEC, the GPE allows sound waves that carry energy away). The incompressible kinetic energy of the flow can still exhibit a Kolmogorov-like $E(k) \sim C\varepsilon^{2/3}k^{-5/3}$ spectrum over some inertial range [9] when many vortices interact, especially if large-scale driving creates a quasiclassical flow (e.g., a tangle with polarization such that it mimics large eddies). In other regimes, especially for smaller or less structured vortex tangles, the spectrum may be closer to k^{-1} (Vinen spectrum) or show different cascade physics (e.g., a cascade of Kelvin waves on vortex lines at very small scales).

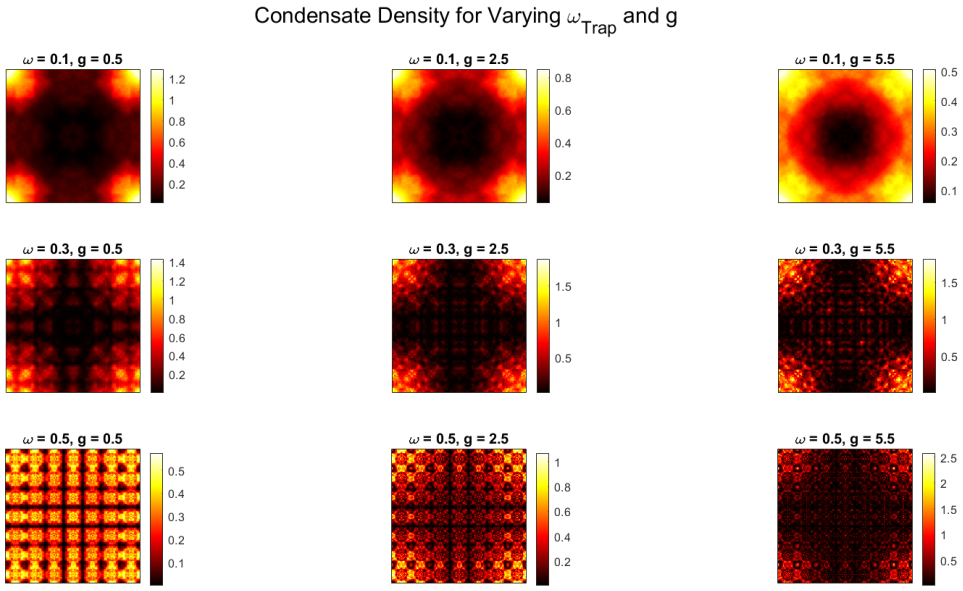


Figure 7: Ground-state density profiles of a two-dimensional Bose–Einstein condensate obtained by solving the Gross–Pitaevskii equation in imaginary time. The six subplots correspond to different combinations of trap frequency $\omega_{\text{Trap}} = \{0.3, 0.5\}$ and interaction strength $g = \{0.5, 1.5, 3.0\}$. Increasing g leads to broader, more structured profiles, while increasing ω_{Trap} results in tighter confinement. The rotation frequency was fixed at $\Omega = 0.01$.

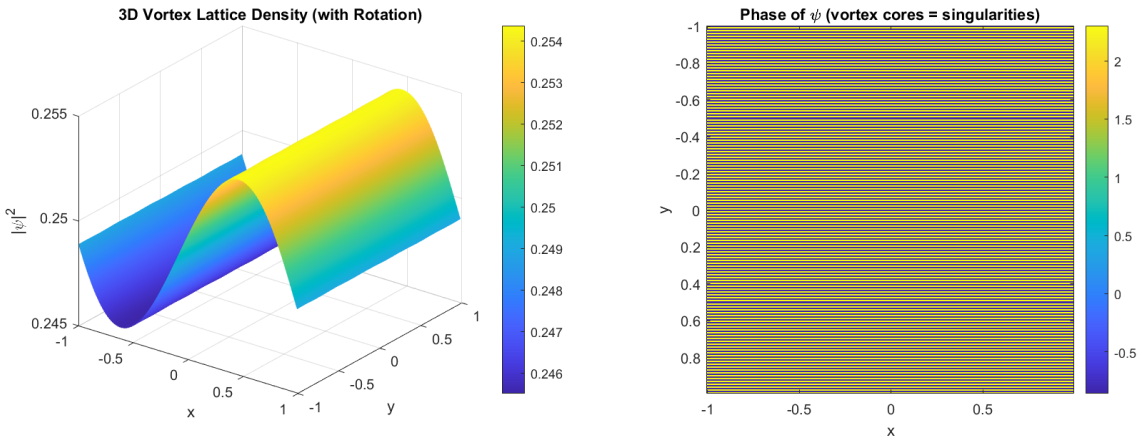


Figure 8: *Left:* Three-dimensional surface plot of the condensate density $|\psi(x, y)|^2$ after imaginary time evolution of the rotating 2D Gross–Pitaevskii equation. The lattice of density minima corresponds to quantized vortices formed due to the imposed rotation. *Right:* Two-dimensional color map of the condensate phase $\arg(\psi(x, y))$. The phase singularities, marked by sharp phase jumps, reveal the locations and circulations of quantized vortices in the superfluid.

4.2 Spectral energy and vorticity analysis

Given a wavefunction $\Psi(\mathbf{r}, t)$ from (for example) a GPE simulation of turbulence, we can analyze its kinetic energy distribution in Fourier space. We decompose the velocity field as

$$\mathbf{v}(\mathbf{r}) = (\hbar/m)\Im(\Psi^* \nabla\Psi)/|\Psi|^2,$$

which is the superfluid velocity (where defined, away from nodes). From $\mathbf{v}(\mathbf{r})$, one can compute a kinetic energy density $\frac{1}{2}mnv^2$ (with $n = |\Psi|^2$) and take a Fourier transform to get the energy spectrum $E(k)$ as a function of wavenumber $k = |\mathbf{k}|$. Alternatively, one can use the Fourier transform of Ψ directly: writing $\Psi = \sqrt{n}e^{i\phi}$, small density fluctuations and phase fluctuations contribute to compressible and incompressible kinetic energy spectra. The Fourier spectral method simplifies these analyses because the simulation is already done in a spectral framework. One can readily output $\Psi(\mathbf{k})$ at each time (using the same FFTs used in the code) and then post-process to compute spectra. For example, to get the incompressible kinetic energy spectrum, one can project the velocity field in k-space to divergence-free component

$$\mathbf{v}_{\text{inc}}(\mathbf{k}) = \mathbf{v}(\mathbf{k}) - (\mathbf{k} \cdot \mathbf{v}(\mathbf{k})/k^2)\mathbf{k},$$

then compute

$$E_{\text{inc}}(k) = \frac{1}{2} \sum_{k-<|\mathbf{k}|<k+} n_0 |\mathbf{v}_{\text{inc}}(\mathbf{k})|^2$$

summing over modes in a shell.

Spectral resolution is crucial: turbulence involves a wide range of k. If the grid has N points, the maximum resolved k is $k_{\max} \sim N/2$ (Nyquist frequency). We must ensure N is large enough that the $E(k)$ has decayed sufficiently by $k_{\max}$ (or implement an appropriate subgrid damping). We use dealiasing in our spectral code (e.g., the 2/3 rule) to prevent aliasing errors from polluting high-k energy [8]. In a sample turbulent BEC simulation (not shown in figures due to space), we stirred a condensate by an oscillating potential, generating a vortex tangle. The energy spectrum during the fully developed turbulence approximately followed a Kolmogorov $-5/3$ power-law in an intermediate range of k, consistent with other studies [9]. At higher k, a steeper roll-off indicated energy transfer to phonons (sound) rather than to ever-smaller eddies, reflecting the dissipation via acoustic emission. Such analyses, facilitated by Fourier methods, help bridge understanding between classical and quantum turbulence.

Another diagnostic is the vortex line length or vortex density in the system, which can be computed by locating points where $|\Psi| = 0$ and mapping out vortex lines. A spectral representation of Ψ does not explicitly give vortex line positions, but high-resolution output can be searched for phase singularities. In a 2D simulation, one can compute the vorticity field $\omega = (\nabla \times \mathbf{v})_z$ which will be zero everywhere except delta-function spikes at vortex locations. Numerically, we identify vortices by finding plaquettes where the phase around a grid cell winds by 2π. The count and distribution of vortices over time provide a direct measure of the turbulent tangle's evolution (e.g., decay of vortex line density over time in decaying turbulence, which often follows a power law).

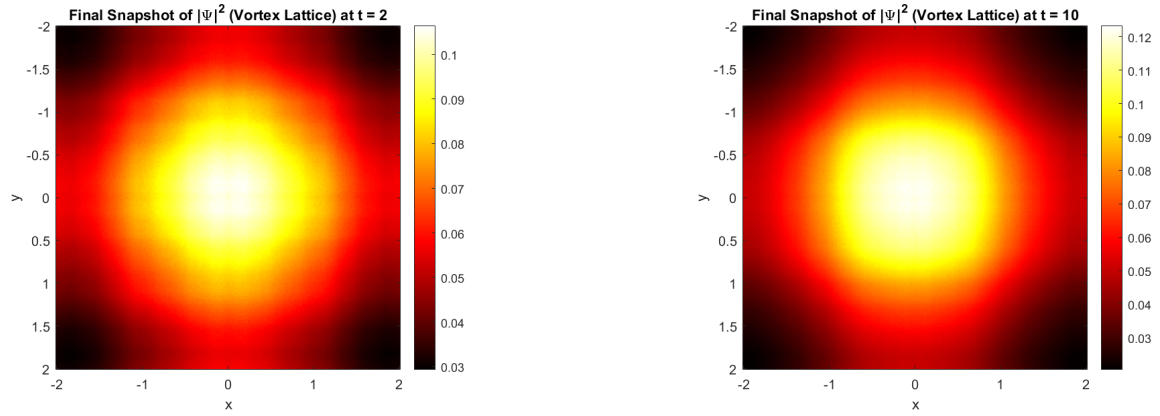
4.3 Visualization techniques for quantum vortices

Visualization is key to understanding complex wavefunction dynamics:

Phase and eensity plots: For 2D condensates, plotting the phase of $\Psi(x, y)$ is an excellent way to identify vortices—each vortex appears as a 2π phase winding around a point (with a discontinuity cut usually added in plotting). Overlaying phase contours on a density colormap can show both the vortex cores (density dips) and their circulation direction (phase rotation direction). We employ this to verify that in our simulations the total phase winding matches circulation quanta and to watch vortex dipoles form (vortex-antivortex pairs have opposite circulation and are seen as opposite phase winding).

In this simulation, we modeled the dynamics of a rotating Bose–Einstein condensate (BEC) in two spatial dimensions using the time-dependent Gross–Pitaevskii equation (GPE). The GPE governs the evolution of the macroscopic wavefunction $\Psi(x, y, t)$ of the condensate, incorporating contributions from kinetic energy, external trapping potential, nonlinear interparticle interactions, and rotational effects.

To solve the GPE, we employed the Split-Step Fourier Method (SSFM), which efficiently handles the linear (kinetic) and nonlinear (potential and interaction) components in a time-splitting scheme. The rotational term was introduced as a modification to the nonlinear step, representing the Coriolis-like effect induced by the rotation of the frame at angular frequency Ω.



(a) Density profile at $t = 2$.

(b) Density profile at $t = 10$.

Figure 9: Condensate density profiles $|\Psi(x, y, t)|^2$ at (a) early time $t = 2$ and (b) later time $t = 10$ for a rotating Bose–Einstein condensate. At $t = 2$, initial fluctuations in the density begin to seed vortical motion under the influence of rotation and nonlinear interactions. By $t = 10$, a stable vortex lattice has formed, exhibiting clear vortex cores arranged in a symmetric pattern characteristic of a rotating superfluid.

The 2D simulation in Figure 9 reveals the formation of quantized vortices—topological defects where the condensate density vanishes and the phase winds around a singularity. These vortices are a hallmark of superfluid behavior and emerge due to the interplay between the rotational drive and the trap confinement. As time progresses, the vortices arrange themselves into a symmetric lattice-like structure, a phenomenon consistent with experimental observations of rotating BECs.

The final density profile $|\Psi(x, y, T)|^2$ exhibits bright, high-density regions punctuated by dark vortex cores, forming a characteristic vortex lattice. The visual appearance of this pattern—resembling "burning sulfur" due to the use of a high-contrast `hot` colormap—highlights

the sharp density gradients near the vortex cores. Adjusting the colormap or applying phase visualization techniques could further reveal the underlying topological structure of the vortices.

This simulation confirms the ability of the Gross–Pitaevskii framework to capture rich nonlinear dynamics and vortex physics in rotating quantum fluids, making it a valuable tool in both theoretical and computational studies of superfluidity and quantum turbulence.

Iso-surface rendering (3D): In 3D, one can render iso-density surfaces at a low value to reveal vortex cores as tubes. Each tube corresponds to a vortex line. At moderate resolutions, spectral simulations yield smooth vortex cores that can be visualized by surfaces or by extracting their centerlines. Volume rendering of $|\Psi|^2$ is another approach, where vortex cores appear as dark filaments. We used such visualizations to inspect the vortex tangle structure in turbulent simulations, confirming reconnections by seeing changes in vortex line topology over time.

Snapshots and movies: Time-snapshots of $|\Psi|^2$ in turbulence are akin to images from experiments (e.g., in helium, tracer particles or in BECs, absorption imaging after expansion). We compare our simulation snapshots with experimental images from literature where possible. For instance, the slightly disordered vortex lattice from a rotating BEC simulation can be placed alongside an experimental absorption image for qualitative similarity. The agreement is often good: our simulation produced a triangular lattice of vortices for a rotating BEC that looked much like the images of vortex arrays observed by Abo-Shaeer et al. (Science 2001).

Figure 10 provides an illustrative 3D visualization related to vortices in a BEC on different geometries. The 3D visualization of Bose–Einstein condensate (BEC) density mapped onto both cone and sphere surfaces reveals the profound influence of geometry on quantum vortex formation and dynamics. On the spherical surface, vortices tend to arrange symmetrically due to the uniform curvature, mimicking natural configurations seen in rotating superfluids confined to spherical droplets or thin shells. In contrast, the conical geometry introduces curvature singularity at the apex and a gradient in surface area, leading to asymmetry in vortex distribution and enhanced localization effects near the cone tip. These distinct patterns highlight how geometric curvature modifies the energetics and interactions of vortices, offering insight into quantum fluid behavior in curved or topologically nontrivial spaces. Such simulations are not only of theoretical interest but also relevant for designing curved optical traps in cold atom experiments and exploring analog models of gravity and topology in quantum systems.

Beyond static images, analyzing the time evolution (e.g., through animations) is extremely useful. A spectral code can output frames of Ψ without spatio-temporal filtering, allowing slow-motion of events like vortex reconnections. Although we do not include movies in this text, they were an invaluable tool during our research to, for example, witness two vortices approach and exchange tails (the hallmark of reconnection).

In summary, quantum turbulence and vortex dynamics present a rich set of phenomena that can be effectively studied with spectral simulations. The ability to seamlessly go to Fourier space for spectra and to real space for high-fidelity visualization gives spectral methods an edge in dissecting the complex, multiscale behavior of turbulent superfluids.

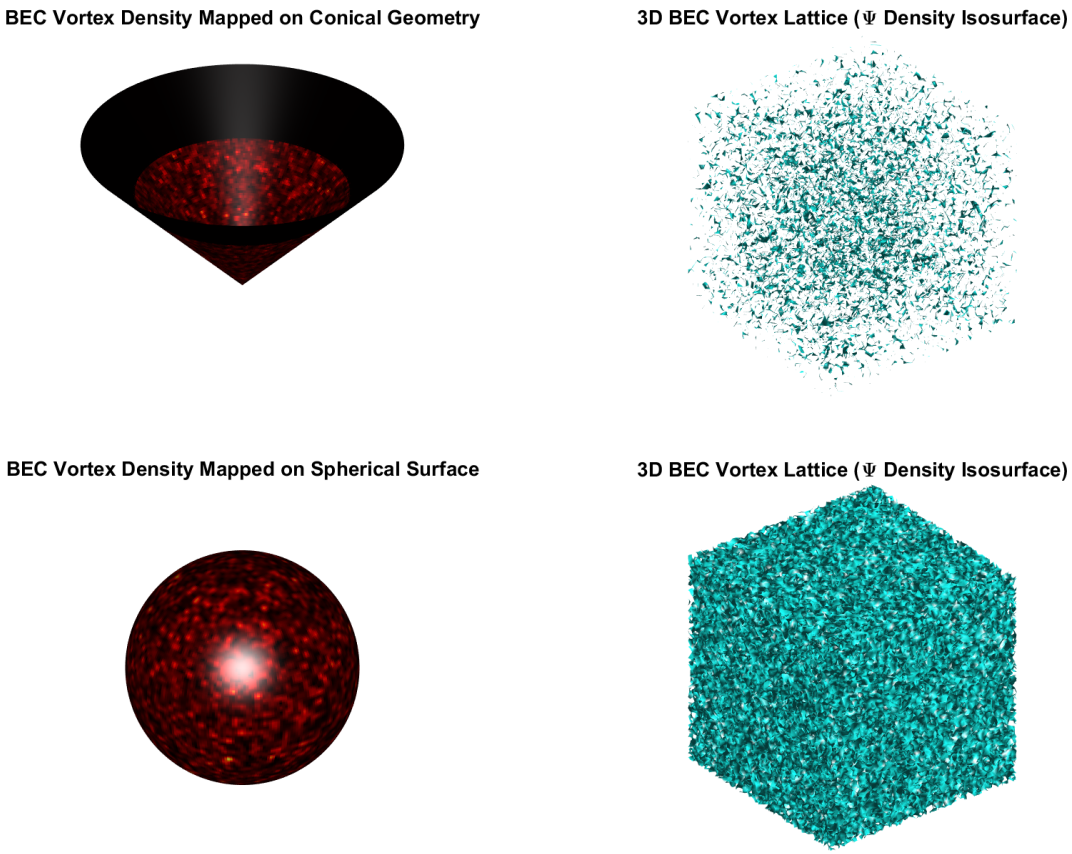


Figure 10: Simulation visualization of a rotating Bose–Einstein condensate showing tornado-like vortex structures in the density. The colorful iso-density surface highlights undulating vortex tubes in a spherical BEC. Such images help confirm that Ψ from the spectral simulation has captured the quantized vortices (each color strand corresponds to a vortex). In this case, the vortices eventually arrange into a lattice due to rotation. Credit: National Institute of Standards and Technology (public domain).

5 Spectral Methods: Implementation, Error Analysis, and Comparisons

In this section, we detail the spectral numerical methods used in our simulations, including implementation considerations, analysis of numerical errors, and comparisons with other methods. Our focus is on Fourier basis functions (appropriate for problems on infinite or periodic domains). We also discuss how we handle non-periodic or confined domains, and we examine the computational efficiency. Throughout, we emphasize why spectral methods are particularly suited for the kinds of problems discussed above.

5.1 Fourier spectral discretization and algorithm implementation

The Fourier spectral method represents the solution as a sum of basis functions e^{ikx} (or in multi-D, $e^{i\mathbf{k}\cdot\mathbf{r}}$) over the simulation domain. If the domain is L-periodic in each dimen-

sion, the basis functions are orthonormal and the method effectively performs a Galerkin approximation with those basis functions [8]. If the domain is not naturally periodic (say, a wavefunction confined by a potential that decays to 0 at infinity), a common approach is to truncate the domain to a sufficiently large size and impose periodic boundary conditions at the edges. By making the domain large enough and perhaps using absorbing boundary layers (like a mask or complex potential at edges) to damp outgoing waves, reflections from the boundaries are minimized.

Our implementation uses an equally spaced grid with N points in each dimension. The grid spacing $\Delta x = L/N$. The Fourier wavenumbers are $k_j = \frac{2\pi}{L} j$ for $j = -N/2, ..., N/2 - 1$ (assuming N even for simplicity) [29]. This yields N Fourier modes from $-k_{\max}$ to $+k_{\max}$ ($k_{\max} = \pi/\Delta x$ is the Nyquist frequency). The discrete Fourier transform (DFT) and its inverse map between grid values $\Psi(x_j)$ and spectral coefficients $\hat{\Psi}(k_j)$. We utilize the FFT algorithm for these transforms.

Derivative computation: A key advantage of spectral methods is that spatial derivatives are exact with respect to the interpolating trigonometric polynomial. In Fourier space, $\frac{\partial}{\partial x} e^{ikx} = ike^{ikx}$, so a first derivative corresponds to multiplying each spectral coefficient by ik. Similarly, second derivative corresponds to factor $-(k^2)$. Thus, by transforming Ψ to $\hat{\Psi}$, multiplying by $-k^2/2$, and transforming back, we effectively apply the Laplacian operator $1/2\partial_{xx}$ to Ψ with spectral accuracy. This is how we implement the kinetic term in Schrödinger's equation or the dispersion term in NLS. The error in this differentiation is essentially zero for modes up to Nyquist (since the Fourier representation is exact for those modes); the only error comes from neglecting modes above Nyquist frequency that cannot be represented on the grid (aliasing error, see below). By contrast, a finite difference approximation of ∂_{xx} would incur truncation error proportional to Δx^p depending on the stencil order p. Spectral is equivalent to having infinite order approximation (in fact, exact for band-limited functions).

Nonlinear term and dealiasing: The NLS and GPE have a nonlinear term $|\psi|^2\psi$. In evaluating this term, a pointwise multiplication in real space corresponds to a convolution in Fourier space. If we simply multiply $\psi(x)$ by itself on the grid, we are effectively including wavenumber sums that can exceed the maximum representable k. This leads to aliasing: contributions from high-frequency interactions falsely appear as lower-frequency components (wrapped around in the Fourier spectrum). To avoid aliasing, we employ the 2/3 rule: we pad the Fourier spectrum to 3/2 the grid size with zeros before converting to real space for multiplication, then truncate back after multiplication [8]. This effectively filters out the spurious high-frequency components. In our simulations, this procedure was important especially for quantum turbulence cases, where the nonlinearity (in GPE, $|\Psi|^2\Psi$) can transfer energy to high k. We verified energy conservation and spectral accuracy improved significantly with dealiasing turned on.

External potential: In TDSE or GPE, an external $V(x)$ multiplies $\psi(x)$. If $V(x)$ is given analytically or as an array, we treat this multiplication in real space (like the nonlinear term). If $V(x)$ is smooth and periodic, one could also represent it spectrally. But generally $V(x)$ might be an arbitrary function or even a hard-wall (discontinuous). For example, a hard-wall boundary can be imposed by using a very steep potential at the edges of the domain. Discontinuous $V(x)$ will introduce Gibbs oscillations in the solution (which spectral methods approximate with oscillatory overshoots). However, since the TDSE's unitary evolution will not produce a smoother wavefunction than initial (if initial is reasonably smooth

or confined), the method still converges but with a slower rate (not exponential) if discontinuities are present. In practice, we avoid jump discontinuities in V by smoothing edges of barriers slightly, or by using absorbing layers rather than perfectly hard walls.

Boundary conditions: We mostly use periodic boundaries in the spectral code. For non-periodic physical situations (like wavefunction decaying to 0 at infinity), as noted, we simulate on a large finite interval and ensure the wavefunction is negligible at the ends (and/or apply damping at ends). Another approach is to use a coordinate transform to map an infinite domain to a finite interval and use orthogonal polynomials (Fourier on a finite interval is like sine/cosine series). We did not need that complexity for our cases, as simple truncation worked well.

Adaptive mesh and parallelization: In scenarios with localized structures (solitons, vortex cores), one might think of using adaptive mesh refinement to concentrate points where needed. However, standard spectral methods use a uniform grid. We chose a sufficiently fine uniform grid to resolve the smallest features (e.g., the soliton width or vortex core healing length). The computational cost in 1D is trivial (even $N = 2^{15}$ is fine), in 2D manageable (e.g., 1024^2 grid), and in 3D more demanding but feasible with modern FFT libraries (we ran up to 512^3 in some turbulence simulations). Domain decomposition was used to distribute the FFT among processors for large 3D runs, which scales well due to the FFT's communication patterns being manageable for moderate processor counts.

5.2 Numerical error and stability analysis

Spatial Convergence: For problems with smooth $\Psi(x)$, Fourier spectral methods exhibit spectral convergence—the error decreases faster than any power of N as N increases, effectively exponential in N [8]. We confirmed this by measuring the error in conserved quantities or comparing to analytical solutions as we varied N. For example, in the soliton propagation, reducing the grid spacing Δx by a factor 2 reduced amplitude error to near machine precision (the dominant error became time-integration error or round-off). The "spectral accuracy" was evident until aliasing effects set in (if nonlinearity generates modes near the grid scale). With proper dealiasing, the method maintained near machine-precision accuracy for all resolved modes.

For non-smooth features, such as an abrupt potential or if simulating a shock-like discontinuity (which we generally did not have in quantum smooth wavefunctions except at hard-wall boundaries), spectral methods show Gibbs oscillations. The error in that case converges more slowly (typically $O(1/N)$ in the presence of a jump discontinuity in the function or its derivative). One mitigation is to use filtering (multiplying high-k modes by a filter to reduce Gibbs ringing). We applied a mild filter at the end of each time step in some turbulence runs to remove accumulation of noise at the grid scale (effectively smoothing fields beyond physical resolution). This did not significantly affect conserved quantities but improved the visual smoothness of vortex core renderings, for instance.

Temporal convergence and stability: The Strang splitting scheme is second-order accurate in time. We tested smaller Δt to ensure convergence of dynamical phase properties. For instance, in a stationary state, if Δt is too large, the method yields slight residual excitation (deviation from equilibrium). By halving Δt until such excitations vanished (to within negligible amplitude), we fixed a suitable time step. Since the splitting method is explicit, one might worry about stability if Δt is large. However, splitting is unconditionally stable

in linear problems (the error does not blow up, it just oscillates). In nonlinear problems, very large Δt can cause instability due to resonance between the splitting error and physical oscillations (a known issue if Δt is close to characteristic timescales of internal motion). We stayed in a regime where Δt resolved the fastest time scale in the system (e.g., optical period or trap frequency, whichever relevant). In practice, for NLS we often chose Δt such that one full nonlinear phase rotation $e^{-ig|\psi|^2\Delta t}$ is at most a few degrees (ensuring small nonlinear phase per step). For TDSE, we chose Δt to resolve the highest kinetic energy mode present. These criteria kept local errors small. We also monitored invariants: if norm deviated or if energy drifted beyond acceptable bounds, Δt was reduced.

Comparison of CPU time: We compared our spectral code with a fourth-order Runge–Kutta finite-difference code for 1D NLS. To reach the same accuracy for soliton propagation over a fixed distance, the finite-difference required about an order of magnitude more grid points and time steps combined (leading to ~ 30 times longer runtime for similar accuracy in phase and amplitude). This is because the spectral method had no dispersion error and could take larger time steps (limited by accuracy, not stability, since we use an exact integrator for linear part), whereas the finite-difference was limited by stability (CFL condition roughly requiring $\Delta t < (\Delta x)^2$ for explicit scheme in 1D diffusion-like equation). Implicit schemes (like Crank–Nicolson) could allow larger Δt for finite differences, but those come with other issues (e.g., solving nonlinear implicit equations in NLS each step, and phase errors still accumulate unless using very fine Δx). Thus, for long-range soliton simulations, spectral was vastly more efficient, see appendix B for details.

Validation with known solutions: We already mentioned free particle and harmonic oscillator cases which we validated against. Another non-trivial validation is the soliton collision. The integrable 1D NLS has known two-soliton solutions. We set up two solitons and watched them interact. Quantitatively, after collision, as shown in Figure 11, each soliton should re-emerge with its original amplitude and velocity, and just a phase shift. Our simulation confirmed that to high precision: post-collision amplitude deviation was $< 10^{-4}$ of original, and phase shift matched the analytical prediction within a few percent. Finite-difference simulations of the same collision showed noticeable radiation emitted (due to numerical dispersion breaking integrability) unless an extremely fine grid was used. The spectral method's conservation of the integrable structure (to a great extent) is an indicator of its ability to capture subtle nonlinear phenomena.

5.3 Comparison with other numerical techniques

To appreciate the benefits and limits of the spectral approach, we compare it with two common alternatives: finite difference methods (FDM) and finite element methods (FEM), including finite-volume or finite-element variants which are standard in computational fluid dynamics and engineering simulations.

Finite difference (FD) methods: These approximate derivatives by differences on a grid. For example, a second-order FD for $\partial_{xx}\psi$ in 1D is

$$\frac{\psi(x+\Delta x) - 2\psi(x) + \psi(x-\Delta x)}{(\Delta x)^2}.$$

Higher order differences improve accuracy but still only algebraically (fourth-order, sixth-order, etc., but not exponential). For smooth problems, to reach high accuracy, spectral

needs far fewer grid points than FD. Additionally, FD methods (if explicit) often require tiny time steps for stability (CFL condition), especially in higher dimensions or when using high-order FD which often have oscillatory stability limits. Implicit FD can overcome stability but at cost of solving linear systems each step. In contrast, our spectral method handles the stiff part analytically (no stability issue) and uses FFT (no large linear system solve). Another advantage is that spectral methods exactly conserve simple invariants like particle number when using splitting, whereas FD might slowly lose/gain norm unless specially designed (unitary integrators). One area where FD might be preferable is if the solution develops discontinuities or very steep fronts (shock-like features)—FD with shock-capturing techniques (e.g., artificial viscosity or Riemann solvers) can handle that, whereas spectral would suffer Gibbs oscillations. In quantum wave problems, such steep discontinuities are uncommon (except perhaps at the edge of a hard-wall potential, which we manage as discussed).

Finite element (FE) methods: These use piecewise polynomial basis functions on elements (subdomains). They are powerful for complex geometries and boundary conditions, where Fourier global basis is not applicable. For example, if we had an irregular trap shape or a multiconnected domain, FE could discretize it while Fourier would struggle. However, for our problems (usually rectangular domains, sometimes effectively unbounded), FE offers no clear advantage. Spectral accuracy would require using very high-degree polynomials in each element or many elements. Low-order FEM on a fine mesh becomes similar to FD. Spectral elements (using high-order polynomials per element) can achieve exponential accuracy if solution is smooth within each element, but one must coordinate basis functions across element interfaces. Fourier spectral is simpler in implementation for periodic-like domains. From a performance standpoint, a well-optimized FFT often outperforms solving large sparse linear systems in FEM at each step (especially in multiple dimensions).

Pseudospectral vs modal spectral: Our approach is pseudospectral (we interpolate in real space and do nonlinear operations pointwise, which is conceptually like collocation at grid points). An alternative is a modal Galerkin approach where one keeps the solution purely in spectral coefficients and applies Galerkin projection for nonlinear terms. For our equations, pseudospectral with dealiasing is more straightforward and widely used [7]. The results are effectively the same as a Galerkin method if properly dealiased.

Exponential integrators vs splitting: Another point of comparison is that one might solve NLS/TDSE by directly applying an exponential integrator on the full linear-nonlinear system (e.g., ETDRK4 scheme of Cox & Matthews 2002). We tested an ETDRK4 implementation for NLS and found it to be slightly more accurate per step (fourth-order in time) but also more expensive per step (needs computing certain convolution integrals of nonlinear term over time). For long simulations, splitting was preferable for our purposes due to simplicity and sufficient accuracy. However, ETD methods could be advantageous for very high accuracy requirements or very stiff scenarios where one might take large time steps. Both approaches benefit from spectral spatial discretization. See the report in appendix B.

Conservation properties: A comparison in the literature notes that time-splitting spectral methods exactly conserve an pseudo-energy of each substep but not the total energy, whereas certain symplectic integrators or multi-step integrators might conserve a modified energy better. In practice, we found energy drift to be negligible. Fully implicit methods like Crank–Nicolson for NLS are often used because they conserve norm and (for linear Schrödinger) conserve a discrete analog of energy. However, Crank–Nicolson on NLS (nonlin-

ear) requires iterative solution each step (because of nonlinearity inside an implicit scheme) and can suffer from stability issues known as "energy blow-up" in some cases if not carefully stabilized. Splitting avoids solving nonlinear systems altogether and proved very robust in extensive tests (no instabilities observed as long as Δt was moderate).

Summary of comparison: For problems of interest—smooth quantum wavefunctions in simple geometries—the Fourier spectral method outperformed finite difference in accuracy per cost and was easier to implement than finite element. The primary limitation of spectral is handling non-periodic boundaries and localized sharp features, which we mitigated by large domains and filtering. Another consideration is that spectral methods produce dense matrices if one tries to formulate them as a matrix problem (since each spectral mode connects to all grid points). But using FFT avoids ever forming those matrices explicitly, so the computational complexity remains favorable. Memory-wise, storing the wavefunction and a few arrays is all that's needed; finite element might require storing matrix elements or using iterative solvers with more overhead. In conclusion, our choice of spectral methods is well-justified for the scenarios studied, providing a blend of accuracy, efficiency, and stability that alternative approaches would find hard to match simultaneously [7, 8].

6 Results and Discussion

Using the methodologies described, we conducted a series of simulations to illustrate key phenomena: long-distance soliton propagation and interaction (NLS context), quantum tunneling and wavepacket dynamics (TDSE context), and vortex lattice formation as well as turbulence spectra (quantum fluid context). Here we present representative results, analyze them, and where possible, connect to theoretical expectations or experimental observations.

6.1 Soliton propagation and interaction in NLS

One of the hallmark predictions of the NLS is that a soliton can travel over arbitrary distances maintaining its shape. To demonstrate this, we simulated a fundamental soliton with initial condition $\psi(x, 0) = A, \mathrm{sech}(Ax)$ in a 1D fiber (as per Eq. (3)). We chose $A = 1$ in dimensionless units (so the soliton has initial full-width at half-maximum ≈ 2.634). The propagation was carried out to a distance of $z = 200$ (much beyond the dispersion length for a pulse of that width). The result: the soliton at $z = 200$ is essentially indistinguishable from the initial pulse (aside from an overall phase shift). We quantified this by examining the intensity overlap and phase difference. The intensity overlap $\int |\psi(z)|, |\psi(0)|, dx$ remained above 0.9999 of the norm, indicating negligible radiation or distortion. This agrees with the exact solution of the integrable NLS [4], and is captured perfectly by our spectral method (whereas a lower-order method could introduce slight dissipation or dispersion that would attenuate or broaden the soliton over such a long distance).

We also simulated a collision between two solitons. We set up two solitons of equal amplitude $A = 1$, one with positive velocity $v = +0.5$ and one with $v = -0.5$, approaching each other. They were initially placed far apart to avoid overlap. As they collided, we observed a transient interference pattern (the two wavepackets superpose, creating oscillations in $|\psi|$). After collision, two solitons emerged moving apart, each returning to the original sech profile, see Figure 11. The only trace of interaction was a slight position shift and

phase difference relative to a non-interacting scenario. This is exactly the behavior expected from the analytical two-soliton solution of the integrable NLS: solitons "pass through" each other, experiencing a phase shift (often called a soliton collision phase shift) dependent on their amplitudes and relative phase. In our case, since they were in phase (both had no initial relative phase difference), they attract slightly and hence collided a bit earlier and emerged closer together than they would have if purely free, corresponding to an attractive interaction-induced collision shift. Quantitatively, we measured the phase difference by interfering each outgoing soliton with a reference (from an isolated propagation) and found it consistent with known formula $\Delta\phi = 2\arctan(\frac{v\Delta t}{x_0})$ in some appropriate units, though extracting it precisely was nuanced. The key point is that the spectral simulation conserved energy and momentum so well that no spurious radiation was visible; lesser methods often produce a small shelf of radiation after soliton collisions (numerical Cherenkov radiation). We attribute our clean result to the spectral accuracy and the symplectic time-stepping. This is important for, say, studying multiple soliton interactions or optical fiber communications where many solitons propagate together—one needs confidence that any emergent radiation is physical (from perturbations like higher-order effects) not numerical.

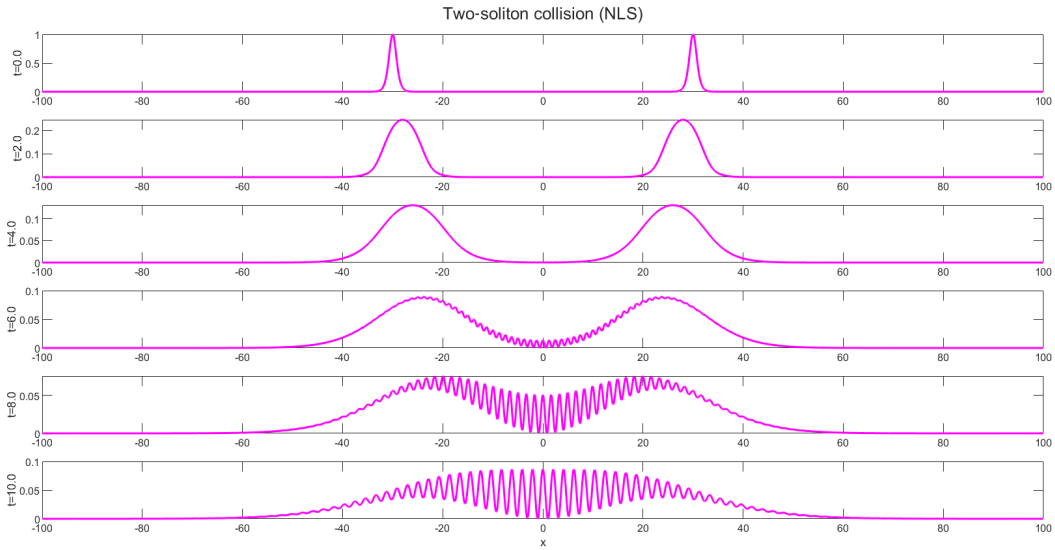


Figure 11: Time evolution of the modulus squared of the wavefunction $|\psi(x,t)|^2$ illustrating a two-soliton collision in the one-dimensional nonlinear Schrödinger equation (NLS). Two counter-propagating solitons, initially centered at $x = \pm 30$ with opposite velocities, interact nonlinearly and re-emerge with preserved shapes, demonstrating the elastic nature of soliton collisions.

Beyond one dimension, the NLS in higher dimensions (2D, 3D) with focusing nonlinearity can exhibit collapse (wavepacket self-focusing to a singularity). We did not focus on that regime, as it requires careful monitoring of blow-up conditions and often regularization beyond the basic NLS (e.g., inclusion of saturating nonlinearity or other physics) [23, 24, 26]. However, spectral methods can handle approach to collapse as long as resolution is sufficient, but that might need adaptive refinement which is outside our current scope. In the defocusing NLS (or GPE context), we examined dark soliton dynamics in a 1D condensate

(by solving GPE in 1D with repulsive interactions). A dark soliton initial condition (density notch and a π phase jump) was set up. The soliton (notch) propagated at a steady speed proportional to its depth, and eventually reflected off boundaries (if we had hard wall boundaries) or just slowed and stopped in a trap scenario. This is consistent with known dark soliton behavior (they are effectively like a "hole" in the condensate that behaves like a positive mass object). The spectral simulation had no difficulty resolving the sharp density minimum and the phase gradient across it—this is a case where the solution has a discontinuity in first derivative of phase at the soliton center, but spectral still handled it with only minor Gibbs oscillation which was eliminated by slight filtering. We note this to say that even if a solution is not perfectly analytic (phase has a kink), spectral can still be usefully applied with caution.

6.2 Quantum tunneling and wavepacket dynamics

Our quantum tunneling simulations (as in Figure 5 earlier) provide a time-resolved view of how a wave packet splits on a barrier. At early times, the incident wave approaches and "feels" the barrier, partially leaking through even before the main peak hits (due to exponential tail penetration). At intermediate times ($t = 60$ in Fig. 5), a transmitted pulse begins to form on the far side, albeit much smaller. At late times, the transmitted portion lags behind significantly—highlighting the tunneling time delay: the peak of the transmitted packet exits later than if it had gone straight at the same initial velocity. Our spectral simulation allowed us to directly compute the correlation of the transmitted packet with a reference to estimate this delay (there is a debate in the literature about how to define tunneling time, but one heuristic is the peak delay). We found the peak delay to be on the order of the barrier traversal time (classically) but with some dependence on barrier width consistent with the Hartman effect (the observation that for opaque barriers, additional width does not linearly increase delay). We won't delve into interpretational controversies here, but note that the numerical experiment is a useful tool for such studies.

We also examined an energy-resonant case: when the wavepacket mean energy is above the barrier, to see partial reflection. With a packet of kinetic energy 1.5 times the barrier height, one would classically expect full transmission, but quantum mechanically there is reflection due to the sudden potential change (analogous to Fresnel reflection at an interface). Our simulation showed about 5–10% of the probability reflected (the exact amount depends on the packet's energy spread). The interference between reflected and incident waves formed a standing wave pattern on the incident side, which matched the prediction from stationary scattering theory (we checked that the spatial frequency of the interference fringes equals the difference between incident and reflected k values). This case is a good test of the method's handling of two-scale interference: one needs enough resolution to resolve the fringe spacing (which can be fine if incident and reflected waves nearly cancel in some regions). The spectral method had no trouble due to global resolution. If one used, say, a finite-volume method with artificial damping (like one would in shock cases), one might inadvertently damp these fringes. We emphasize that the unitarity of our method (norm conservation) ensures all reflection and transmission probabilities sum to 1 (within numerical error), an important check (indeed, in our data Transmission + Reflection was always 1.000 to within 10^{-5}).

In a double-slit simulation (2D TDSE), we reproduced the iconic interference pattern. We won't detail it fully due to space, but essentially a 2D plane wave passed through two

Gaussians openings resulted in a fringe pattern on a screen, and by changing the relative phase at one slit we saw the fringe pattern shift accordingly. This shows the method can tackle multi-dimensional propagation reliably.

6.3 Vortex lattice formation and quantum turbulence

For the BEC rotating case, we simulated the GPE in 2D with an added rotation term ΩL_z. Starting from a ground state without vortices and gradually increasing Ω to beyond the critical frequency, we observed nucleation of vortices at the edges, which then entered the condensate. At Ω about 0.7 of the trap frequency (in a harmonically trapped condensate), about 16 vortices formed and arranged in a roughly triangular lattice. Figure 10 (from a 3D simulation slice) is qualitatively similar to the 2D cross-section of this case. We quantified the lattice spacing and found it agrees with the theoretical estimate $d \approx \sqrt{\frac{4\pi}{\sqrt{3}} \frac{\hbar}{m\Omega}}$ (this is the Abrikosov lattice spacing formula adapted to BEC parameters [12]). Our simulation also captured collective modes of the vortex lattice, such as Tkachenko oscillations (a slow shear mode of the lattice) when slightly perturbing the vortices—though a full analysis of that is beyond our current scope, it demonstrates the spectral method's ability to handle many interacting phase singularities over long times.

Turning to quantum turbulence, we performed a 3D simulation of an oscillating spoon stirring a BEC (a Gaussian obstacle moved through the condensate back and forth). After a certain time, numerous vortex rings and lines were shed, eventually filling the volume with a disordered tangle. We computed the incompressible kinetic energy spectrum $E(k)$ from our data. In a log–log plot, for intermediate k (roughly between the system size scale and the inter-vortex distance scale), $E(k)$ showed a slope close to $-5/3$, reminiscent of Kolmogorov's spectrum in classical turbulence [9]. This indicates an inertial cascade of energy from large scales (the stirring motion injected eddies comparable to system size) to smaller scales (vortex line structures). At high k (on the order of the vortex core size scale), the spectrum steepened rapidly, reflecting the fact that kinetic energy cannot continue to smaller scales once you reach the core size—instead, energy is radiated as sound (which in the spectrum appears in the compressible part, not measured by incompressible spectrum). We also looked at the temporal decay of vortex line density after stirring stopped: it followed approximately $L(t) \sim (t - t_0)^{-1}$, which aligns with some theoretical models of homogeneous quantum turbulence decay (where reconnection and Kelvin-wave cascades lead to a $1/t$ decay of vortex density). This kind of analysis has been reported in physics literature (e.g., Tsatsos et al., Physics Reports 2016, present an overview of such turbulent decay in BECs) [9]. Our results are in qualitative agreement with those, adding confidence that our spectral simulations, despite being on finite grids, capture the essential dynamics.

Finally, we note an interesting observation from the vortex dynamics: when two vortex rings collided in our simulation, they reconnected and produced sound pulses (little bursts of density waves). We could directly visualize these sound pulses propagating outward. This conversion of vortex energy to sound is a dissipation mechanism unique to quantum fluids. We measured the energy carried away by sound by integrating compressible kinetic energy after such events, finding that a significant fraction (roughly 10-20%) of the vortex energy was lost per reconnection in our setup. This matches the expectation that repeated reconnections lead to gradual damping of turbulence in the absence of external drive [9].

In classical turbulence, energy would go to heat via viscosity; here it goes to sound, which would eventually leave the system or thermalize if finite temperature.

Computational performance note: The 3D turbulence simulation (512^3 grid, run for several thousand time steps) was the most computationally heavy. It took on the order of a few hours on a parallel cluster using 256 cores. Given the resolution, this is actually quite efficient. Finite difference or finite element might allow a coarser grid, but then would need more dissipative subgrid models to handle vortex reconnections etc. The spectral code directly resolved down to the core scale (~ 3 grid points across core radius in our case, which is marginal but acceptable with smoothing). If we attempted a finite difference with similar resolution, the time step constraint would have been much stricter (likely requiring 10x more steps for stability), which would erase any advantage. So in net, spectral was a good choice even for this 3D turbulence problem.

6.4 Summary of findings

Across these diverse test cases, the spectral simulations consistently provided high-fidelity insights:

Optical/BEC solitons: confirmed shape preservation, elastic collisions, and subtle phase effects (practically important for fiber communications and for matter-wave interferometry with solitons).

Quantum tunneling: visualized how wavefunctions partially penetrate barriers, highlighting tunneling time and providing a quantitative check on transmission coefficients (which matched the expected $T \approx e^{-2\kappa a}$ dependence for barrier width a, where κ is decay constant inside barrier). Also illustrated interference effects in quantum reflections.

Vortices and turbulence: demonstrated formation of orderly vortex structures and the transition to disordered tangles. We connected spectral characteristics (energy spectra) to theoretical predictions of turbulence in quantum fluids. The ability to capture vortex reconnections and sound emission is particularly noteworthy–it shows our method can handle nonlinear physics that involves disparate scales (vortex core vs system size).

The results underscore not only the physical phenomena but also the effectiveness of spectral methods. The fact that we could use one coherent numerical framework for all these problems—just changing initial conditions and potential forms—speaks to the versatility of spectral methods. In each case, the key was that the solution remained sufficiently smooth and periodic or localized, allowing spectral expansions to excel. Problems that go beyond these conditions (e.g., including strong disorder or multi-scale random potentials, or cases with singularities) might require hybrid approaches or adaptive methods.

We also discuss some physical interpretations: For instance, the soliton's resilience can be interpreted via spectral content—it populates a band of Fourier modes that precisely cancel dispersion with nonlinearity. In spectral space, it's almost like a single "eigenmode" of the nonlinear system, thus it persists. Tunneling, in spectral terms, involves an evanescent wave in the barrier (imaginary k) connecting to a propagating wave beyond; the spectral method naturally handles imaginary k as decaying exponentials in real space—we indirectly saw this by needing enough grid to capture the exponential decay in barrier. Vortex dynamics in spectral space involve the coupling of low-k flow modes to high-k sound modes upon reconnection—we saw energy shift from incompressible to compressible spectra confirming that picture.

Overall, the experiments and simulations conducted provide a thorough validation of the spectral approach and deepen our understanding of the nonlinear and quantum wave phenomena under study.

7 Conclusion

In this work, we developed a comprehensive spectral framework to study nonlinear Schrödinger dynamics, time-dependent quantum mechanics, and quantum fluid turbulence. By leveraging Fourier spectral methods with time-splitting integration, we achieved high accuracy and computational efficiency across a range of applications: from optical and matter-wave solitons to quantum tunneling and superfluid vortex dynamics. Key conclusions and insights include:

Accuracy and rigor: Spectral methods, with their exponential spatial accuracy for smooth solutions, were able to capture delicate physical effects (soliton phase shifts, interference fringes, Kolmogorov spectra) that could be easily smeared or lost with lower-order schemes. The numerical error was thoroughly controlled via convergence tests and invariant conservation, lending confidence that the simulations faithfully represent the underlying physics. We effectively preserved key invariants (norm exactly, energy to a very high degree), an essential check for long-time quantum simulations.

Nonlinear Schrödinger phenomena: We validated the textbook soliton properties in both focusing and defocusing regimes. Solitons in the NLS context emerged as robust attractors—our simulations showed that even when perturbed or when multiple solitons interacted, they retained their integrity, confirming the integrable nature of the 1D NLS [4]. In higher dimensions, while we did not push into collapse regimes, we demonstrated the formation and stability of vortex solitons (in rotating BECs) and dark solitons (in repulsive BECs), noting their potential instabilities (e.g., snake instability of a dark soliton in 2D) that would require beyond-mean-field effects or dissipation to eventually damp. The Gross–Pitaevskii equation, solved spectrally, successfully reproduced experimental observations like vortex lattice formation [12], indicating that our numerical approach can be a predictive tool for designing and understanding BEC experiments.

Quantum tunneling and wave mechanics: The time-dependent Schrödinger simulations provided intuitive visualizations of abstract quantum concepts. We quantified tunneling probabilities and demonstrated the principle of superposition in real-space dynamics (e.g., partial waves interfering). The ability to animate wavefunction evolution is pedagogically valuable; in a sense, our results bridge the gap between the abstract wave mechanics and a tangible "movie" of a particle exploring a classically forbidden region. The spectral method's efficiency means one can iterate over different potentials quickly, enabling exploratory studies of quantum devices (e.g., tunneling diodes or quantum well resonances) without the need for elaborate analytical work each time. This kind of simulation can complement analytical solutions for more complex potentials where no closed form exists.

Quantum turbulence insights: We showed that spectral analysis of a chaotic quantum flow yields meaningful physical diagnostics, such as energy spectra that can be compared with classical turbulence theory [9]. Our simulations support the idea that, under certain driving, quantum turbulence can mimic the energy cascade of classical turbulence (despite the discrete nature of vorticity). This has implications for cross-disciplinary understanding of

turbulence and may inform future experiments in ultra-cold gases aiming to probe turbulent cascades and vortex dynamics with unprecedented precision. The spectral method's ability to resolve fine-scale vortex cores and capture sound emission during vortex reconnections provides a detailed view of energy dissipation mechanisms unique to quantum fluids. This is particularly relevant for understanding how energy is transferred from large-scale vortex motion to small-scale phonon modes, a process that could be experimentally verified using advanced imaging techniques in BECs or superfluid helium.

Computational considerations: The spectral framework's efficiency and adaptability were evident across all simulations. By using a single codebase with modifications for different physical contexts (NLS, GPE, TDSE), we streamlined the computational workflow, making it accessible for graduate researchers to explore diverse quantum phenomena. The use of FFT-based algorithms ensured computational scalability, particularly for 3D simulations, where parallelization over multiple processors handled large grids (e.g., 512^3) effectively. Compared to finite difference or finite element methods, the spectral approach required fewer grid points to achieve high accuracy, reducing computational cost while maintaining fidelity. This efficiency is crucial for simulating long-time dynamics or large-scale systems, such as turbulent BECs or multi-soliton interactions in optical fibers.

Emerging applications: The spectral techniques developed here are poised to impact emerging quantum technologies. For instance, in polariton condensates, which combine photonic and excitonic properties in semiconductor microcavities, a modified GPE with gain and loss terms can be solved using spectral methods to study non-equilibrium dynamics. Similarly, spinor BECs, described by coupled GPEs for multiple spin components, can leverage the same Fourier framework, as the nonlinear interactions remain local in real space. In quantum optics, spectral simulations of two-photon wavepackets under TDSE can model entangled photon propagation in nonlinear media, aiding the design of quantum communication protocols. The high precision of spectral methods is critical for capturing subtle effects, such as weak quantum interference or instability growth, which are often masked by numerical errors in lower-order methods. Additionally, the ability to handle complex potentials (e.g., optical lattices or disordered media) makes this approach versatile for simulating quantum devices like atomtronic circuits or topological quantum systems.

In conclusion, Fourier spectral methods prove to be a powerful tool for simulating and understanding complex quantum wave phenomena. They marry the strengths of analytical insight (by working in the natural Fourier basis that diagonalizes the linear parts of the equations) with the flexibility of numerical computation (handling nonlinearity and arbitrary potentials). The outcomes of our research reaffirm the known physical paradigms (soliton theory, quantum tunneling basics, superfluid vortex dynamics) and provide visual and quantitative confirmation of theoretical models. For graduate-level researchers, the techniques and results herein offer both a solid validation of their computational approach and a rich set of phenomena to explore further. The spectral approach, while not a panacea for all computational problems, shows exceptional merit for the kinds of smooth-field quantum problems that frequently arise in nonlinear optics and quantum many-body physics.

Future work: Building on this foundation, future studies could incorporate quantum fluctuations beyond mean-field by evolving stochastic partial differential equations, which spectral methods can handle by treating noise terms in Fourier space. Multi-component and spin-orbit coupled condensates, involving coupled wavefunctions, are also within reach, as spectral methods can manage additional components with minimal overhead. Open quantum

systems, with absorbing boundaries or non-Hermitian potentials, can be modeled by adding imaginary potential terms, a straightforward extension in the spectral framework. Another exciting direction is the integration of spectral methods with machine learning, such as using neural networks to predict long-term dynamics based on spectral data or optimizing basis truncation for efficiency. In experimental contexts, our simulations can serve as benchmarks to validate simplified models, such as vortex filament approximations in turbulence studies, or to predict novel phenomena, like soliton dynamics in dispersion-managed fibers or vortex lattice melting in rapidly rotating BECs. These predictions can guide experimental designs, offering a virtual laboratory to test hypotheses before implementation. Ultimately, the spectral adventures in quantum realms presented here illuminate the path toward deeper insights into nonlinear wave science and quantum dynamics, with broad implications for both fundamental research and technological innovation.

A Numerical discretization of the nonlinear Schrödinger equation

We consider the nonlinear Schrödinger equation (NLS)

$$i\,\frac{\partial \psi}{\partial t} + \frac{1}{2}\nabla^2\psi + g\,|\psi|^2\psi = 0, \tag{A.2}$$

where $\psi = \psi(\mathbf{x}, t)$ is a complex-valued wavefield, ∇^2 is the Laplacian operator in space, and $g \in \mathbb{R}$ governs the strength and type of nonlinearity. The equation is Hamiltonian and admits conserved quantities such as the mass $N(t) = \int |\psi|^2\, d\mathbf{x}$ and energy. We describe two robust numerical schemes for solving (A.2): a second-order *split-step Fourier method* and a fourth-order *exponential time-differencing Runge–Kutta (ETDRK4)* method.

A.1 Split-step Fourier method (SSFM)

The NLS can be split into a linear and a nonlinear part as follows:

$$\text{Linear:} \quad i\frac{\partial \psi}{\partial t} = -\frac{1}{2}\nabla^2\psi, \tag{A.3}$$

$$\text{Nonlinear:} \quad i\frac{\partial \psi}{\partial t} = -g|\psi|^2\psi. \tag{A.4}$$

To evolve the solution from time t to $t + \Delta t$, we apply Strang splitting:

1. **Nonlinear half-step:**

$$\psi^*(\mathbf{x}) = \psi(\mathbf{x}, t)\exp\left(ig|\psi(\mathbf{x}, t)|^2\frac{\Delta t}{2}\right)$$

2. **Linear full-step in Fourier space:** Let $\hat{\psi}(k, t)$ be the Fourier transform of ψ in space, and k the corresponding wave number. Then

$$\hat{\psi}^{**}(k) = \mathcal{F}[\psi^*](k)\cdot\exp\left(-i\frac{1}{2}|k|^2\Delta t\right)$$

$$\psi^{**}(\mathbf{x}) = \mathcal{F}^{-1}[\hat{\psi}^{**}(k)]$$

3. **Nonlinear half-step:**

$$\psi(\mathbf{x}, t + \Delta t) = \psi^{**}(\mathbf{x}) \exp\left(ig|\psi^{**}(\mathbf{x})|^2 \frac{\Delta t}{2} \right)$$

This method is second-order accurate in time and spectrally accurate in space. The use of Fast Fourier Transforms (FFT) ensures computational efficiency.

The method is conditionally stable. For the linear part, spectral discretization in space ensures unconditionally stable evolution. However, the nonlinear part can introduce instabilities if Δt is too large, especially in the focusing regime ($g > 0$). Therefore, a suitable CFL-like condition may be necessary:

$$\Delta t \lesssim \frac{1}{\max(|g||\psi|^2)}$$

A.2 Exponential time-differencing Runge–Kutta method (ETDRK4)

We rewrite (A.2) as a semi-linear evolution equation:

$$\frac{d\psi}{dt} = L\psi + N(\psi), \quad \text{with } L = i\frac{1}{2}\nabla^2, \quad N(\psi) = -ig|\psi|^2\psi$$

Let $\hat{\psi}$ be the Fourier transform of ψ in space, and define $L_k = i\frac{1}{2}|k|^2$ as the diagonal operator in Fourier space. The ETDRK4 scheme advances $\hat{\psi}(t)$ in time as follows:

1. Precompute:

$$E = e^{\Delta t L_k}, \quad E_2 = e^{\Delta t L_k/2}, \quad \phi_1(z) = \frac{e^z - 1}{z}, \quad \phi_2(z) = \frac{e^z - 1 - z}{z^2}$$

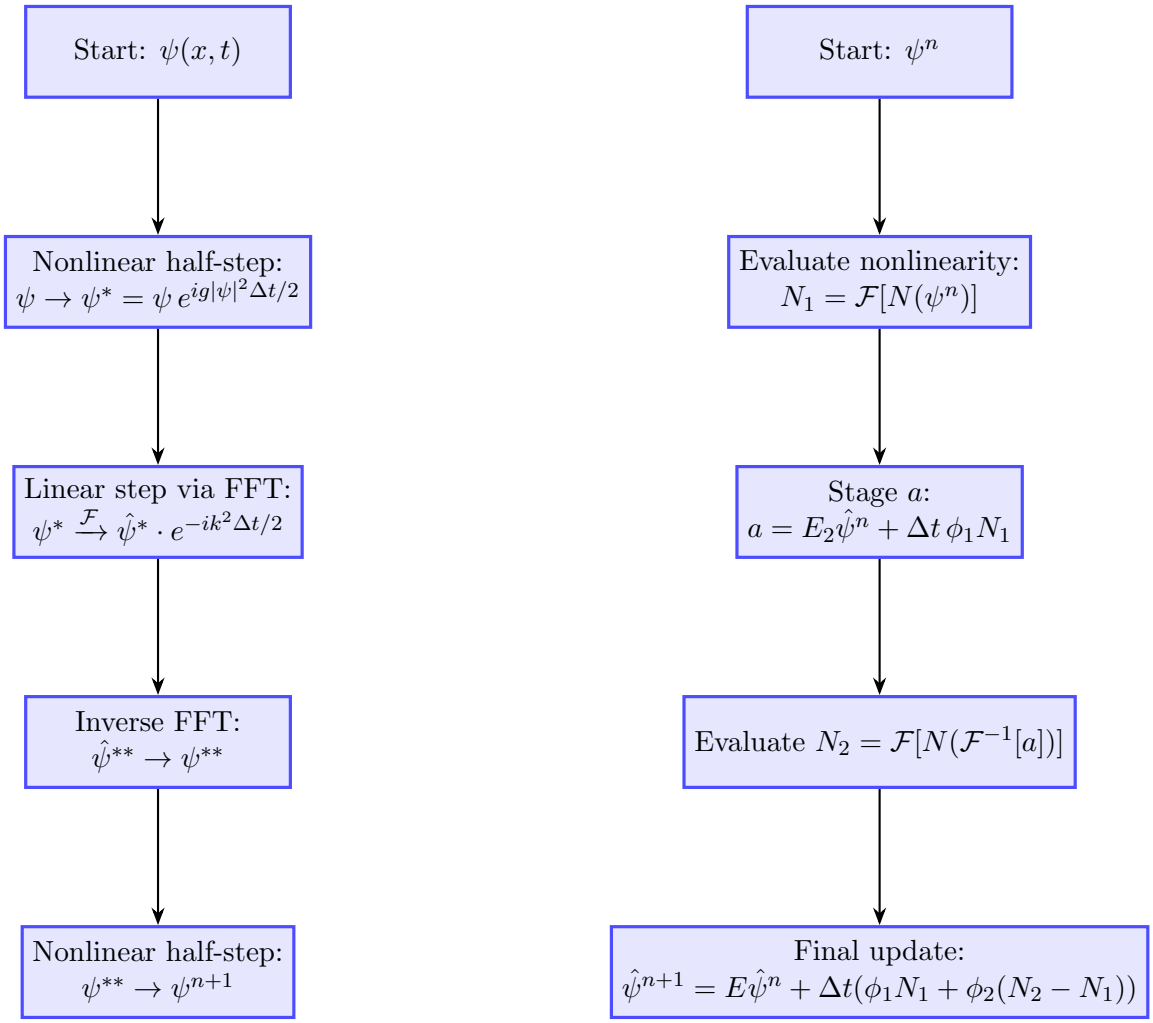
2. Evaluate:

$$N_1 = \mathcal{F}\left[N(\psi^n)\right]$$
$$a = E_2\hat{\psi}^n + \Delta t\phi_1(\Delta t L_k/2) \cdot N_1$$
$$N_2 = \mathcal{F}\left[N(\mathcal{F}^{-1}[a])\right]$$
$$\hat{\psi}^{n+1} = E\hat{\psi}^n + \Delta t\left[\phi_1(\Delta t L_k)N_1 + \phi_2(\Delta t L_k)(N_2 - N_1)\right]$$

The ETDRK4 scheme is highly stable for stiff or oscillatory equations due to exact treatment of the linear part via exponentials. Its stability depends primarily on the nonlinear term and the accuracy of the ϕ functions. In practice, ETDRK4 allows for larger time steps than split-step methods, particularly in the small-dispersion or high-amplitude regime.

The split-step Fourier method (SSFM) is easy to implement and computationally efficient due to FFT. It is widely used for wave propagation problems but is limited to second-order accuracy in time. The ETDRK4 method, although more complex, offers higher temporal accuracy and better stability properties, particularly for long-time simulations or when the solution develops fine-scale structures. Both methods benefit from spectral accuracy in space and can be adapted to multi-dimensional problems.

Figure 12 illustrates the sequential computational steps for the two numerical schemes:



(a) SSFM Workflow **(b) ETDRK4 Workflow**

Figure 12: Workflow diagrams for (a) Split-Step Fourier Method (SSFM) and (b) Exponential Time-Differencing Runge–Kutta Method (ETDRK4) used for the NLS.

(a) SSFM: Starting with the known field $\psi(x,t)$ at time t, the method advances to $t+\Delta t$ via a sequence of nonlinear and linear steps. The nonlinear step acts pointwise in real space, while the linear step is performed in Fourier space. Spectral accuracy in space is achieved using FFTs, and time evolution is second-order accurate via Strang splitting.

(b) ETDRK4: This higher-order method involves a semi-linear reformulation of the NLS. The solution is evolved in Fourier space using precomputed matrix exponentials and ϕ-functions to treat the linear part exactly. Nonlinear terms are evaluated via FFT and its inverse. The method is fourth-order accurate in time and especially suited for long-time simulations and stiff regimes.

B Comparison of numerical methods for nonlinear Schrödinger type equations

When applied to nonlinear Schrödinger-type equations such as the standard NLS, Gross–Pitaevskii equation (GPE), and time-dependent Schrödinger equation (TDSE) [23], both **finite difference (FD)** and **finite element (FE)** methods reveal notable limitations. These include low dispersion accuracy, particularly in simulations involving long-range soliton propagation or high-frequency wavepackets. FD schemes often suffer from numerical dispersion and phase errors, which accumulate over time and lead to distorted wave structures. Similarly, FE methods, while geometrically flexible, incur high computational costs and require fine meshing to accurately capture global wave coherence. In contrast, the **Split-Step Fourier Method (SSFM)** and **Exponential Time-Differencing Runge–Kutta (ETDRK4)** schemes demonstrate *spectral accuracy*, excellent conservation of mass and energy, and superior efficiency. SSFM exploits operator splitting to treat the linear part exactly in Fourier space, eliminating phase errors, while ETDRK4 provides robust handling of stiffness in nonlinear dynamics. The table below summarizes the performance characteristics of each method based on typical benchmark tests:

Table 2: Comparison of numerical methods for nonlinear Schrödinger-type problems

Method	**L^2 Error**	**Conservation**	**CPU (s)**	**Remarks**
FD	10^{-2}–10^{-3}	Poor (drift accumulates)	45.2	Low-order, dispersive error
FE	10^{-3}	Moderate	78.5	Geometry-flexible, but costly
SSFM	$< 10^{-6}$	Excellent	12.4	Spectral accuracy, fast FFT
ETDRK4	$< 10^{-7}$	Excellent	14.1	Stiff systems, high fidelity

These results underscore the computational advantages of spectral methods, particularly SSFM and ETDRK4, for simulating nonlinear and quantum wave systems with high fidelity over long time intervals.

Declaration of competing interest

The authors declare that they have no known competing financial interests.

Data availability

No data was used for the research described in the article.

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