Exploration of the Nonlinear Schrödinger Equation

Alexis Saucerman, Riley Prendergast, Andy Chiv, Dr. Stathis Charalampidis

Department of Mathematics, California Polytechnic State University, San Luis Obispo

Background:

The nonlinear Schrödinger equation (NLSE) is a special nonlinear partial differential equation (PDE): $i\psi_t = -\frac{1}{2}\psi_{xx} + |\psi|^2\psi + V(x)\psi$ often seen in Physics. The function ψ is the so-called wave-function, and $V(x) = \frac{1}{2}\Omega^2 x^2$ represents the external potential where Ω is the trap's strength. Its presence has the effect of confining particles in space. Solutions to this PDE are found by the separation of variables ansatz $\psi(x,t) = \phi(x)e^{-i\mu t}$ where ϕ(x) is the steady-state part of the solution, and μ is the chemical potential (effectively controlling the number of atoms in the condensate).

This equation has applications in many areas of physics, including atomic physics, water waves, and nonlinear optics. The equation we focused on in this project is used for studying Bose-Einstein condensation (BEC), a state of matter in which atoms are cooled down to 0 Kelvin, and thus share same quantum properties.

In this project, we studied the existence, stability, and spatio-temporal dynamics of solutions to the NLSE. The tools we used in this project included Newton's method and the four stage, fourth-order Runge-Kutta (RK4) method.

Existence of Steady States:

Steady-state solutions satisfy the BVP: $0 = -\frac{1}{2}\phi'' + |\phi|^2\phi + V(x)\phi - \mu\phi$ supplemented by zero Dirichlet boundary conditions (BCs), and can be found by Newton's method. Linearization of the above BVP results in a Sturm-Liouville problem which yields discrete values for μ given by $\mu = (n + \frac{1}{2})\Omega$ with n ≥ 0 and ϕ_0(x) using the Hermite polynomials of degree n. Thus, the initial guess in our Newton's Method is (μ, ϕ_0(x)) . In our study, we set Ω = 1. The latter highlights the number of zero-crossings in ϕ(x) that we present below. **Figure 1** corresponds to the case with n = 0; **Figures 2 & 3** corresponds to n = 1 and n = 2, respectively.

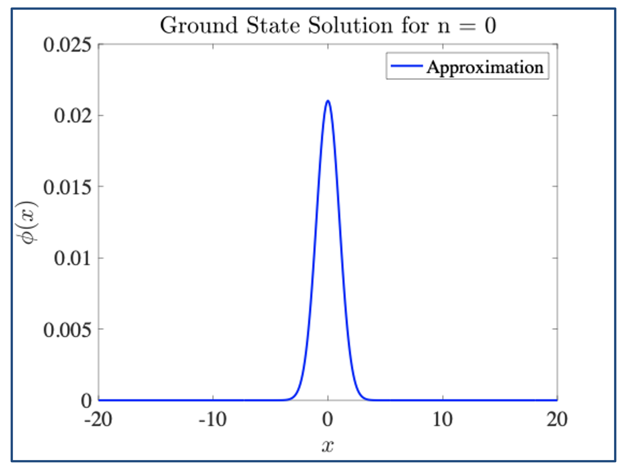

Figure 1

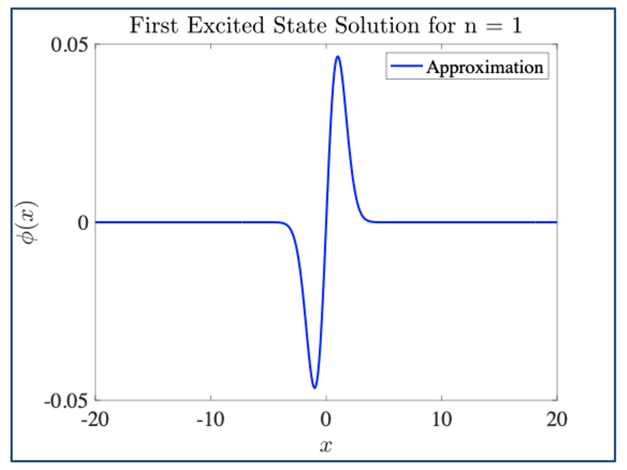

Figure 2

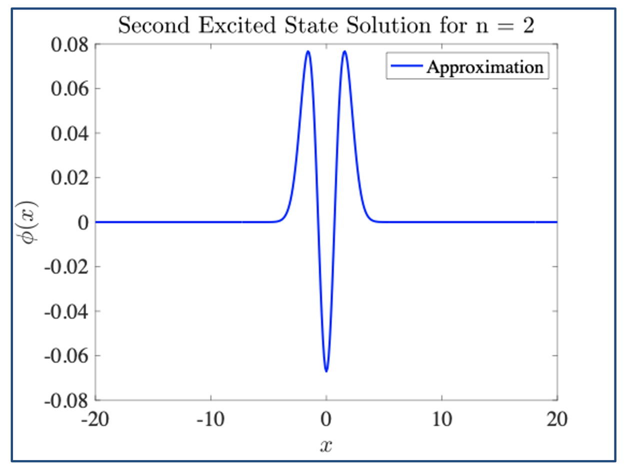

Figure 3

Stability Analysis:

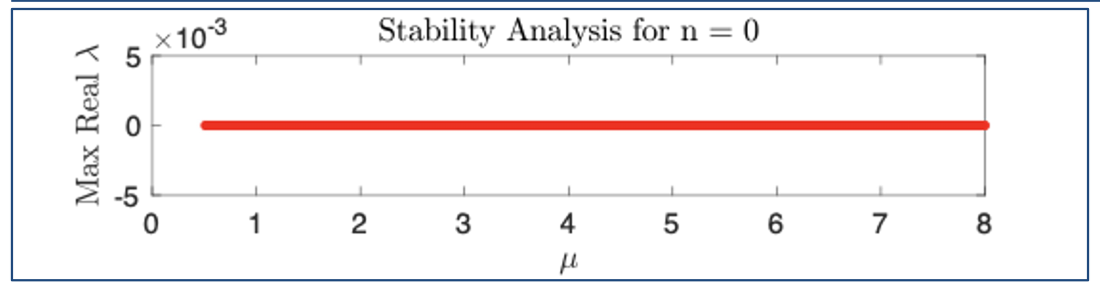

Figure 4

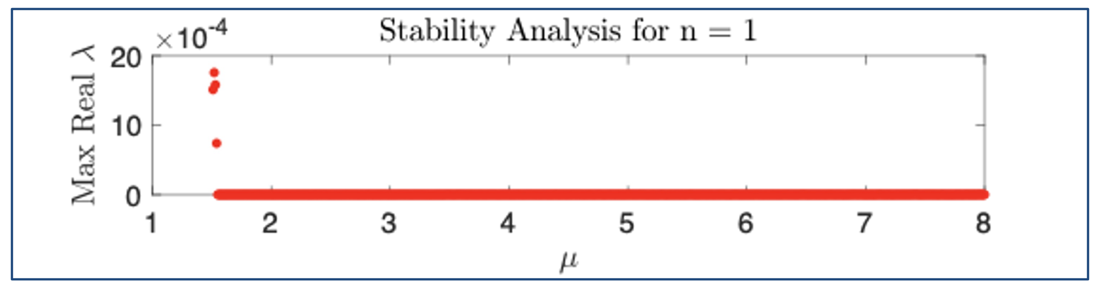

Figure 5

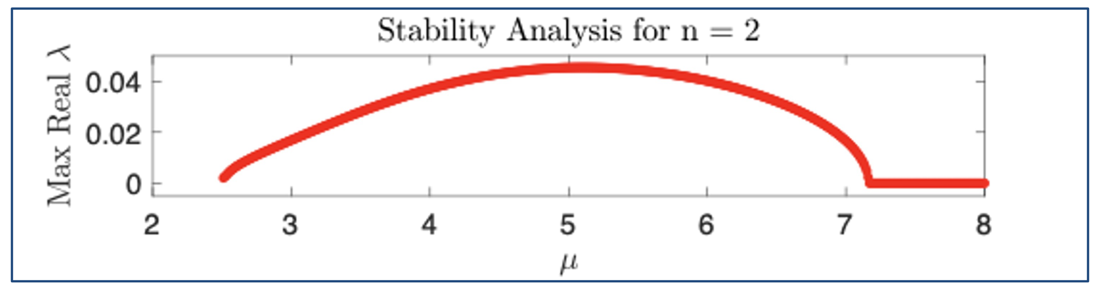

Figure 6

To determine the stability trait of the solutions we studied, the perturbation ansatz: $\tilde{\psi}(x,t) = e^{-i\mu t}[\phi(x) + \epsilon(a(x)e^{\lambda t} + \bar{b}(x)e^{\bar{\lambda}t}]$ which results in the following eigenvalue problem.

$$i\lambda \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} -\frac{1}{2}\frac{d^2}{dx^2} + 2|\phi(x)|^2 - \mu + V(x) & \phi(x)^2 \\ -\bar{\phi}(x)^2 & -(-\frac{1}{2}\frac{d^2}{dx^2} + 2|\phi(x)|^2 - \mu + \bar{V}(x)) \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix}$$

We plotted the maximum real λ against μ. An unstable solution has a nonzero real λ where a stable solution does not. Starting from the linear limit, we traced branches of solutions for different n. In **Figure 4**, the solutions are all stable over μ. **Figures 5 & 6** illustrate the instabilities in the n = 1 and n = 2 branches, respectively. It can be discerned that the states become more prone to instabilities as n increases.

Dynamics:

We used the time integrator RK4 method to evaluate the solutions of the NLSE. These findings are important because although many solutions exist for the NLSE, only some of them are stable over time, and thus applicable to physical applications.

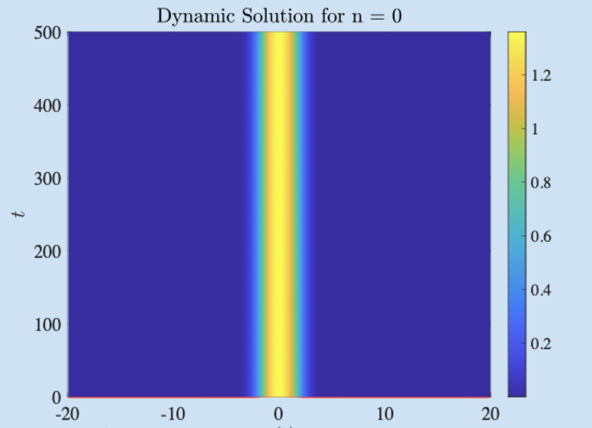

Figure 7

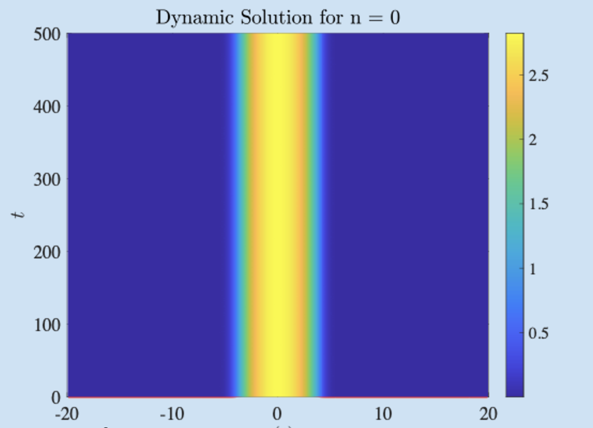

Figure 8

- these plots are the spatio-temporal evolution for n = 0 at different values of μ
- the profiles remain stable over time, supporting our spectral stability analysis

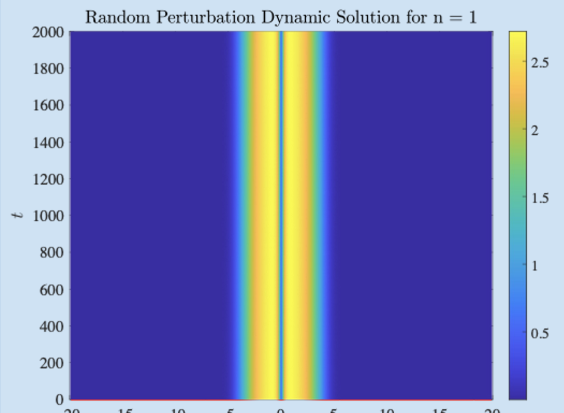

Figure 9

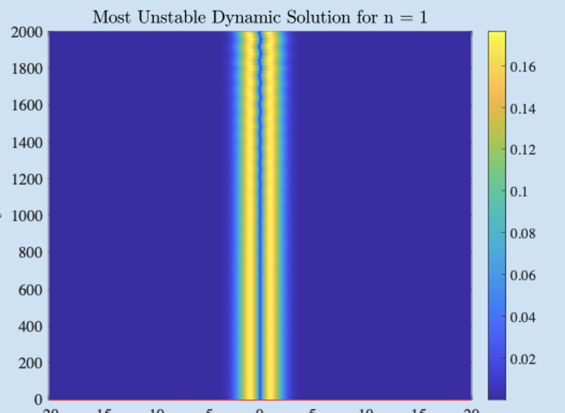

Figure 10

- above are stable and unstable dynamics of n = 1
- the solutions at μ = 8 remain stable
- at μ = 1.52, an oscillatory instability manifests at t = 1000 where the real part of λ is of order 10^{-3}

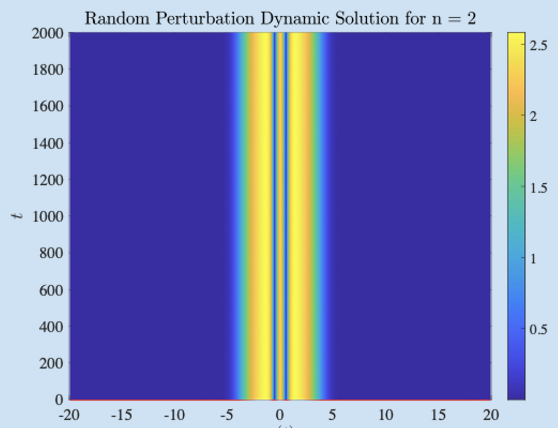

Figure 11

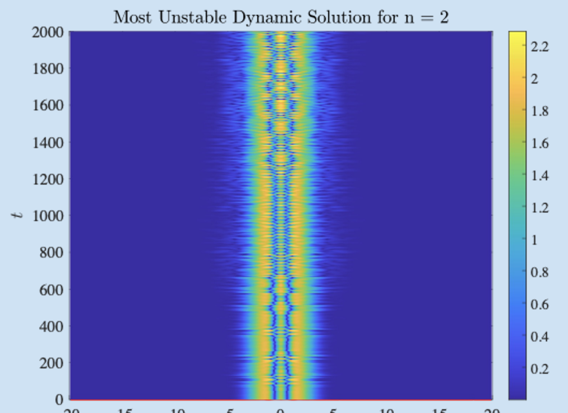

Figure 12

- above are stable and unstable dynamics of n = 2
- the solutions at μ = 8 remain stable
- at μ = 5.1, the instability occurs at t = 100, due to the maximal real part of λ being of order 10^{-2}

Perturbations:

Due to imperfections of experimental initial conditions in BECs, it is important to explore whether solutions are robust or not. To that effect, we investigate numerically whether perturbations added to steady states force an instability in their time evolution or not. We used two types of perturbations: a random perturbation (for stable solutions) and the one specified by the most unstable eigendirection (for unstable solutions).

Moving Forward:

It is important to note the limitations of using zero Dirichlet BCs. Although the NLSE is defined on the real line, we truncated the domain into a finite one and supplemented the problem with the aforementioned BCs. This was possible due to the presence of the external potential V(x) which forces the solution outside of the BCs to be zero. However, the interplay between the finiteness of the computational domain and BCs employed may shed some light on any potential changes in the stability analysis results we obtained in this project. It is more natural to consider other types of BCs, including the modulus-squared Dirichlet (MSD) boundary conditions as this would be more accurate in representing the characteristics of the solutions and their spectrum.

References:

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