CHAOS IN BOSE-EINSTEIN CONDENSATES

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Abstract

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The Gross-Pitaevskii equation (GPE) is a nonlinear Schrödinger equation used in modeling Bose-Einstein condensates (BECs). Using Lyapunov exponents, chaos was characterized in the GPE in the one-dimensional case. The GPE was simulated using Python using both spectral and finite-difference methods in space and an adaptive Runge-Kutta solver was used to evolve the equation in time. When a turbulent state is perturbed, positive Lyapunov exponents were found. There was a proportionality found between positive Lyapunov exponents and the nonlinear coupling constant of the GPE, g. Further research can be done to analyze this proportionality.

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Chapter One

Introduction

The Schrödinger equation is a linear differential equation that describes how quantum mechanical objects evolve in time and space. Any quantum mechanical object can be described by its corresponding wavefunction, governing its probability density. This complex wavefunction exists in a mathematical space known as Hilbert space, differing from a Euclidian space by its inner product and infinite dimensionality [1].

Bose-Einstein condensates (BECs) are formed by bosonic gases at low densities near absolute zero temperatures, resulting in the occupation of the lowest quantum state. The collapse to the lowest quantum state is due to the indistinguishability and bosonic nature of these particles [2]. This additional state of nature was predicted by Einstein and Bose in the early twentieth century [3]. This state of matter is a purely quantum phenomena and are a recent research interest since its experimental realization of rubidium-87 by Cornell and Wieman in 1995 [4]. Although we can model BECs using the Schrödinger equation, problems lay when the particle count is increased.

Systems of many bodies can be difficult to model as the wavefunction grows exponentially to account for Coulombic interaction. Several approximations can be used to reduce the modeling complexity. For a many-body Schrödinger equation, a mean-field pseudopotential approximation can be employed to reduce the complexity from exponential to a constant complexity, as well as using a Hartree-Fock approximation [5]. This resulting nonlinear

Schrödinger equation is known as the Gross-Pitaevskii equation (GPE), capable of accurately modeling BECs routinely produced experimentally [5].

Chaos is the apparent disorder and irregular motion of a dynamical system—more formally, the exponential divergence of a trajectory in time [6]. Chaos can be characterized through Lyapunov exponents, where the sign of the exponent denotes the chaos in a system. A positive maximal exponent characterizes chaos, as it implies an exponential diverging growth. A zero maximal exponent is found when no chaos is present in a system.

An example of chaotic motion can be seen in the the Lorenz attractor, resulting in positive Lyapunov exponents [7]. The Lorenz system is composed of a set of interdependent, nonlinear differential equations, initially used to model atmospheric convection by Edward Lorenz [7]. As two points with slightly different initial conditions evolve in time in this system, they may have wildly varying trajectories. Using the distance between these two points in time, their Lyapunov exponent can be calculated. This process can be repeated for long durations in time and for several different initial conditions. From this set of Lyapunov exponents, the maximal exponent can be taken to represent the chaos within this system. As there are no classical trajectories for calculating Lyapunov exponents in Hilbert space, there are several potential metrics that emulate these trajectories and allow a difference to be found. We will use the L^2 norm to measure distances in the Hilbert space.

The correspondence principle states that quantum mechanics should reproduce classical mechanics in the limit of higher states, as stated by Bohr [8]. Yet, here lies a puzzling conundrum: the world of classical mechanics is chaotic, but the Schrodinger equation is fundamentally linear and cannot exhibit chaos. This is an unsolved problem in physics and several theories exist [9]. Although this paper does not discuss the source of quantum chaos, it will instead look towards the effects of GPE parameters on quantum chaos in BECs.

Previous works have demonstrated chaos in Bose-Einstein condensates through positive Lyapunov exponents [10–12]. This work aims to replicate these results in one-dimension using both spectral and finite-difference methods, as well as discusses the effect of GPE parameters on the Lyapunov exponent. Additionally, this paper discusses numeric errors in both the finite difference method and the adaptive Runge-Kutta solver.

Chapter Two

Background

In this chapter, we will begin to introduce the fundamentals of quantum mechanics with the Schrödinger equation. We will justify the extension of the Schrödinger equation to the Gross-Pitaevskii equation for Bose-Einstein condensates. Next, we will introduce the mathematical description of chaos and how chaos can be characterized with Lyapunov exponents. Numerical methods will be introduced, which will later be applied to the nonlinear Schrödinger equation to evolve it using computer simulation.

2.1 Schrödinger equation

The Schrödinger equation is mathematical description of how quantum mechanical objects evolve through time and space. It asserts that quantum objects are governed by a wave nature calculatable with a differential equation in complex space. This wave is used to calculate the probability of the object existing in a particular location at a time. The equation takes form as a second order linear partial differential equation, defined in one-dimension as

$$i\hbar\frac{\partial}{\partial t}\Psi(x,t) = \hat{H}\left|\Psi\right\rangle = \left[\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x,t)\right]\Psi(x,t), \tag{2.1}$$

for a wavefunction $\Psi(x,t)$ and a potential $V(x,t)$. This equation is the *time-dependent* Schrödinger equation. For a constant potential in time and an assumption of separability, we can manipulate (2.1) and define the *time-independent* Schrödinger equation as

$$E\Psi(x) = \hat{H}\left|\Psi\right\rangle = \left[\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]\Psi(x). \tag{2.2}$$

If we take an example of an electron in the vicinity of another electron in one-dimension and account for Coulomb forces, the potential will be proportional to $1/x$. For a system of N-many electrons, the time-independent Schrödinger equation for one electron will take the form

$$E\Psi(x) = \left[\frac{\hbar^2}{2m_e}\frac{\partial^2}{\partial x^2} - \frac{e}{4\pi\epsilon_0}\sum_i^N \frac{1}{d_i}\right]\Psi(x),$$

for a distance between particles d_i. The potential term contains a sum over the distance of all particles. This becomes computationally problematic for the many-particle case, as it requires recalculating the potential for each particle during each integration step. We will now turn to approximations made in the Gross-Pitaevskii equation that simplifies the Schrödinger equation for this many-particle case of bosonic gases.

2.2 Gross-Pitaevskii equation

As the Schrödinger equation describes one object, it becomes impractical to use it to model multiple interacting objects. This is due to the exponential growth of terms in the equation with the addition of each interaction. The Gross-Pitaevskii equation successfully patches the Schödinger equation for Bose-Einstein condensates (BECs) with the addition of a nonlinear term [5]. This model makes several assumptions to achieve lower term complexity in the many-body Schrödinger equation. First, this model assumes diluteness and weak particle interaction, allowing the omission of quantum fluctuations. Next, the equation assumes a mean-field pseudopotential seen by particles. These approximations allow a macroscopic many-body Schödinger equation of form

$$-i\hbar\frac{\partial\Psi}{\partial t} = \left[\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x,t) + g|\Psi|^2\right]\Psi. \tag{2.3}$$

In the equation, note the addition of the nonlinear term with coupling constant g. This constant is given by

$$g = \frac{4\pi\hbar^2 a_s^2}{m}, \tag{2.4}$$

where a_s is the s-wave scattering length characterizing atomic interactions in the low energy limit [13]. This value can be determine experimentally, with ^{87}Rb and ^{23}Na having $a_s = 5.8\,\mathrm{nm}$ and $2.8\,\mathrm{nm}$ respectively [5]. Additionally, as this is a macroscopic wavefunction, the normalization is now the number of particles in the condensate, i.e.

$$N = \int |\Psi|^2 \,\mathrm{d}x\,. \tag{2.5}$$

2.3 Chaos and Lyapunov exponents

Chaos is a term commonly used in everyday speech, but can be hard to define mathematically. When a droplet of cream is added to coffee, the cream diffuses and creates a pattern in the coffee. If the droplet were instead placed in a slightly different location, a new pattern emerges. This system can be completely deterministic, yet exhibit chaos and unpredictability. (TODO: use a better analogy.) Chaos is found in unstable systems, where similar initial conditions can lead to wildly different outcomes. This can be characterized mathematically using Lyapunov exponents.

Lyapunov exponents of a dynamical system tracks the rate of separation of two initially similar trajectories. The maximal Lyapunov exponent (MLE) along vector $\mathbf{Z}(t)$ perturbed from initial vector $\mathbf{Z}_0$ is defined as

$$\lambda = \lim_{t\to\infty} \frac{1}{t} \ln \frac{|\delta\mathbf{Z}(t)|}{|\delta\mathbf{Z}_0|}. \tag{2.6}$$

A well-known example of Lyapunov exponents is through the Lorenz system. This system consists of a set of interdependent nonlinear differential equations, initially used to model atmospheric convection [7]. Typically for the Lorenz system, two attractors are seen, shown in Figure 2.1. There exists a curve between the two attractors that is unstable, where minuscule changes along the curve will lead to the system switching lobes. This is seen in Figure 2.2, where an initial point is perturbed slightly, and the distances between the two points is measured through time. An approximation of the maximal Lyapunov exponent is shown in the dashed red line.

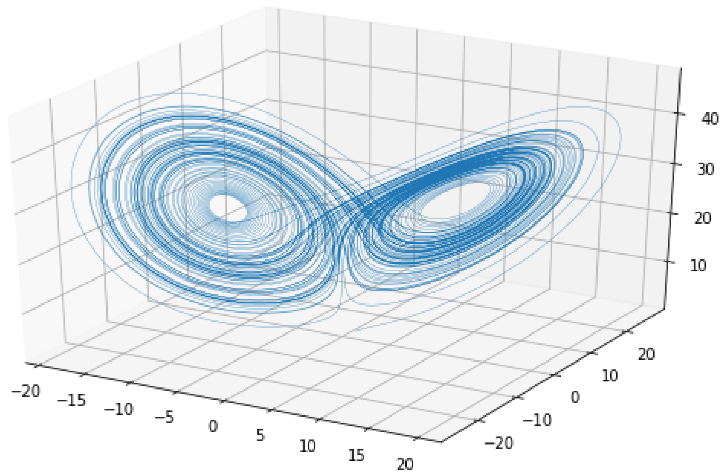

Figure 2.1 The Lorenz attractor in three dimensions with parameters $\sigma = 10$, $\beta = 8/3$, $\rho = 28$.

Lyapunov exponents in Hilbert space

In order to find Lyapunov exponents in Hilbert space L^2 as required for quantum wavefunctions, we must devise a metric to find calculate distances. The L^2 norm of the wavefunctions is an obvious choice for this and has been used in prior works [10]. This distance metric follows

$$d^{(2)}(\psi_1, \psi_2; t) = \frac{1}{2} \langle \psi_1 - \psi_2 | \psi_1 - \psi_2 \rangle = \frac{1}{2} \int \mathrm{d}x \, |\psi_1(x,t) - \psi_2(x,t)|^2. \tag{2.7}$$

An alternative metric is distance between densities,

$$d(\psi_1, \psi_2; t) = \int \mathrm{d}x \left(|\psi_1|^2 + |\psi_2|^2 - 2\psi_1^* \psi_2 \right). \tag{2.8}$$

Both of these metrics will be used in this paper to calculate distances between wavefunctions.

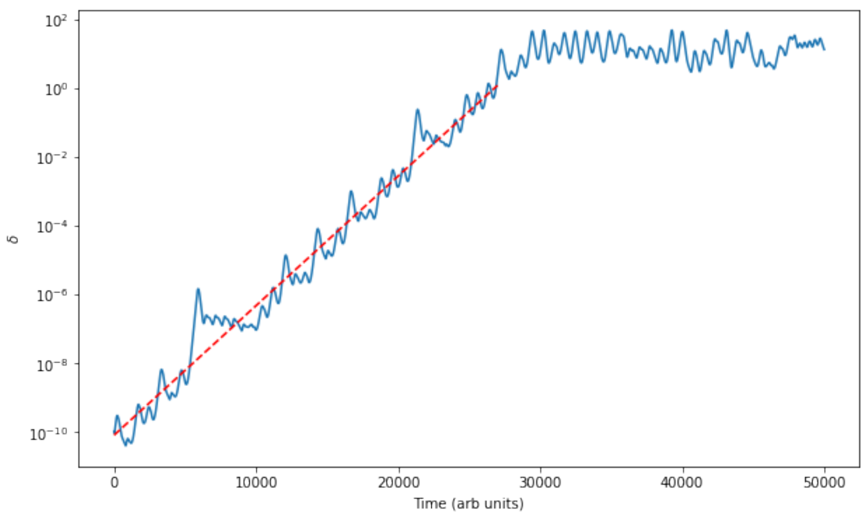

Figure 2.2 The difference in trajectories through time of two nearby points, with an approximation of the MLE (dashed red). The plateau near the top is due to the maximal separation possible from the constraints of the system.

2.4 Numerical methods

Numerical methods are procedures to solve a numerical problem. To see how the GPE evolves in time, the continuous spatial and time components must first be sliced into many smaller discrete—this is known as discretization. TODO: write this out more.

In this paper, we will use Runge-Kutta (RK) methods for approximate solutions of the GPE. We will use the `solve_ivp` function provided by SciPy as an implementation of the explicit Runge-Kutta method of order 5. This function has controllable tolerances, allowing an estimation of an error due to temporal discretization.

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