CHAOS OF BOSE-EINSTEIN CONDENSATES IN ONE-DIMENSION

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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 $a_s = 5.8\,\text{nm}$ and $2.8\,\text{nm}$ 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.

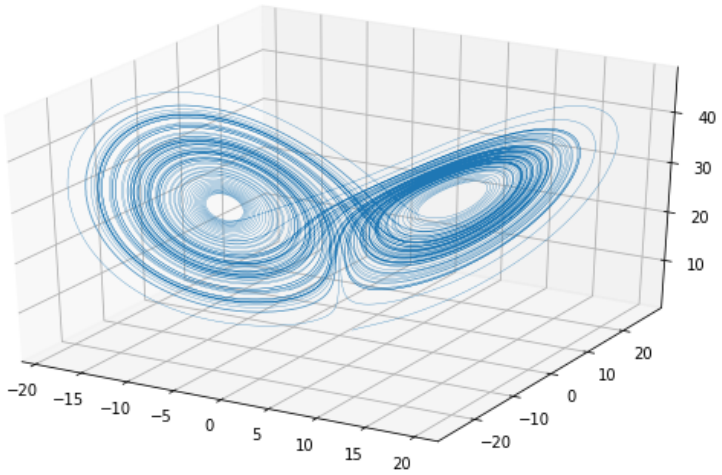

Figure 2.1 The Lorenz attractor in three dimensions with parameters $\sigma = 10$, $\beta = 8/3$, $\rho = 28$.

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.

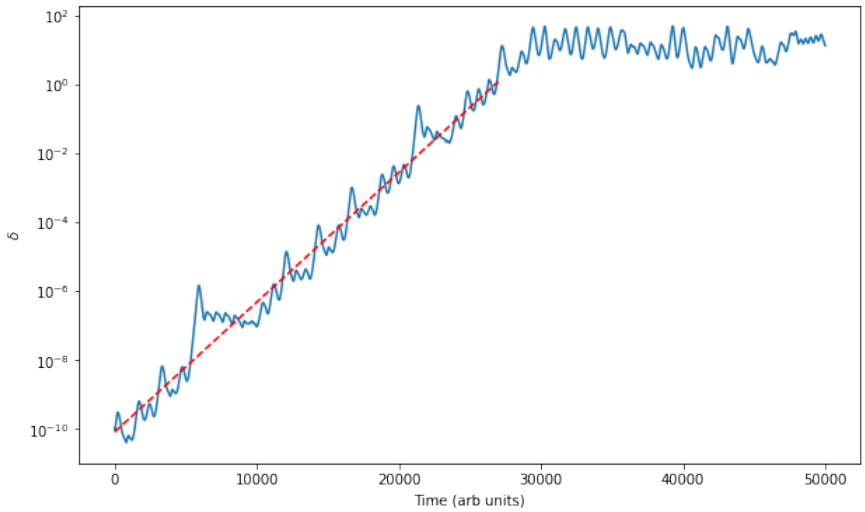

Figure 2.2 The difference in trajectories through time of two nearby points, with an approximation of the MLE (dashed red). The plateau near the top is due to the maximal separation possible from the constraints of the system.

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.

Chapter Three

Procedures

First, the Gross-Pitaevskii equation is simulated using Python using a spatial finite difference method. This used Numpy to discretize the wavefunction and `solve_ivp` is used to evolve the wavefunction through time. This wavefunction is perturbed by superimposing a small sinusoid and both functions are allowed to evolve independently. The difference of these wavefunctions is recorded and a Lyapunov exponent can be calculated.

3.1 Numerical Derivatives

For the spatial discretization, a 2D diagonal matrix was used to calculate the first derivative. To begin, recall the definition of a derivative,

$$f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}. \tag{3.1}$$

To approximate the limit, we can take h to be a small finite value relative to the target function $f(x)$. This equation is known as the *forward difference*, as h is *forward* of x. In a similar fashion, the backward difference is given as

$$f'(x) = \lim_{h \to 0} \frac{f(x-h) - f(x)}{h}. \tag{3.2}$$

Both the forward and backward differences can be averaged for a more accurate central difference approximation,

$$f'(x) = \lim_{h \to 0} \frac{f\left(x + \frac{h}{2}\right) - f\left(x - \frac{h}{2}\right)}{h}. \tag{3.3}$$

For the second-order central difference approximation, it can be shown either directly or through the Taylor expansion

$$f''(x) = \lim_{h \to 0} \frac{f(x+h) - 2f(x) + f(x-h)}{h^2}. \tag{3.4}$$

Note that this method has some truncation error due to the Taylor expansion. Additional higher-order terms can be added for better precision at the expense of computational cost. TODO: expand on this.

3.1.1 Matrix formulation

In the second-order central difference approximation, each term at point x depends on the previous and next spatial term. As the derivative operator is linear and many Python libraries support matrices including Numpy, it will be optimal to convert the second-order derivative operator to a matrix. For a given function $f(x)$ discretized over x, the second derivative can be calculated using matrices,

$$\begin{aligned} |f''(x)\rangle &= \hat{D}\,|f(x)\rangle \\ \begin{pmatrix} f''(x_0) \\ f''(x_1) \\ f''(x_2) \\ \vdots \\ f''(x_{N-1}) \end{pmatrix} &= \frac{1}{h^2} \begin{pmatrix} -2 & 1 & & & & \\ 1 & -2 & 1 & & & \\ & 1 & -2 & 1 & & \\ & & \ddots & \ddots & \ddots & \\ & & & 1 & -2 & 1 \end{pmatrix} \begin{pmatrix} f(x_0) \\ f(x_1) \\ f(x_2) \\ \vdots \\ f(x_{N-1}) \end{pmatrix}. \end{aligned} \tag{3.5}$$

For periodic boundary conditions, the first term of the derivative must wrap around and use the last term in the derivative calculation, and vice versa. This results in modifying (3.5) to

$$\begin{pmatrix} f''(x_0) \\ f''(x_1) \\ f''(x_2) \\ \vdots \\ f''(x_{N-1}) \end{pmatrix} = \frac{1}{h^2} \begin{pmatrix} -2 & 1 & & & & 1 \\ 1 & -2 & 1 & & & \\ & 1 & -2 & 1 & & \\ & & \ddots & \ddots & \ddots & \\ 1 & & & 1 & -2 & 1 \end{pmatrix} \begin{pmatrix} f(x_0) \\ f(x_1) \\ f(x_2) \\ \vdots \\ f(x_{N-1}) \end{pmatrix}. \tag{3.6}$$

From this matrix, the one-dimensional Laplacian term in the Gross-Pitaevskii equation can be approximated.

3.2 Gross-Pitaevskii equation and time evolution

From the second derivative matrix (3.6), the Python function 3.1 can be used to evolve the time-dependent Gross-Pitaevskii equation over time with `solve_ivp`. This function solves the (2.3) for $\frac{\partial \Psi}{\partial t}$. Using this function, the Runge-Kutta method can be applied as an adaptive solver and the time evolution can be observed. Additionally, the relative and absolute tolerances can be lowered in the solver to ensure high precision.

Listing 3.1 The `solve_ivp` wrapper function for the Gross-Pitaevskii equation. This function approximates (2.3).

```
1  def compute_dpsi_dt(t, psi):
2      """ Return dpsi/dt for the GPE. """
3      phase = 1 / (1j * hbar * cooling_phase / np.abs(cooling_phase))
4      n = abs(psi)**2
5      return phase * (-hbar / 2 / m * (D2 @ psi) + (V(x) + g * n) * psi)
```

3.3 Initial many-body wavefunction

Before perturbing the wavefunction when calculating the Lyapunov exponent, an initial wavefunction must be generated. Here, a function was used to generate sinusoidal noise with Dirichlet boundary conditions. This function allows the noise independent of the dimensions of the lattice spacing. This function is shown in Listing 6.1.

3.4 Lyapunov exponent calculation

To calculate the Lyapunov exponent of the Gross-Pitaevskii equation, first we must generate a wavefunction and a perturbed copy, then evolve both through time and calculate the difference in Hilbert space. An initial wavefunction is generated using Listing 6.1. A perturbed wavefunction is created by superimposing a small-amplitude sinusoid on the initial function. Both functions are evolved independently and the difference in wavefunctions are calculated over time using (2.8). After a set time, the perturbed wavefunction is "pulled back" and is reset to another superimposed sinusoid over the non-perturbed wavefunction. This process is repeated several times to ensure a maximal exponent can be found. The Lyapunov exponent is calculated for each iteration by taking a exponential fit of the differences as a function of time.

To ensure numerical (error?) is minimized, after evolving the wavefunction through time, the wavefunction is evolved backwards through time. The difference between the original wavefunction and the reverse-time-evolved function must be within a small tolerance to ensure (accuracy?).

Additionally, for the $g = 0$ case, the Gross-Pitaevskii equation is the regular linear Schrödinger equation. This case is linear and should give no chaotic motion, with a zeroth Lyapunov exponent. TODO: expand on this more.

3.5 Experimental values

In the simulations, the constant $\hbar = 1$ and the lattice is divided into 400 segments. Under these units, the maximum time step size is set to 0.01. The perturbation amplitude is set to 1×10^{-5}. When varying g, the system is allowed to evolve for 1 time unit with 100 steps. This process is repeated 5 times per g value.

Chapter Four

Findings

The Gross-Pitaevskii equation exhibits numerical chaos when an initial turbulent state evolves in zero potential. Chaos is seen for positive values of g. For positive nonlinear coupling constant g, the relationship between the Lyapunov exponent is seemingly linear, as shown in Figure 4.1. For negative g, there is no clear relationship. Shown in Figure 4.2, applying a linear regression results in

$$\lambda(g) = (0.04996 \pm 0.00206)\, g + (0.0197 \pm 0.0125)\,. \tag{4.1}$$

4.1 Error analysis

Several steps were taken to ensure error is minimized. TODO: discuss solver tolerances, floating point error, etc.

Role of solver tolerances

The Gross-Pitaevskii equation with coupling constant $g = 0$ returns the Schrödinger equation, a linear differential equation. The Lyapunov exponent for this case was found to be zero for high-precision absolute and relative solver tolerances of 1×10^{-10} and smaller, as expected. For lower-precision tolerances, the solver fails, as shown in Figure 4.3.

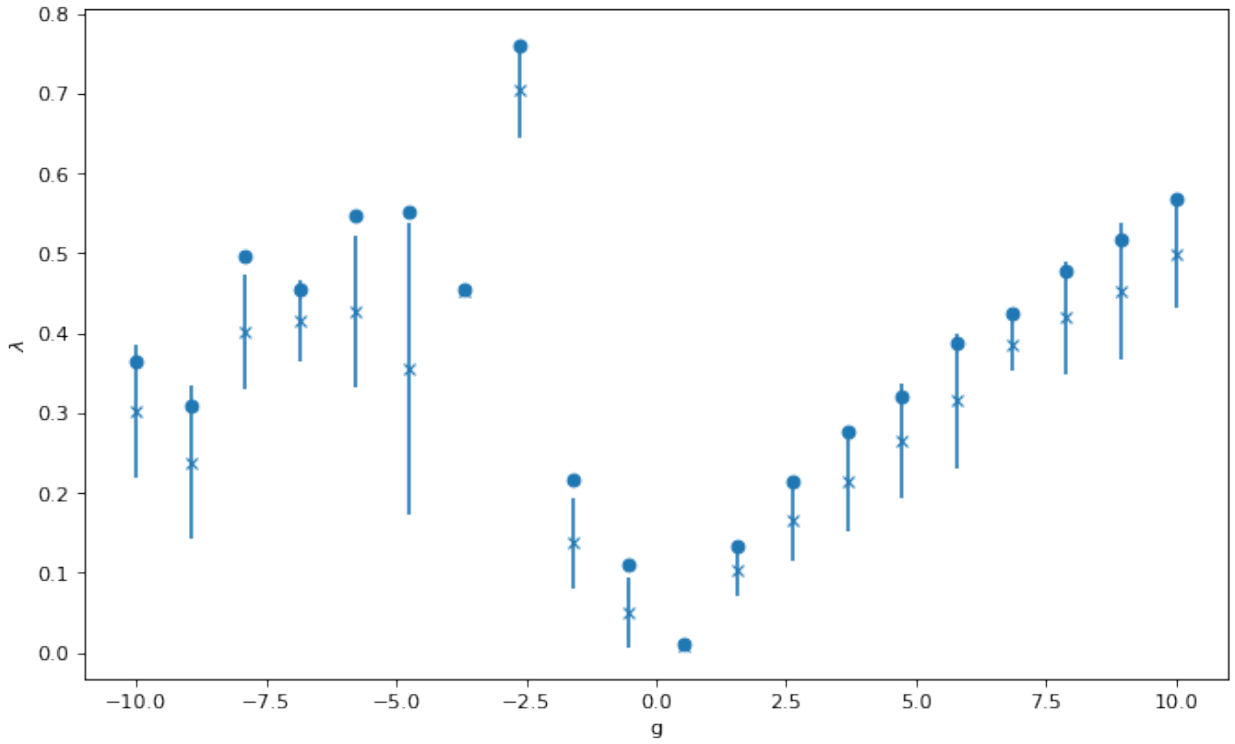

Figure 4.1 The effect of g on the Lyapunov exponent. Note that the dot depicts the approximate maximal Lyapunov exponent (MLE) and the cross represents the mean.

Role of machine precision and spatial derivative error

The machine precision of floating point numbers as defined in IEEE754 is the limiting precision on numbers in the simulated Gross-Pitaevskii equation [14]. This value is calculated to be

$$\epsilon = 2.22 \times 10^{-16}. \tag{4.2}$$

The leading error in the Taylor expansion of the spatial derivative is

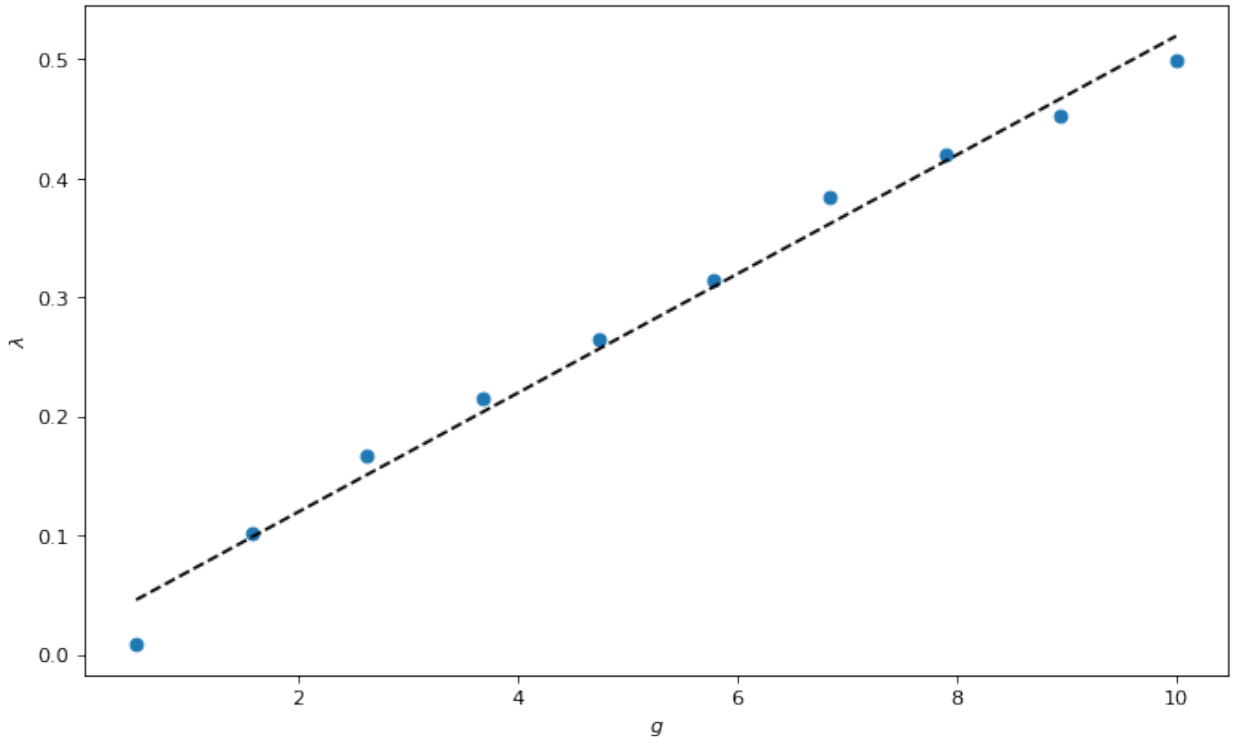

Figure 4.2 Linear fit on coupling constant g versus the Lyapunov exponent.

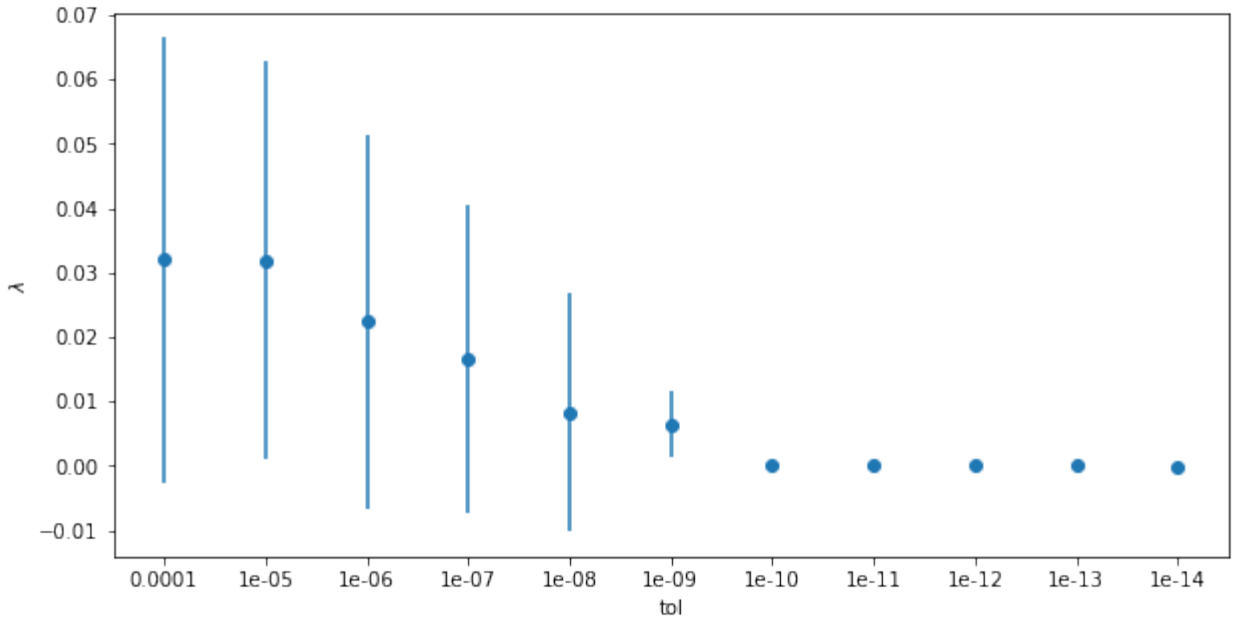

Figure 4.3 Effect of solver tolerances on the Lyapunov exponent for the non-chaotic Schrödinger equation.

Chapter Five

Summary and Conclusions

The Gross-Pitaevskii equation in one-dimension has shown to have positive Lyapunov exponents, implying chaotic motion in Bose-Einstein condensates. The nonlinear coupling constant term is seemingly the cause of this chaos, understandably as chaos cannot arise from linearity. It is still unclear how chaos arises in classical mechanics, but it could be due to interaction in the many-particle case. Additional research is necessary to expand to the case of two- and three-dimensions.

Chapter Six

Appendices

Listing 6.1 Fourier noise function.

```
def fourier_noise(n_modes=4, dirichlet=True, seed=3):
    """ Generates random sinuosodal noise independent of box size """

    np.random.seed(seed)
    n = np.arange(n_modes) - n_modes // 2

    # ks = 2*np.pi * np.fft.fftfreq(N, dx)
    # ks[inds] = 2*np.pi * n /L
    # np.where(...)

    # create list of wavenumbers for the modes to generate
    ks = 2 * np.pi * n / L

    # create random amplitudes for each mode (-0.5, 0.5)
    As = (np.random.random(n_modes) - 0.5) * 2

    # random phases too
    phases = np.random.random(n_modes) * 2 * np.pi

    # box space
```

```
21      _x = (1 + np.arange(N)) * dx
22
23      if dirichlet:
24      # for dirichlet, the end points are zero (as each mode is guaranteed to
            fit in the box, as phase=0)
25      # although: there is no complex phase here, so: will this generate
            turbulance as the phase is uniform?
26      psi = sum(_A * (np.exp(1j * _k * _x) - np.cos(_k * _x))
27      for _A, _k in zip(As, ks))
28      else:
29      # basically do a fourier series but of these specific modes, i.e. sum up
             each sine wave
30      # the ends may not be zero here
31      psi = sum(_A * np.exp(1j * (_k * _x + _phase))
32      for _A, _k, _phase in zip(As, ks, phases))
33
34      return psi
```

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