Bosenova Simulation

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Field Session 2007 - June 20, 2007

Introduction

This project has as its goal the exploration of a numerical method for finding solutions of four coupled, partial differential equations that describe a current theory of the Bosenova phenomenon.

Bose-Einstein Condensates

To begin, we need to discuss some of the physics, to give a background for this project. The Bosenova is a phenomenon of Bose-Einstein Condensates. Bose-Einstein Condensates are composed of a large number of atoms (millions) that are super-cooled, down to a temperature on the order of 100 nano-Kelvin, putting them all into the same quantum mechanical state, the lowest energy state. Because they all occupy the same state, these atoms start to act synchronously, as one large quantum-mechanical system. This allows experimental physicists to probe a macroscopic system that has quantum properties. See Figure 1 for a graphical representation of a condensate forming.

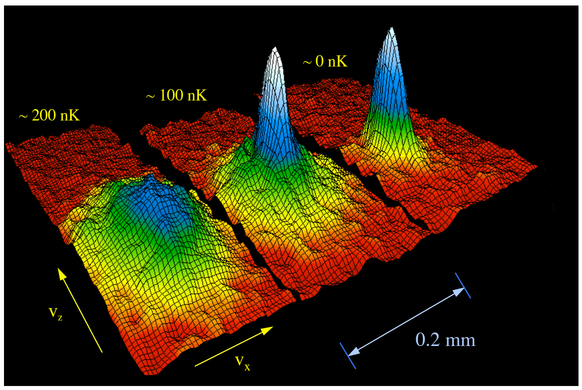

Figure 1: Bose-Einstein Condensate Forming

This is exciting and relevant because it allows physicists to explore quantum phenomena such as tunneling and entanglement in systems that are far more accessible experimentally, because of their size, than any quantum systems previously available. There are also phenomena that only occur in Bose-Einstein Condensates. One of these phenomena is the Bosenova.

Bosenova

The Bosenova has been observed at the JILA/NIST laboratory in Boulder, Colorado. It is a Bose-Einstein Condensate trapped in a magnetic field, in which the magnetic field is tuned (using so-called Feshbach resonances) so the atoms in the condensate are mutually attractive. This causes the Bose-Einstein Condensate to collapse. What is interesting about this experiment is the conclusion of the collapse. Instead of simply becoming smaller - as the particles clump together - as experimentalists expected, the condensate explodes, like a mini version of the super-nova of the cosmological variety. Experimentalists named the phenomena precisely because of these similarities. It also provides a simple laboratory model of the phenomena of a super-nova, giving good reason to study it.

There are currently no demonstrably accurate theoretical models for this phenomena. This could be due to a number of reasons, one of which is wrong theoretical models, or inaccurate numerical simulations of those theoretical models. This project looks to solve some of possible numerical problems that could be hindering the demonstration of the accuracy of the models.

Theoretical Formulation of Problem

Dr. Lincoln Carr (my physics advisor on this project), and his colleagues have created a theoretical formulation of the problem. As such, this problem will not be reformulated. The following are the partial differential equations that the theory supposes govern the Bosenova phenomenon.

$$\begin{aligned} i\hbar\frac{\partial\tilde{\phi}_a(R)}{\partial t} &= \left\{-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial R^2}+V_a(R)+U\left[\frac{|\tilde{\phi}_a(R)|^2}{R^2}+\frac{2\tilde{G}_N(R,0,0)}{R}\right]\right\}\tilde{\phi}_a(R) \\ &\quad+\left[\frac{U\tilde{G}_A(R,0,0)}{R}+\frac{g\tilde{\phi}_m(R)}{R}\right]\tilde{\phi}_a^*(R) \end{aligned} \tag{1}$$

$$\begin{aligned} i\hbar\frac{\partial\tilde{\phi}_m(R)}{\partial t} &= \left\{-\frac{\hbar^2}{4m}\frac{\partial^2}{\partial R^2}+2V_a(R)\right\}\tilde{\phi}_m(R) \\ &\quad+\frac{g}{2}\left\{\frac{\left(\tilde{\phi}_a(R)\right)^2}{R}+\tilde{G}_A(R,0,0)\right\} \end{aligned} \tag{2}$$

$$\begin{aligned} i\hbar\frac{\partial\tilde{G}_N(R,k,\ell)}{\partial t} &= -ik\frac{\hbar^2}{m}\left\{\left[\frac{\partial\tilde{G}_N(R,k,\ell+1)}{\partial R}-\frac{\tilde{G}_N(R,k,\ell+1)}{R}\right]\frac{\ell+1}{2\ell+3}\right. \\ &\quad\left.+\left[\frac{\partial\tilde{G}_N(R,k,\ell-1)}{\partial R}-\frac{\tilde{G}_N(R,k,\ell-1)}{R}\right]\frac{\ell}{2\ell-1}\right\} \\ &\quad+\left\{U\left[\frac{\left(\tilde{\phi}_a(R)\right)^2}{R^2}+\frac{\tilde{G}_A(R,0,0)}{R}\right]+g\frac{\tilde{\phi}_m(R)}{R}\right\}\tilde{G}_A^*(R,k,\ell) \\ &\quad-\left\{U\left[\frac{\left(\tilde{\phi}_a^*(R)\right)^2}{R^2}+\frac{\tilde{G}_A^*(R,0,0)}{R}\right]+g\frac{\tilde{\phi}_m^*(R)}{R}\right\}\tilde{G}_A(R,k,\ell) \end{aligned} \tag{3}$$

$$\begin{aligned} i\hbar\frac{\partial\tilde{G}_A(R,k,\ell)}{\partial t} &= \left\{-\frac{\hbar^2}{4m}\frac{\partial^2}{\partial R^2}+\frac{\hbar^2k^2}{m}+2V_a(R)\right. \\ &\quad\left.+4U\left[\frac{|\tilde{\phi}_a(R)|^2}{R^2}+\frac{\tilde{G}_N(R,0,0)}{R}\right]\right\}\tilde{G}_A(R,k,\ell) \\ &\quad+\left\{U\left[\frac{\left(\tilde{\phi}_a(R)\right)^2}{R^2}+\frac{\tilde{G}_A(R,0,0)}{R}\right]+g\frac{\tilde{\phi}_m(R)}{R}\right\} \\ &\quad\times\left[R\delta_{\ell,0}+\left\{\begin{array}{ll}2, & \ell\text{ even}\\ 0, & \ell\text{ odd}\end{array}\right\}\tilde{G}_N(R,k,\ell)\right] \end{aligned} \tag{4}$$

Note that this set of equations uses the following coordinate system (with small catch I will explain momentarily):

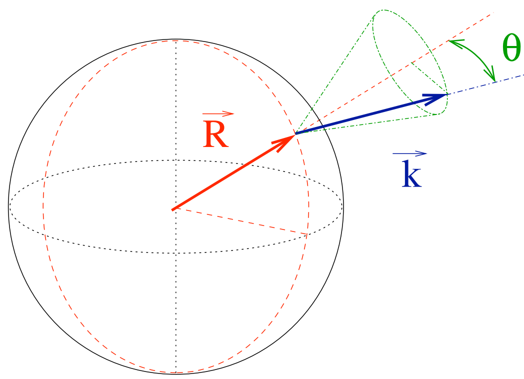

Figure 2: Coordinate System

Where $\vec{R}$ is the center of mass coordinate, $\vec{k}$ is the Fourier transformed relative coordinate, and θ is the angle between the two vectors. We can use spherical symmetries of our system to get the following transformations: $\vec{R} \rightarrow \|\vec{R}\| = R$, $\vec{k} \rightarrow \|\vec{k}\| = k$, and the catch: θ is also Fourier transformed to get the ℓ component of $\tilde{G}_N(R, k, \ell)$ and $\tilde{G}_A(R, k, \ell)$, where ℓ is the frequency of the partial wave in Fourier space.

- $\tilde{\phi}_a(R)$ is the atomic mean field. This represents the average density of the atoms in the condensate. As the condensate collapses, this field will decrease in value.
- $\tilde{\phi}_m(R)$ is the molecular mean field. This represents the average density of the atoms and molecules outside of the condensate. The values in this field will increase as the condensate collapses.
- $\tilde{G}_N(R, k, \ell)$ and $\tilde{G}_A(R, k, \ell)$ are the normal and anomalous densities, respectively. They have to do with correlations between different parts of the condensate.

Numerical Methods

As mentioned before, this project is principally concerned with the implementation of numerical methods to solve this set of time-dependent partial differential equations. We will use a method called the Method of Lines. We look at using finite differences and pseudo-spectral methods for the derivatives in space, and Runge-Kutta for the time integration.

Methods of Lines

The Method of Lines is a numerical method for the integration of time dependent partial differential equations. It discretizes the spatial dimensions of the problem as shown in Figure 3, and integrates each of those discrete components in time to find solutions to the PDEs.

For instance, we might have the following PDE:

$$\frac{\partial}{\partial t}\phi(x,t) = \left[\frac{\partial^2}{\partial x^2} + V\right]\phi(x,t)$$

If we discretize the spatial portion using 3-point second derivatives, we get the following system of coupled ordinary differential equations:

$$\begin{aligned}
\tfrac{\partial}{\partial t}\phi_1(t) &= \tfrac{\phi_0(t)-2\phi_1(t)+\phi_2(t)}{dR^2} + V\phi_1(t)\\
\tfrac{\partial}{\partial t}\phi_2(t) &= \tfrac{\phi_1(t)-2\phi_2(t)+\phi_3(t)}{dR^2} + V\phi_2(t)\\
&\vdots\\
\tfrac{\partial}{\partial t}\phi_i(t) &= \tfrac{\phi_{i-1}(t)-2\phi_i(t)+\phi_{i+1}(t)}{dR^2} + V\phi_i(t)
\end{aligned} \tag{5}$$

we can integrate these in time with the Runge-Kutta method.

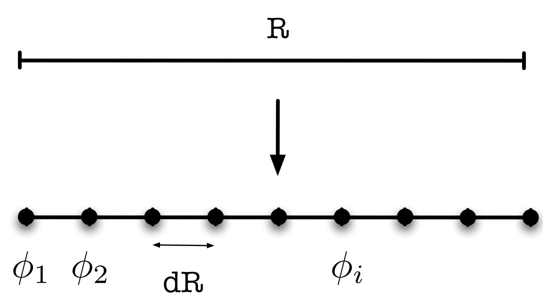

Figure 3: Method of Lines

We do something very similar to this in our code. There are some technicalities associated with the 3-dimensional nature of our system, but this method generalizes easily. And the derivatives in our problem only have to be taken with respect to R.

Pseudo-spectral Derivatives

Pseudo-spectral derivatives take advantage of the following fact:

$$\frac{\partial^2}{\partial x^2} f(x) = \mathfrak{F}^{-1}[p^2 \mathfrak{F}[f(x)]]$$

where

$$\mathfrak{F}, \mathfrak{F}^{-1}$$

are the Fourier transform and inverse Fourier transform, respectively. So, instead of using finite differences to calculate discrete derivatives, we use a discrete Fourier transform to transform our discretized function into the conjugate Fourier space, multiply by an appropriate constant p^2 and then use an inverse discrete Fourier transform to get back to coordinate space. This process gives us the derivative of the discretized function.

Runge-Kutta Time Integration

Runge-Kutta uses multiple intermediate time-steps to approximate a single temporal derivative. We are using a fourth order Runge-Kutta. As shown in Figure 4, the following happens:

- The first time step is taken using the derivative at time t_i, $\delta\phi_1$, with length $\frac{1}{2}\delta t$.
- Then the derivative at $\phi_{\delta\phi_1}(t_i + \frac{1}{2}\delta_t)$, $\delta\phi_2$ is found.
- Again, a time step of length $\frac{1}{2}\delta t$ is taken, but using the derivative $\delta\phi_2$, at which point the derivative is again found, giving $\delta\phi_3$.
- Once more, we take a step using $\delta\phi_3$, but this time of length δt, and find the derivative there as well, $\delta\phi_4$.
- Finally, we get the final derivative, $\bar{\delta\phi}$, which we use to take the full time step of length δt.

$$\bar{\delta\phi} = \frac{\delta\phi_1 + 2\delta\phi_2 + 2\delta\phi_3 + \delta\phi_4}{6}$$

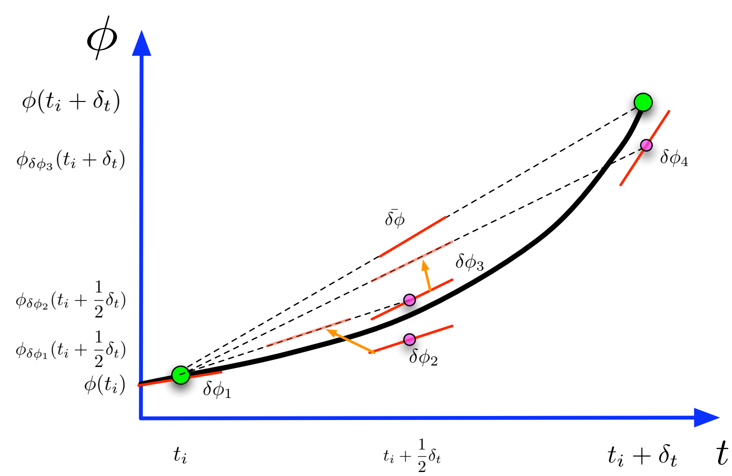

Figure 4: Runge-Kutta Time Integration

The fourth order Runge-Kutta gives and error of $O(\delta t^4)$.

Numerical Method Summary

We can use the methods outlined above to solve the PDEs in equations (1) - (4), discretizing in space with the Method of Lines, and integrating the resulting ODEs with Runge-Kutta. A formal derivation of this process is beyond the scope of this report, but the results of the derivation are in the included code.

Results

The results are at the same time heartening and disheartening. With 3-point derivatives, we get the following in the propagation of the ϕ_a PDE, with no references to the other PDEs. This propagation ought to be stable, with little to no error. As is obvious in Figure 5, it is not. There are numerical errors in the implementation.

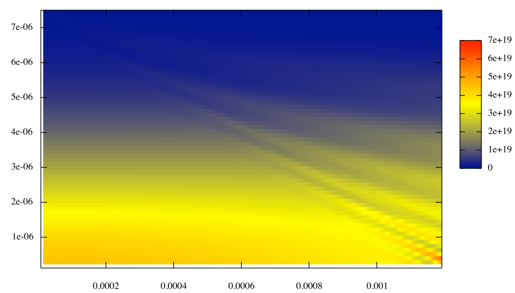

Figure 5: 3 point derivatives propagation of ϕ_a

Because of this, we implemented 5-point derivatives, with the following propagation. As you can see in Figure 6, the results are much better, with stable propagation. However, there are still small numerical errors (seen better in printouts of the data), that plague this code.

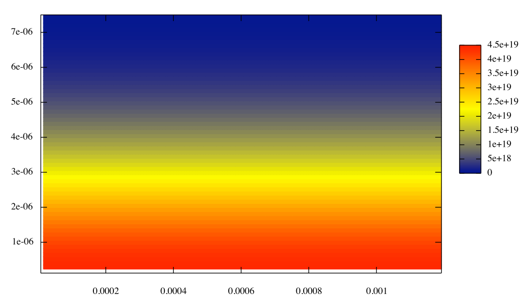

Figure 6: 5 point derivatives propagation of ϕ_a

Because of those errors, we decided to implement an even more accurate discrete derivative, pseudo-spectral derivatives, as described above. These derivatives had the exact same error characteristics as the 5-point derivatives, thus not improving the simulation. See Figure 7.

Given these results, we must investigate further the cause of these errors, perhaps implementing this simulation using a different method. As such, the initial goals of this project were not fully fulfilled. However,

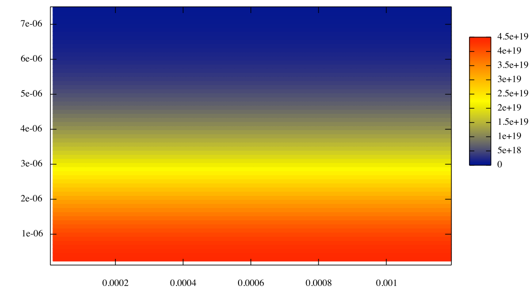

Figure 7: Psuedo-spectral derivatives propagation of ϕ_a

this should not be seen as a failure. This is a research project, and must be understood as such. These circumstances have merely closed a few doors, and we shall have to investigate more possibilities in the future.

Deliverables

The code associated with this project will be submitted on a CD. This is the deliverable.

Future Work and Use of Code

Because of the unsatisfactory nature of the conclusions reached with this project, more investigation is required. Dr. Carr and the members of his group will be continuing this research, investigating the possible problems with this code, and potentially moving on to other methods of simulation.

This code is a small part of a larger investigation into the properties of this phenomenon known as the Bosenova. It will allow Dr. Carr and his students (graduate and undergraduate) to research this phenomenon more deeply, and gain insight into how it works.