Project Report for IDC605

Solving The Gross-Pitaevskii Equation using Spectral Method

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1 Abstract

In this project, I'll solve the Gross-Pitaevskii equation using spectral methods. I've used two time spitting spectral schemes which are Lie splitting and strang splitting method both in 1-D and 2-D. I'll try to compare various potential operators for the one-dimensional (1D) and two-dimensional (2D) Gross-Pitaevskii equation (GPE) for Bose-Einstein condensates with some smooth inital conditions.

2 Introduction

The Gross–Pitaevskii equation (GPE, named after Eugene P. Gross and Lev Petrovich Pitaevskii) describes the ground state of a quantum system of identical bosons using the Hartree–Fock approximation and the pseudopotential interaction model. The Gross-Pitaevskii equation (GPE), a nonlinear Schrödinger equation (NLSE) for the macroscopic wave functions, governs the properties of a BEC at temperatures T far below the critical condensation temperature T_c. The GPE includes a term for the trap potential as well as the mean field interaction between atoms in the gas which manifests as a nonlinear term. Attractive interactions as well as repulsive interactions are accounted for in the GPE through the use of a focussing constant which may be positive (focussing) or negative (defocussing).

3 Form of the Equation

The equation has the form of the Schrödinger equation with the addition of an interaction term. The coupling constant g is proportional to the s-wave scattering length a_s of two interacting bosons:

$g = \frac{4\pi\hbar^2 a_s}{m}$. where $\hbar$ is planck constant and m is the mass of boson.

The time-dependent Gross–Pitaevskii equation is

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

where Ψ is the wavefunction, or order parameter, and V is the external potential (e.g. a harmonic trap)

The number of particles is related to the wavefunction by $N = \int |\Psi(\mathbf{r})|^2 d^3r$. The single particle wave function $\psi(\mathbf{r})$ obeys the normalization condition:

$$\int_{R^3} |\psi(\mathbf{r})|^2 dr = 1$$

.

4 Dimensionless Equation

Throughout the project I've used the normalized form of gross-pitaevskii equation with harmonic potential. I've introduced the following parameters:

$$\tilde{t} = \omega_s t, \quad \tilde{\mathbf{r}} = \frac{\mathbf{r}}{x_s}, \quad \tilde{\psi}(\tilde{\mathbf{r}}, \tilde{t}) = x_s^{3/2}\psi(\mathbf{r}, t)$$

Also, I represent

$$\tilde{V}(\tilde{\mathbf{r}}) = \frac{V(\mathbf{r})}{E_s}$$

Where, $E_s = \hbar w_s$ ans ω_s is characteristic(trap) frequency. The GPE will reduce to following:

$$i\hbar w_s \frac{\partial\tilde{\psi}(\tilde{\mathbf{r}}, \tilde{t})}{\partial\tilde{t}} = (-\frac{\hbar^2}{2mx_s^2}\nabla^2 + E_s\tilde{V}(\tilde{\mathbf{r}}) + gx_s^{-3}|\tilde{\psi}(\tilde{\mathbf{r}}, \tilde{t})|^2)\tilde{\psi}(\tilde{\mathbf{r}}, \tilde{t})$$

$$Or, \qquad i\frac{\partial\tilde{\psi}(\tilde{\mathbf{r}}, \tilde{t})}{\partial\tilde{t}} = (-\frac{\hbar}{2mx_s^2\omega_s}\nabla^2 + \tilde{V}(\tilde{\mathbf{r}}) + \frac{g}{\hbar x_s^3 w_s}|\tilde{\psi}(\tilde{\mathbf{r}}, \tilde{t})|^2)\tilde{\psi}(\tilde{\mathbf{r}}, \tilde{t})$$

x_s is the characteristic length of the condensate. For my simplicity, I remove the ˜ from every variable from equation. Now, it has form:

$$i\frac{\partial\psi(\mathbf{r}, t)}{\partial t} = \left(-\frac{\alpha}{2}\nabla^2 + V(\mathbf{r}) + \kappa|\psi(\mathbf{r}, t)|^2\right)\psi(\mathbf{r}, t)$$

where, $\alpha = \frac{\hbar}{mx_s^2 w_s}$ and $\kappa = \frac{g}{hx_s^3 w_s}$ or $\frac{4\pi\hbar a_s}{mx_s^3 w_s}$. Healing length x_h is defined as

$$x_h := \left(\frac{8\pi|a_s|}{x_s^3}\right)^{-1/2}$$

For ground state,

$$\alpha = 1 \Rightarrow x_s = \sqrt{\frac{\hbar}{mw_s}}$$

$\kappa < 0$ implies attractive interaction while $\kappa > 0$ implies repulsive interaction.

5 Solving the Equation

Equation involves the partial differential term w.r.t spatial parameters. So, first we use spatial discretization. Taking euquation to fourier space (1-D), it has following from:

$$i\frac{\partial\widehat{\psi_l}}{\partial t} = \frac{\alpha\mu_l^2}{2}\widehat{\psi_l} + (\widehat{V\psi})_l + \kappa\widehat{|\psi|^2}\psi_l$$

where, $\mu_l = \frac{2\pi l}{b-a}$ and

$$\widehat{\psi_l} = \sum_{j=0}^{M-1} \psi_j e^{-i\mu_l(x_j-a)}, l = \frac{M}{2}, ..., \frac{M}{2} - 1$$

Also,

$$\psi = \frac{1}{M} \sum_{l=M/2}^{l=M/2-1} \widehat{\psi_l} e^{i\mu_l(x_j-a)}$$

I've chosen spatial mesh size$\Delta x = \frac{(b-a)}{M}$ and time step size $t_{n+1} - t_n = \Delta t > 0$ where $a \leq x \leq b$. if we substitute ψ by below equation following by multiplication of whole equation by $e^{i\frac{\alpha}{2}\mu_l^2 t}$:

$$\tilde{\widehat{\psi_l}} = \widehat{\psi_l} e^{i\frac{\alpha}{2}\mu_l^2 t}$$

Now, equation would look like:

$$\frac{\partial \tilde{\widehat{\psi_l}}}{\partial t} = -i \left\{ (\widehat{V\psi})_l + (\kappa \widehat{|\psi|^2\psi})_l \right\} e^{i\frac{\alpha}{2}\mu_l^2 t}$$

Note that: $\frac{\partial \tilde{\widehat{\psi_l}}}{\partial t} = \frac{d\tilde{\widehat{\psi_l}}}{dt}$. So, this equation is now in the form of ODE. we can use any stable scheme to solve this equation conserving $\int |\psi|^2 dx = 1$

5.1 Leapfrog method

It is the method which can conserve $\int |\psi|^2 dx = 1$ over the iteration. which can be stated as:

$$\tilde{\widehat{\psi_l}}^{n+1} = \tilde{\widehat{\psi_l}}^{n-1} - 2i\Delta t \left\{ (\widehat{V\psi})_l^n + (\kappa \widehat{|\psi|^2\psi})_l^n \right\} e^{i\frac{\alpha}{2}\mu_l^2 t_n}$$

$$\Rightarrow \widehat{\psi_l}^{n+1} e^{i\frac{\alpha}{2}\mu_l^2 t_{n+1}} = \widehat{\psi_l}^{n-1} e^{i\frac{\alpha}{2}\mu_l^2 t_{n-1}} - 2i\Delta t \left\{ (\widehat{V\psi})_l^n + (\kappa \widehat{|\psi|^2\psi})_l^n \right\} e^{i\frac{\alpha}{2}\mu_l^2 t_n}$$

$$\Rightarrow \widehat{\psi_l}^{n+1} = \widehat{\psi_l}^{n-1} e^{-i\alpha\mu_l^2 \Delta t} - 2i\Delta t \left\{ (\widehat{V\psi})_l^n + (\kappa \widehat{|\psi|^2\psi})_l^n \right\} e^{-i\frac{\alpha}{2}\mu_l^2 \Delta t}$$

This equation can be solved using leapfrog but stability is the issue here. It is not stable for any mesh size and time step although it is time reversible. For initial condition for calculation of $\hat{\psi}_l^1$ we may use euler-forward scheme. Note that if we do $\hat{\psi}_l^1 = \hat{\psi}_l^0$ it will introduce the error of $O(\Delta t)$ order. You can choose initial configuration like as follows:

$$\psi(x,0) = \frac{1}{(\pi)^{\frac{1}{4}}} e^{\frac{-x^2}{2}}.$$

Euler forward for ψ_j^1 is as follows.

$$\psi_l^1 = \psi_l^0 e^{-i\alpha\mu_l^2 \Delta t/2} - i\Delta t \left\{ (\widehat{V\psi})_l^0 + (\kappa \widehat{|\psi|^2\psi})_l^0 \right\} e^{-i\frac{\alpha}{2}\mu_l^2 \Delta t}$$

6 Alternate Solution

I present time-splitting trigonometric spectral approximations of the problem, with periodic boundary conditions. We first split the Dimensionless GPE Equation using Lie-Splitting Method (**LS**) and combine splitting step using standard Strang splitting (**SS**). he time-splitting spectral schemes LS and SS are unconditionally stable. In fact,under any mesh size Δt and time step Δx. For the simplicity of notation we shall introduce the method for the case of one space dimension ($D = 1$). The analysis in the next section will also focus on the case $D = 1$. Generalizations to $D > 1$ are straightforward for tensor product grids and the results remain valid without modifications. Also, this method conserves $\int |\psi|^2 dx$ term.

6.1 Lie Splitting

The GPE euqation is solved into two parts. First solves:

$$i\frac{\partial \psi}{\partial t} = -\frac{\alpha}{2}\frac{\partial^2 \psi}{\partial x^2}$$

we'll discretize this equation in space by spectral method and will be intergrated in time exaclty. Fourier transformation of above equation:

$$i\frac{\partial \widehat{\psi_l}}{\partial t} = \frac{\alpha \mu_l^2}{2}\widehat{\psi_l}$$

Now this is an ODE can be exactly solvable. It has a solution of the form:

$$\psi_j = \frac{1}{M}\sum_{l=-M/2}^{M/2-1} e^{-i\alpha \Delta t \mu_l^2/2}\widehat{\psi_l} e^{i\mu_l(x_j - a)}$$

Now, the 2^{nd} part of the equation is

$$i\frac{\partial \psi}{\partial t} = V\psi + \kappa|\psi^2|\psi$$

which is again a ODE and can be solved exactly. We can engulf the potential term by multiplying whole equation by e^{iVt} and then substituting $\hat{\psi} = \psi e^{iVt}$.

6.2 The Strang Splitting Spectral Method

As in the previous method, GPE eqn to be split into two parts. This time, from time $t = t_n$ to $t = t_n + 1$, we combine the splitting steps via the standard Strang splitting:

$$\psi_j^* = e^{-iV\Delta t/2}\psi_j^n$$

$$\psi_j^{**} = \frac{1}{M}\sum_{l=-M/2}^{M/2-1} e^{-i\alpha \Delta t \mu_l^2/2}\widehat{\psi_j^*} e^{i\mu_l(x_j - a)}, j = 0, 1, 2, ..., M-1$$

$$\psi_j^{n+1} = e^{-i(V+\kappa|\psi_j^{**}|^2)\Delta/2}\psi_j^{**}, j = 0, 1, 2, 3....., M-1$$

where $\widehat{\psi_j^*}$ is the fourier coefficient of ψ_j^*, i.e $\widehat{\psi_j^*} = \sum_{j=0}^{M-1}\psi_j^* e^{-i\mu_l(x_j - a)}$. The overall time discretization error comes solely from the splitting, which is $O(\Delta t^2)$.

7 Simulations

I look at the graphs of the solutions to the GPE at various times and for various potentials. Only two simulation snap shown here, other can be accessed through links provided in links & Simulation section.

7.1 1-D Simulation

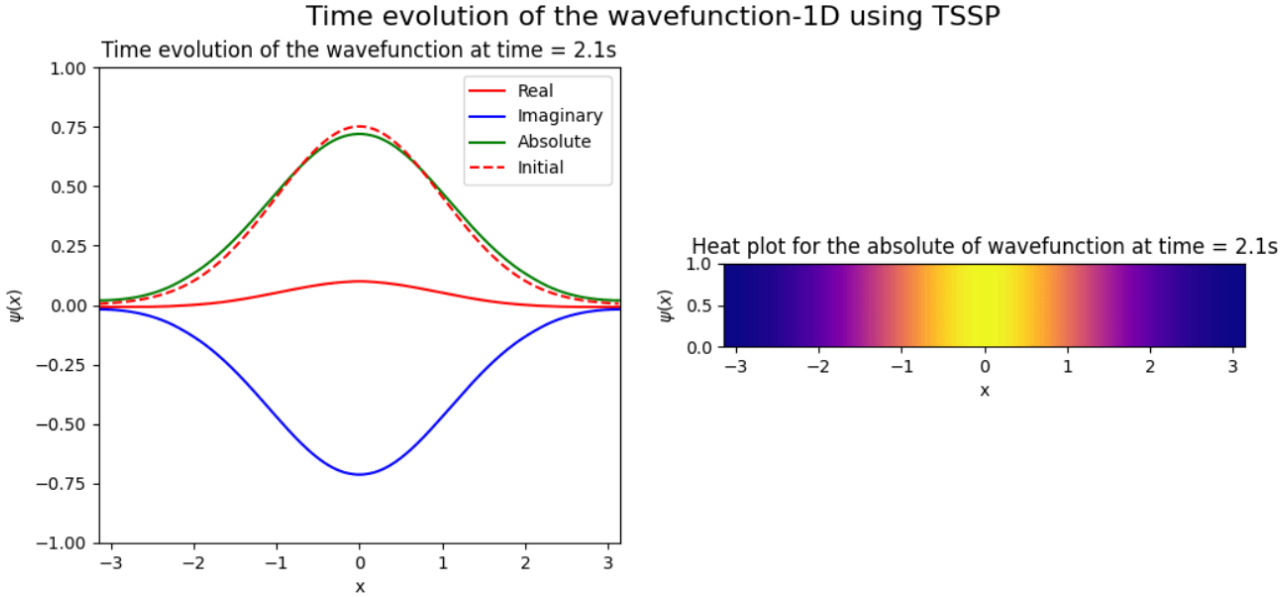
I've chosen the Gaussian Initial Condition for 1-D. It can be represented as follows:

$$\psi(x,0) = \frac{1}{(\pi)^{1/4}} e^{\frac{-x^2}{2}}$$

we can verify that $\int_{-\infty}^{\infty} |\psi(x,0)|^2 dx = 1$.

7.1.1 Visualizations

For this simulation the values are $\alpha = \kappa = 1.$ and $V(x) = \frac{x^2}{2}$.



for above graph are shown for particle confined in $-\pi \leq x \leq \pi$, grid mesh size $\Delta x = \frac{2\pi}{500}$ and time step $\Delta t = 0.01$.

7.2 2-D Simulation

Again, I've chosen the Gaussian Initial Condition for 2-D. It can be represented as follows:

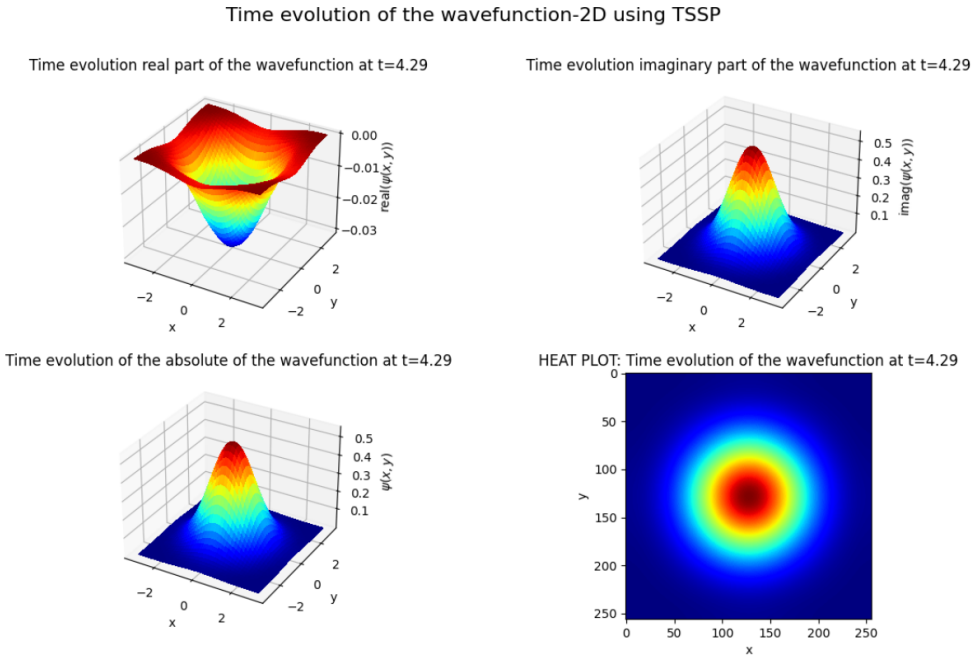
$$\psi(x,y,0) = \frac{1}{\sqrt{\pi}} e^{\frac{-(x^2+y^2)}{2}}$$

we can verify that

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} |\psi(x,y,0)|^2 dxdy = 1$$

7.2.1 Visualizations

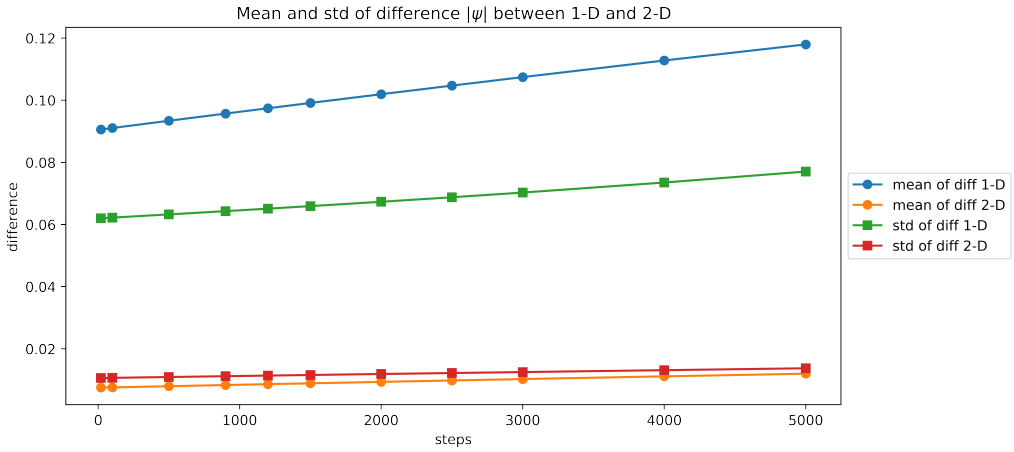
For this simulation the values are $\alpha = \kappa = 1.$ and $V(x, y) = \frac{x^2+y^2}{2}$.



for above graph are shown for particle confined in $-\pi \leq x \leq \pi, -\pi \leq y \leq \pi$, grid mesh size $\Delta x = \Delta y = \frac{2\pi}{256}$ and time step $\Delta t = 0.01$.

8 Comparison B/W Leapfrog & TSSP

I'll compare the TSSP method with Leapfrog method. Errors in the discretization of the space variable are investigated. For the Gaussian starting condition from before, a very short time step (t =.0001) (for stability) is selected, and the spatial discretization is taken as same for both the methods. The following graph shows the mean and std-dev of difference in values of $|\psi|$ among methods for 1-D and 2-D.



9 Code & Simulation links

Spectral Method 1D simulation
Leapfrog Method 1D simulation
Spectral Method 2D simulation
Leapfrog Method 2D simulation

9.1 Programming code

9.1.1 TSSP Code for 1-D equation

```
L = 2*np.pi #Length of the domain
N = 500 #Number of Grid points
DX = L/N #Grid spacing
GRID = np.arange(-L/2,L/2,DX, dtype=complex) #Grid points
DT = 0.01 #Time step
alpha = 1
kappa = 1
mu_sq  = (2*np.pi*np.fft.fftfreq(N, d=DX))**2 #Fourier frequencies

def update(frame):
    global psi
    #print(np.sum(np.abs(psi)**2)*DX)
    psi  = np.fft.fft(psi*np.exp(-0.5j*DT*potential(GRID)))
    psi = np.exp(-0.5j*DT*alpha*mu_sq)*psi
    psi = np.fft.ifft(psi)
    psi = psi*np.exp(-0.5j*DT*(kappa*np.absolute(psi)**2 + potential(GRID)))
```

9.1.2 TSSP Code for 2-D equation

```
L = 2*np.pi
N = 256
DX = L/N
GRID = np.meshgrid(np.arange(-L/2,L/2,DX), np.arange(-L/2,L/2,DX))
GRID_X, GRID_Y = GRID
DT = 0.01
alpha = 1
kappa = 1
mu = np.meshgrid(2*np.pi*np.fft.fftfreq(N, d=DX),2*np.pi*np.fft.fftfreq(N, d=DX))
mu_sq = mu[0]**2 + mu[1]**2

def update(frame):
    global psi
    psi  = np.fft.fft2(psi*np.exp(-0.5j*DT*potential(GRID)))
    psi = np.exp(-0.5j*DT*alpha*mu_sq)*psi
    psi = np.fft.ifft2(psi)
    psi = psi*np.exp(-0.5j*DT*(kappa*np.absolute(psi)**2 + potential(GRID)))
    ax.clear(), ax1.clear(), ax2.clear(), ax3.clear()
```

Whole code can be referenced through Github link.

10 Conclusion

The Gross-Pitaevskii method produces non-analytic solutions in the study of Bose-Einstein condensation, which must be solved numerically. Many approaches have been developed to solve this nonlinear Schrodinger equation, but the Strang Splitting method, in particular, has been proved to be extremely accurate and light on computer systems.

Leapfrog is unstable at some initial parameter for my when I took $\Delta = 0.001$ I got stable result whereas for $\Delta t = 0.01$ the model is diverging after 9385 steps in time.

10.1 Time Taken by Computer Program

1-D Leapfrog, steps = 1000, dt = 0.01

real	4m16.810s
user	4m22.187s
sys	0m8.725s

2-D Leapfrog, steps = 1000, dt = 0.01

real	19m45.575s
user	48m45.180s
sys	23m41.725s

1-D TSSP , steps = 1000, dt = 0.01

real	3m21.334s
user	3m26.126s
sys	0m7.157s

2-D TSSP , steps = 1000, dt = 0.01

real	18m6.690s
user	46m57.602s
sys	23m52.085s

References

[1] Galati, Luigi, "Numerical Solutions to the Gross-Pitaevskii Equation for Bose-Einstein Condensates" (2013). Electronic Theses and Dissertations. 844.

[2] Bao, Weizhu, Numerical Solution of the Gross-Pitaevskii Equation for Bose-Einstein Condensation.