Project of Computational Mathematics

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1 Abstract

In this essay, we try to apply three methods to solve two-dimension Gross Pitaevskii equations numerically, including explicit finite difference method, Time Splitting Spectrum Method and Fourier spectral method. Firstly, the explicit finite difference method fails to match the reference answer because of lacking of boundary condition. Secondly, the answer given by TSSP matches the picture in Bao's article, and $|\Psi(0,0)|^2$ decease to zero with oscillations. Moreover, when we try to apply Fourier spectral method to these equations, we find FSM is not suitable for Gross–Pitaevskii equations. Finally, we discuss the advantages and disadvantages of different methods.

2 Description of the problem

For 3d Gross–Pitaevskii equation(GPE),

$$i\varepsilon\frac{\partial\psi(x,t)}{\partial t} = -\frac{\varepsilon^2}{2}\nabla^2\psi(x,t) + V_d(x)\psi(x,t) + \kappa_d|\psi(x,t)|^2\psi(x,t)$$

Choose $d = 2$, we solve the problem on $[-10, 10]^2$, with mesh size $h = \frac{1}{51.2}$ and time step $k = 0.00005$. Do computations for the following cases:

1. $O(1)-$ intersections, $\varepsilon = 1.0, \gamma_y = 1.0, kappa_2 = -2.0,$
   $\psi(x, y, 0) = \frac{1}{\sqrt{(\pi\varepsilon)}}exp(-(x^2 + y^2)/(2\varepsilon)$;

2. Strong intersections, $\varepsilon = 0.3, \gamma_y = 1.0, kappa_2 = -1.9718,$
   $\psi(x, y, 0) = \frac{1}{\sqrt{(\pi\varepsilon)}}exp(-(x^2 + y^2)/(2\varepsilon)$;

3 Numerical Methods

In order to solve this problem, we apply three numerical methods to solve these equations, including finite difference method(FDM), Time Splitting

Spectrum Method(TSSP) and Fourier spectrum method(FSM). And we analysis and compare their convergence and convergent rate.

3.1 Explicit Finite Difference Method

Firstly, we try to discretize equation(1) with simply finite scheme.As the dimension of these problem is too large(about 10^{12}),which leads to it is hard to solve the related linear system, therefore, it is impossible to use implicit or semi-implicit method, such as Crank-Nicolson finite difference method. Discretize equation(1) as follows:

$$i\varepsilon\frac{\psi_{ij}^{n+1}-\psi_{i,j}^{n}}{k} = -\frac{\varepsilon^2}{2}(\psi_{i+1,j}^{n}-4\psi_{i,j}^{n}+\psi_{i-1,j}^{n}+\psi_{i,j+1}^{n}+\psi_{i,j-1}^{n})+\frac{1}{2}(x_i^2+y_j^2)\psi_{i,j}^{n}-2|\psi_{i,j}^{n}|^2\psi_{i,j}^{n}$$

with boundary condition $\psi_{0,:}^{n} = \psi_{N,:}^{n} = \psi^{n}:, 0 = \psi_{:,N}^{n} = 0$

3.1.1 Numerical Results of FDM

The above scheme is executed with Matlab(R2018b) in MacbookPro(CPU:). For case I: $\varepsilon = 1.0, \gamma_y = 1.0, kappa_2 = -2.0, \delta t = 0.005, h = 0.02$,Fig1 shows the magnitude of $|\Psi|^2$ decrease to 0 very fast without any oscillations when t goes from 0 to 40. This fast decay means FDM ignores some details of Gross–Pitaevskii equation,then is not suitable for this equations.

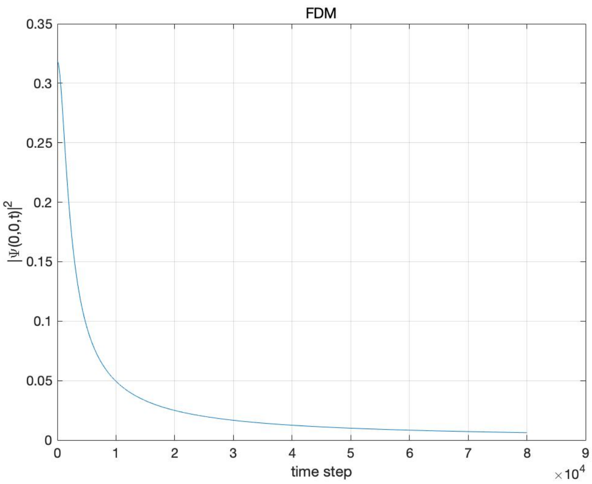


Figure 1: $\Psi(0, 0, t)$

3.2 Time Splitting Spectrum Method

As Bao(2003) mentioned TSSP is unconditionally stable, time reversible, conserves the total particle number and it is time transverse-invariant.Then we apply TSSP method for these 2d GPE as follows. For time-splitting spectrum method, the 2d GPE is solved in two splitting steps. One solves first:

$$i\varepsilon\frac{\partial\psi(x,y,t)}{\partial t} = -\frac{\varepsilon^2}{2}(\psi(x,y,t)_{xx} + \psi(x,y,t)_{yy})$$

for the time step of length k, followed by solving

$$i\varepsilon\frac{\partial\psi(x,y,t)}{\partial t} = \frac{x^2+y^2}{2}\psi(x,y,t) + \kappa_2|\psi(x,y,t)|^2\psi(x,y,t)$$

Therefore, from t_n to t_{n+1}, combine the splitting steps via the standard Strang splitting:

$$\psi^*_{j,s} = exp(-i((x_j^2+y_s^2)/2 + \kappa_2|\psi_{j,s}|^2)k/(2\varepsilon))\psi^n_{j,s}$$

$$\psi^{**}_{j,s} = \frac{1}{MN}\sum_{p=-N/2}^{N/2+1}\sum_{l=-M/2}^{M/2+1} exp(-i\varepsilon k(\mu_l^2+\mu_p^2)/2)\hat{\psi}^*_{l,p}exp(i(\mu_l(x_j-a)+\mu_p(y_s-a)))$$

,

$$\psi^{n+1}_{j,s} = exp(-i((x_j^2+y_s^2) + \kappa_2|\psi^{**}_{j,s}|^2)k/(2\varepsilon))\psi^{**}_{j,s}$$

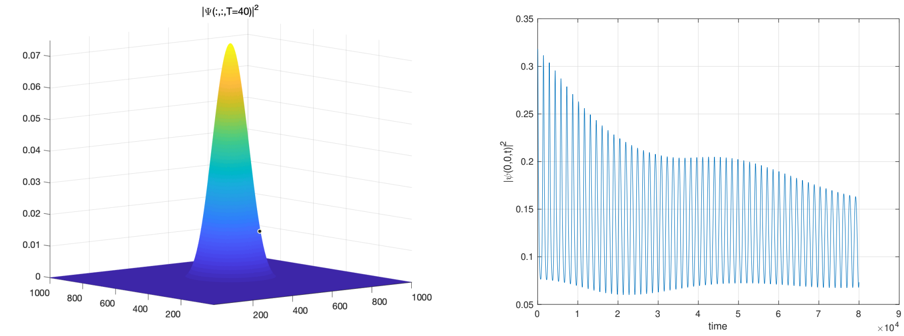
$j = 0, 1, 2, 3, ..., M-1, S = 0, 1, 2, 3, ..., N-1.$
where $\hat{\psi}^*_{l,p}$ is the Fourier coefficients of ψ^*,

$$\mu_l = \frac{2\pi l}{b-a}, \mu_p = \frac{2\pi p}{b-a}, \hat{\psi}^*_{j,s} = \sum_{p=-N/2}^{N/2+1}\sum_{l=-M/2}^{M/2+1}\psi^*_{j,s}exp(-i(\mu_l(x_j-a)+\mu_p(y_s-a)))$$

3.2.1 Numerical Results of TSSP

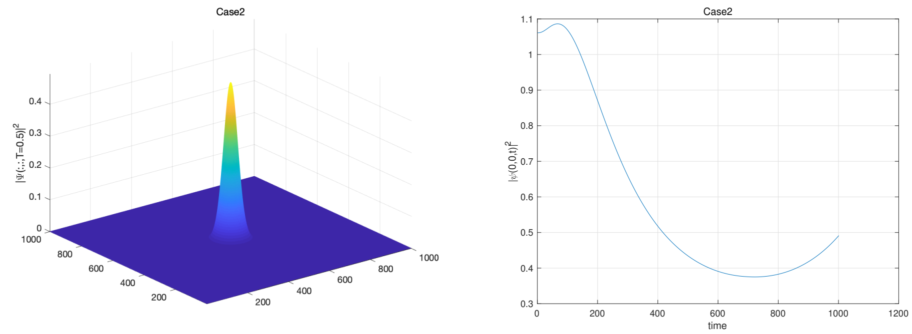
The numerical results is showed in Fig2.As the performance limitation of personal computer, we increase δt from 0.00005 to 0.0005, the running time for calculate $|\Psi(T=40)|^2$ is about 6298 seconds. Fig2 shows, $|\Psi(T=40)|^2$ is very similar to the picture showed in Bao's article and the right figure shows that the energy decrease to zero with oscillations as time goes to infinite, which is according to theoretical analysis.

Unfortunately,as Fig3 shows the results of Case II do not match the reference answer in Bao's essay.



(a) $T = 40$ (b) $|\Psi|^2$

Figure 2: TSSP for Case I



(a) $T = 0.5$ (b) $|\Psi|^2$

Figure 3: TSSP for Case II

3.3 Fourier Spectral Method

Inspired by the TSSP method, we try to apply Fourier Spectral method to the original equation directly. For Fourier spectrum method,

$$i\varepsilon\frac{\partial\psi(x,y,t)}{\partial t} = -\frac{\varepsilon^2}{2}(\psi(x,y,t)_{xx}+\psi(x,y,t)_{yy})+\frac{x^2+y^2}{2}\psi(x,y,t)+\kappa_2|\psi(x,y,t)|^2\psi(x,y,t)$$

However, when we derive the iteration formula we find it is hard to apply Fourier Spectral method directly because of the existence of term $\frac{x^2+y^2}{2}$, which means FSM is not suitable for this kind of PDEs.

4 Discussions

For implicit and semi-implicit finite difference methods, their performances depend on the dimension of the related linear system even if they preserve the convergence and stability, moreover, even though explicit finite difference method is fast, it might diverge. And these finite method require the boundary condition, however, the boundary condition is not available, such as Case I. We analysis the failure of explicit FDM is induced by setting the boundary to zero coercively.

For TSSP method, this method is powerful for many kinds of nonlinear Schroedinger equation because it splits a complicated PDE into an ODE and a simple PDE. Especially, TSSP splits 2d GPE into a very simple ODE and a heat equation, both of them could be solved very fast and accurately.

5 References

[1] Weizhu Bao, Dieter Jaksch and Peter A.Markowich, Numerical Solution of the Grosss-Pitaevskii Equation for Bose-Einstein Condensation.

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[3] https://en.wikibooks.org/wiki/Parallel_Spectral_Numerical_Methods/Examples_in_Matlab

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