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Sinc Collocation Numerical Methods for Solving Two-Dimensional Gross-Pitaevskii Equations with Non-Homogeneous Dirichlet Boundary Conditions

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Abstract. This paper presents the numerical solution of the time-dependent Gross-Pitaevskii Equation describing the movement of quantum mechanics particles under non-homogeneous boundary conditions. Due to their inherent non-linearity, the equation generally can not be solved analytically. Instead, a highly accurate approximation to the solutions defined in a finite domain is proposed, using the Crank-Nicolson difference method and Sinc Collocation numerical methods to discretize separately in time and space. Two Sinc numerical approaches, involving the Sinc Collocation Method (SCM) and the Sinc Derivative Collocation Method (SDCM), are easy to implement. The results demonstrate that Sinc numerical methods are highly efficient and yield accurate results. Mainly, the SDCM decays errors faster than the SCM. Future work suggests that the SDCM can be extensively applied to approximate solutions under other boundary conditions to demonstrate its broad applicability further.

AMS subject classifications: 65N35, 81Q05

Key words: Quantum mechanics, spectral method, time-dependent partial differential equation, boundary value problem.

1 Introduction

1.1 Gross-Pitaevskii equation

In modern physics, the Gross-Pitaevskii Equation (GPE) as an important partial differential equation (PDE) has earned central importance due to its applications. For instance,

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it is remarkable to describe the phenomenon of a Bose-Einstein Condensate [1, 2] representing the phase transition where a macroscopic number of particles all go into the same quantum state while cooling them below the critical transition temperature [3]. In this paper, we consider the two-dimensional generalized Gross-Pitaevskii Equation given by:

$$iu_t+\alpha u_{xx}+\alpha u_{yy}+f(x,y)u+\rho|u|^2u=0,\quad (x,y)\in\Omega,\quad t\geq 0, \tag{1.1}$$

with the initial condition and Dirichlet boundary conditions:

$$\begin{aligned}&u(x,y,t=0)=g(x,y,0),\\&u(x,y,t)=\Theta(x,y,t),\quad (x,y)\in\Gamma,\quad t>0,\end{aligned}$$

where $i=\sqrt{-1}$ is the imaginary unit, α is a real constant, t is the time variable with $t\geq 0$, $(x,y)\in\mathbb{R}^2$, Ω denotes a bounded and open domain in $\mathbb{R}^2$, Γ is the simple closed curve bounding the region Ω, $u=u(x,y,t)$ is a complex-valued wave function, $|u|^2$ is named as the atomic density, $|u|^2u$ is the so-called cubic nonlinearity, and ρ is a given dimensionless constant describing the strength of interaction (negative for the repulsive or defocusing interaction and positive for the attractive or focusing interaction). In this case, the interactions are weak enough that the predictions made by this equation are very reliable [4]. The external potential function $f(x,y)$, the function $g(x,y,t)$ and $\Theta(x,y,t)$ are all known real-valued functions. The special case of $\rho=0$ in Eq. (1.1) corresponds to the well-known Schrödinger Equation (SCE). Also, when $f(x,y)=0$, it becomes the standard Non-Linear Schrödinger Equation (NLSE). Therefore, the GPE incorporates the properties of the SCE and the NLSE.

1.2 Literature review

Even though Gross, E. P. [5] and Pitaevskii, L. P. [6] separately presented the GPE in 1961, the academic research on Eq. (1.1) has not been paused, especially in its numerical solutions. That results from the truth that analytical solutions are hard to figure out. Even if the GPE given by Eq. (1.1) has an exact resolution, it usually exhibits large temporal and spatial gradients, including solition solutions, breather solutions, and bound states with multiple modes [7]. Thus, employing efficient and effective numerical methods is vital to identify solutions' qualitative and quantitative characteristics.

An extensive study in theoretical analyses and numerical simulations for the GPE has existed in the literature. As one of the typical techniques, Eq. (1.1) is solved in two time-splitting steps. The process relies on identical small time steps and eliminates the nonlinear mechanisms influenced in the spatial domain for numerical solutions [2, 8, 9]. Due to the limitation of the technique, wide-ranging researches are intended to discretize the GPE in time and space, respectively, for acquiring numerical solutions. With this regard, the Finite Difference Method (FDM) is a sweeping way to discretize in the temporal dimension. Especially, the Crank-Nicolson Method (CNM) is a prominent numerical treatment with the second-order accuracy for discretizing the time derivative [10]. In