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An efficient and conservative compact finite difference scheme for the coupled Gross–Pitaevskii equations describing spin-1 Bose–Einstein condensate

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A B S T R A C T

The coupled Gross–Pitaevskii system studied in this paper is an important mathematical model describing spin-1 Bose-Einstein condensate. We propose a linearized and decoupled compact finite difference scheme for the coupled Gross–Pitaevskii system, which means that only three tri-diagonal systems of linear algebraic equations at each time step need to be solved by using Thomas algorithm. New types of mass functional, magnetization functional and energy functional are defined by using a recursive relation to prove that the new scheme preserves the total mass, energy and magnetization in the discrete sense. Besides the standard energy method, we introduce an induction argument as well as a lifting technique to establish the optimal error estimate of the numerical solution without imposing any constraints on the grid ratios. The convergence order of the new scheme is of $O(h^4+\tau^2)$ in the L^2 norm and H^1 norm, respectively, with time step τ and mesh size h. Our analysis method can be used to high dimensional cases and other linearized finite difference schemes for the two- or three-dimensional nonlinear Schrödinger/Gross–Pitaevskii equations. Finally, numerical results are reported to test the theoretical results.

1. Introduction

At a temperature much lower than the critical temperature T_c, the spin-1 Bose–Einstein condensate (BEC) are well described by the following coupled Gross–Pitaevskii equations (CGPEs) [8,14,21,30–34]:

$$i\hbar\partial_t\psi_1(\mathbf{x},t)=\left[-\frac{\hbar^2}{2m}\nabla^2+V(\mathbf{x})+(C_0+C_2)\left(|\psi_1|^2+|\psi_0|^2\right)+(C_0-C_2)|\psi_{-1}|^2\right]\psi_1 + C_2\overline{\psi}_{-1}\psi_0^2,\quad \mathbf{x}\in\mathbb{R}^3,\quad t>0, \tag{1.1}$$

$$i\hbar\partial_t\psi_0(\mathbf{x},t)=\left[-\frac{\hbar^2}{2m}\nabla^2+V(\mathbf{x})+(C_0+C_2)\left(|\psi_1|^2+|\psi_{-1}|^2\right)+C_0|\psi_0|^2\right]\psi_0 + 2C_2\psi_{-1}\overline{\psi}_0\psi_1,\quad \mathbf{x}\in\mathbb{R}^3,\quad t>0, \tag{1.2}$$

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$$i\hbar\partial_t\psi_{-1}(\mathbf{x},t) = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{x}) + (C_0+C_2)\left(|\psi_{-1}|^2 + |\psi_0|^2\right) + (C_0 - C_2)|\psi_1|^2\right]\psi_{-1} + C_2\psi_0^2\overline{\psi}_1, \quad \mathbf{x}\in\mathbb{R}^3, \quad t>0, \tag{1.3}$$

where $\mathbf{x} = (x, y, z)$ is the spatial cartesian coordinate vector, t is time, $\hbar$ is the plank constant, m is the atomic mass, $V(\mathbf{x})$ is the external trapping potential, and $\Psi(\mathbf{x},t) = (\psi_1(\mathbf{x},t), \psi_0(\mathbf{x},t), \psi_{-1}(\mathbf{x},t))^\top$ is the three-component wave function. When a harmonic trap potential is considered,

$$V(\mathbf{x}) = \frac{m}{2}(\omega_x^2x^2 + \omega_y^2y^2 + \omega_z^2z^2), \tag{1.4}$$

with ω_x, ω_y and ω_z being the trap frequencies in the $x-$, $y-$ and $z-$ direction, respectively. $\overline{f}$ denotes the conjugate of the complex-valued function f. There are two atomic collision terms $C_0 = \frac{4\pi\hbar^2}{3m}(a_0 + 2a_2)$ and $C_2 = \frac{4\pi\hbar^2}{3m}(a_2 - a_0)$ expressed in terms of the $s-$wave scattering lengths a_0 and a_2 for a scattering channel of total hyperfine spin 0 (antiparallel spin collision) and spin 2 (parallel spin collision), respectively. The usual mean-field interaction C_0 is positive for repulsive interaction and negative for attractive interaction. The spin-exchange interaction C_2 is positive for antiferromagnetic interaction and negative for ferromagnetic interaction. The wave function is normalized according to

$$||\Psi||^2 := \int_{\mathbb{R}^3}|\Psi(\mathbf{x},t)|^2d\mathbf{x} = \int_{\mathbb{R}^3}\sum_{l=-1}^{1}|\psi_l(\mathbf{x},t)|^2d\mathbf{x} := \sum_{l=-1}^{1}||\psi_l||^2 = N, \tag{1.5}$$

where N is the total number of particles in the condensate.

By introducing the dimensionless variables: $t\to t/\omega_m$ with $\omega_m = \min\{\omega_x, \omega_y, \omega_z\}$, $\mathbf{x}\to\mathbf{x}a_s$ with $a_s = \sqrt{\frac{\hbar}{mw_m}}$ and $\psi_l \to \sqrt{N}\psi_l/a_s^{3/2}$ $(l = -1, 0, 1)$, one can get the dimensionless CGPEs from (1.1)–(1.3) as [9,32,34]:

$$i\partial_t\psi_1(\mathbf{x},t) = \left[-\frac{1}{2}\nabla^2 + V(\mathbf{x}) + (\beta_n+\beta_s)(|\psi_1|^2 + |\psi_0|^2) + (\beta_n-\beta_s)|\psi_{-1}|^2\right]\psi_1 + \beta_s\overline{\psi}_{-1}\psi_0^2, \tag{1.6}$$

$$i\partial_t\psi_0(\mathbf{x},t) = \left[-\frac{1}{2}\nabla^2 + V(\mathbf{x}) + (\beta_n+\beta_s)(|\psi_1|^2 + |\psi_{-1}|^2) + \beta_n|\psi_0|^2\right]\psi_0 + 2\beta_s\psi_{-1}\overline{\psi}_0\psi_1, \tag{1.7}$$

$$i\partial_t\psi_{-1}(\mathbf{x},t) = \left[-\frac{1}{2}\nabla^2 + V(\mathbf{x}) + (\beta_n+\beta_s)(|\psi_{-1}|^2 + |\psi_0|^2) + (\beta_n-\beta_s)|\psi_1|^2\right]\psi_{-1} + \beta_s\psi_0^2\overline{\psi}_1, \tag{1.8}$$

where $\beta_n = \frac{Nc_0}{a_s^3\hbar\omega_m} = \frac{4\pi N(a_0+2a_2)}{3a_s}$, $\beta_s = \frac{Nc_2}{a_s^3\hbar\omega_m} = \frac{4\pi N(a_2-a_0)}{3a_s}$ and $V(\mathbf{x}) = \frac{1}{2}(\gamma_x^2x^2 + \gamma_y^2y^2 + \gamma_z^2z^2)$ with $\gamma_x = \frac{\omega_x}{\omega_m}$, $\gamma_y = \frac{\omega_y}{\omega_m}$, $\gamma_z = \frac{\omega_z}{\omega_m}$. Similar to those in a single-component BEC [4,6,14,21], in a disk-shaped condensation, i.e., $\omega_x\approx\omega_y$ and $\omega_z\gg\omega_x$ ($\Leftrightarrow\gamma_x$, $\gamma_y\approx 1$ and $\gamma_z\gg 1$ with $\omega_m = \omega_x$), the three-dimensional (3D) CGPEs (1.6)–(1.8) can be reduced to 1D CGPEs. In this paper, we mainly consider the numerical method for the dimensionless CGPEs in one dimension. We here consider the 1D CGPEs on a bounded computational domain $[a, b]\times[0, T]$,

$$i\partial_t\psi_1(x,t) = \left[-\frac{1}{2}\partial_{xx} + V(x) + (\beta_n+\beta_s)(|\psi_1|^2 + |\psi_0|^2) + (\beta_n-\beta_s)|\psi_{-1}|^2\right]\psi_1 + \beta_s\overline{\psi}_{-1}\psi_0^2, \quad (x,t)\in(a,b)\times(0,T], \tag{1.9}$$

$$i\partial_t\psi_0(x,t) = \left[-\frac{1}{2}\partial_{xx} + V(x) + (\beta_n+\beta_s)(|\psi_1|^2 + |\psi_{-1}|^2) + \beta_n|\psi_0|^2\right]\psi_0 + 2\beta_s\psi_{-1}\overline{\psi}_0\psi_1, \quad (x,t)\in(a,b)\times(0,T], \tag{1.10}$$

$$i\partial_t\psi_{-1}(x,t) = \left[-\frac{1}{2}\partial_{xx} + V(x) + (\beta_n+\beta_s)(|\psi_{-1}|^2 + |\psi_0|^2) + (\beta_n-\beta_s)|\psi_1|^2\right]\psi_{-1} + \beta_s\psi_0^2\overline{\psi}_1, \quad (x,t)\in(a,b)\times(0,T], \tag{1.11}$$

with boundary condition

$$\psi_l(a,t) = \psi_l(b,t) = 0, \quad l = -1, 0, 1, \quad t\in(0,T], \tag{1.12}$$

and initial condition

$$\psi_l(x,0) = \phi_l(x), \quad l = -1, 0, 1, \quad x\in[a,b], \tag{1.13}$$