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Optimal H^1-Error Estimates for Crank-Nicolson Finite Difference Scheme for Gross-Pitaevskii Equation with Angular Momentum Rotation Term

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Abstract. Optimal H^1-error estimates for a Crank-Nicolson finite difference scheme for $2D$-Gross-Pitaevskii equation with angular momentum rotation term are derived. The analysis is based on classical energy estimate method and on the lifting technique. With no constraint on the grid ratio, we show that the convergence rate of approximate solutions is equivalent to $\mathscr{O}(\tau^2 + h^2)$, consistent with numerical results of the existing studies.

AMS subject classifications: 65M06, 65M12

Key words: Gross-Pitaevskii equation with angular momentum rotation, finite difference method, conservation laws, error estimate.

1. Introduction

Let Ω be a bounded domain in $\mathbb{R}^d$, $d = 2,3$, $\mathbf{x} = (x, y) \in \mathbb{R}^2$ or $\mathbf{x} = (x, y, z) \in \mathbb{R}^3$ and t is time variable. We consider the finite difference method for the initial-boundary problem for d-dimensional Gross-Pitaevskii (GP) equation with angular momentum rotation (AMR)

$$\mathrm{i}\partial_t \psi = \left[-\frac{1}{2}\Delta + V(\mathbf{x}) - \gamma L_z + \beta |\psi|^2 \right] \psi, \quad \mathbf{x} \in \Omega \subset \mathbb{R}^d, \quad t > 0, \tag{1.1}$$

$$\psi(\mathbf{x}, 0) = \psi_0(\mathbf{x}), \quad \mathbf{x} \in \Omega, \tag{1.2}$$

$$\psi(\mathbf{x}, t) = 0, \quad \mathbf{x} \in \partial\Omega, \quad t \geqslant 0, \tag{1.3}$$

where $V(\mathbf{x})$ and $\psi(\mathbf{x}, t)$ are, respectively, real- and complex-valued functions, γ and β constants, and $\psi(\mathbf{x}, t)$ is an unknown complex-valued wave function.

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This equation plays an important role in modeling a rotating Bose-Einstein condensate (BEC) — cf. Ref. [8]. Note that V corresponds the external trap potential and, in most experiments, it is chosen as a harmonic potential — i.e. as a quadratic polynomial. The dimensionless constant γ is associated with the angular speed of a laser beam in experiments, and the dimensionless constant β characterises the interaction of particles in the rotating BEC. It is positive for repulsive interaction and negative for attractive ones. Moreover, L_z is the z-component of the angular momentum defined by

$$L_z = -\mathrm{i}(x\partial_y - y\partial_x) = -\mathrm{i}\partial_\theta,$$

where (r,θ) and (r,θ,z) are polar coordinates in $2D$- and cylindrical coordinates in $3D$-domains, respectively.

The GP equation with AMR has been vigorously studied. In particular, Lieb and Seiringer [6] showed that rotating Bose gas is correctly described by this equation and Hao *et al.* [4] investigated its well-posedness and dynamical properties. In fact, one can easily show that the initial-boundary value problem (1.1)-(1.3) preserves total mass

$$M(\psi(\cdot,t)) := \int_\Omega |\psi(\mathbf{x},t)|^2 dx dy \equiv M(\psi_0), \qquad t \geqslant 0,$$

and energy

$$E(\psi(\cdot,t)) := \int_\Omega \left[\frac{1}{2}|\nabla\psi|^2 + V(\mathrm{x})|\psi|^2 - \gamma\bar{\psi}L_z\psi + \frac{\beta}{2}|\psi|^4\right] d\mathbf{x} \equiv E(\psi_0), \qquad t \geqslant 0,$$

where $\bar{\psi}$ refers to the conjugate of ψ.

For nonlinear Schrödinger (NLS) equations (which include $1D$-GP equation), the unconditional and optimal error estimates of the conservative difference method have been established in Ref. [13]. Note that the proofs in Ref. [13] heavily rely on discrete conservative property and discrete $1D$-version of the Sobolev inequality

$$\|f\|_{L^\infty} \leqslant C_\Omega \, \|f\|_{H^1}, \quad f \in H^1(\Omega), \quad \Omega \subset \mathbb{R}.$$

In 2 and 3 dimensions such an inequality is not available, which causes serious difficulties with a priori uniform estimate of the numerical solutions. Therefore, the error estimates of finite difference methods for two-dimensional GP equation with AMR are less studied. For linear Schrödinger $2D$-equations, Liao and Sun [7] established a maximum norm error estimate of a compact difference scheme. However, this approach cannot be directly used in nonlinear problems. On the other hand, Bao and Cai [2] applied a classic CNFD scheme to the GP equation with AMR. It is unconditionally stable and conserves mass and energy at the discretised level. To approximate the nonlinearity, some authors used a cut-off technique [1, 9, 11] and obtained an L^∞ priori estimate for the numerical solution. Nevertheless, a week condition on the time-step size is involved in the corresponding error analysis. For $\gamma \neq 0$, the error estimate in the discrete H^1-norm is only $\mathscr{O}(h^{3/2} + \tau^{3/2})$, while numerical experiments show that the convergence rate can be as fast as $\mathscr{O}(h^2 + \tau^2)$. Thus the H^1-error