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LOD-MS for Gross-Pitaevskii Equation in Bose-Einstein Condensates

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Abstract. The local one-dimensional multisymplectic scheme (LOD-MS) is developed for the three-dimensional (3D) Gross-Pitaevskii (GP) equation in Bose-Einstein condensates. The idea is originated from the advantages of multisymplectic integrators and from the cheap computational cost of the local one-dimensional (LOD) method. The 3D GP equation is split into three linear LOD Schrödinger equations and an exactly solvable nonlinear Hamiltonian ODE. The three linear LOD Schrödinger equations are multisymplectic which can be approximated by multisymplectic integrator (MI). The conservative properties of the proposed scheme are investigated. It is mass-preserving. Surprisingly, the scheme preserves the discrete local energy conservation laws and global energy conservation law if the wave function is variable separable. This is impossible for conventional MIs in nonlinear Hamiltonian context. The numerical results show that the LOD-MS can simulate the original problems very well. They are consistent with the numerical analysis.

AMS subject classifications: 65M06, 65M12, 65Z05, 70H15

Key words: LOD-MS, Gross-Pitaevskii equation, local one-dimensional method, midpoint method, conservation laws.

1 Introduction

The existence of the Bose-Einstein Condensate (BEC) was predicted in the early 1920s by Bose and Einstein. It was experimentally created and confirmed until 1995 in atomic

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gas at ultra low temperature [7]. The BEC phenomena can be reported by the mean-field theory in physics and can be modeled by the well-known Gross-Pitaevskii (GP) equation [9,18]

$$i\hbar u_t = -\frac{\hbar^2}{2m}\nabla^2 u + \overline{V}_d(\mathbf{x})u + \frac{4\pi\hbar^2 a_s}{m}|u|^2 u, \quad \mathbf{x}\in\mathbb{R}^d, \; t\geqslant 0, \tag{1.1}$$

where m is the atomic mass, $\hbar$ is the Planck constant, a_s is the s-wave scatting length ($a_s>0$ for repulsive interaction and $a_s<0$ for attractive interaction), and $\overline{V}_d(\mathbf{x})$ is the external potential imposed on the physical system.

For convenience, it is necessary to scale GP equation (1.1) into the dimensionless form

$$iu_t = -\frac{1}{2}\nabla^2 u + V_d(\mathbf{x})u + \beta_d|u|^2 u, \quad \mathbf{x}\in\mathbb{R}^d, \; t\geqslant 0, \tag{1.2}$$

where β_d is a real constant, and $V_d(\mathbf{x})$ is the external potential acting on the physical system which can be periodic

$$V_d(\mathbf{x}) = \begin{cases} 1-\sin^2 x, & d=1, \\ 1-\sin^2 x\sin^2 y, & d=2, \\ 1-\sin^2 x\sin^2 y\sin^2 z, & d=3, \end{cases}$$

or harmonic

$$V_d(\mathbf{x}) = \begin{cases} \frac{\gamma_x^2 x^2}{2}, & d=1, \\ \frac{\gamma_x^2 x^2+\gamma_y^2 y^2}{2}, & d=2, \\ \frac{\gamma_x^2 x^2+\gamma_y^2 y^2+\gamma_z^2 z^2}{2}, & d=3, \end{cases}$$

with the trapped frequencies $\gamma_x,\gamma_y,\gamma_z$ in x-, y- and z-direction, respectively.

We consider the Cauchy problem of GP equation (1.2) with the initial value

$$u(\mathbf{x},0) = u^0(\mathbf{x}), \quad \mathbf{x}\in\mathbb{R}^d. \tag{1.3}$$

By direct calculation, one can derive that the GP equation (1.2)-(1.3) endows with the following two important invariants: the first one is mass invariant

$$\mathcal{Q}(t) = \int_{\mathbb{R}^d}|u(\mathbf{x},t)|^2 \mathrm{d}\mathbf{x} = \int_{\mathbb{R}^d}|u(\mathbf{x},0)|^2 \mathrm{d}\mathbf{x} = \mathcal{Q}(0), \tag{1.4}$$

and the second one is energy invariant

$$\mathcal{E}(t) = \int_{\mathbb{R}^d}\left[\frac{1}{2}|\bigtriangledown u(\mathbf{x},t)|^2 + V_d(\mathbf{x})|u|^2 + \frac{\beta_d}{2}|u|^4\right]\mathrm{d}\mathbf{x} = \mathcal{E}(0). \tag{1.5}$$

Significant progress on numerical simulation of BEC phenomena has been made over the last ten years (see [2–4,8,14,20,23,24,27] and references therein). In [2–4], Bao et al.