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Regularized Numerical Methods for the Nonlinear Schrödinger Equation with Singular Nonlinearity

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Dedicated to Professor Tao Tang on the occasion of his 60th birthday.

Abstract. We present different regularizations and numerical methods for the nonlinear Schrödinger equation with singular nonlinearity (sNLSE) including the regularized Lie-Trotter time-splitting (LTTS) methods and regularized Lawson-type exponential integrator (LTEI) methods. Due to the blowup of the singular nonlinearity, i.e., $f(\rho)=\rho^\alpha$ with a fixed exponent $\alpha<0$ goes to infinity when $\rho\to 0^+$ ($\rho=|\psi|^2$ represents the density with ψ being the complex-valued wave function or order parameter), there are significant difficulties in designing accurate and efficient numerical schemes to solve the sNLSE. In order to suppress the round-off error and avoid blowup near $\rho=0^+$, two types of regularizations for the sNLSE are proposed with a small regularization parameter $0<\varepsilon\ll 1$. One is based on the local energy regularization (LER) for the sNLSE via regularizing the energy density $F(\rho)=\rho^{\alpha+1}/(\alpha+1)$ locally near $\rho=0^+$ with a polynomial approximation and then obtaining a local energy regularized nonlinear Schrödinger equation via energy variation. The other one is the global nonlinearity regularization which directly regularizes the singular nonlinearity $f(\rho)=\rho^\alpha$ to avoid blowup near $\rho=0^+$. For the regularized models, we apply the first-order Lie-Trotter time-splitting method and Lawson-type exponential integrator method for temporal discretization and combine with the Fourier pseudospectral method in space to numerically solve them. Numerical examples are provided to show the convergence of the regularized models to the sNLSE and they suggest that the local energy regularization performs better than directly regularizing the singular nonlinearity globally.

AMS subject classifications: 35Q55, 35Q60, 65M15, 81Q05

Key words: Nonlinear Schrödinger equation, singular nonlinearity, local energy regularization, global nonlinearity regularization, convergence rate, Lie-Trotter time-splitting, Lawson-type exponential integrator.

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1. Introduction

The nonlinear Schrödinger equation (NLSE) is a prototypical dispersive partial differential equation (PDE) playing an important role in different areas of physics, chemistry and engineering. The relevant applications vary from Bose-Einstein condensate (BEC) [6,35], nonlinear optics [1,3] to plasma and particle physics [6,40].

In general, the time-dependent NLSE is in the following form [16,38,40]:

$$\begin{aligned} &i\partial_t\psi(\mathbf{x},t) = -\Delta\psi(\mathbf{x},t) + \lambda f\left(|\psi(\mathbf{x},t)|^2\right)\psi(\mathbf{x},t), && \mathbf{x}\in\Omega, \quad t>0, \\ &\psi(\mathbf{x},0) = \psi_0(\mathbf{x}), && \mathbf{x}\in\overline{\Omega}, \end{aligned} \tag{1.1}$$

where $i=\sqrt{-1}$ is the complex unit, t is time, $\mathbf{x}\in\mathbb{R}^d$ $(d=1,2,3)$ is the spatial coordinate, $\psi := \psi(\mathbf{x},t)\in\mathbb{C}$ is the dimensionless wave function or order parameter, $\psi_0 := \psi_0(\mathbf{x})$ is a given complex-valued initial data, $\lambda\neq 0$ is a given real constant with $\lambda>0$ for repulsive or defocusing interaction and $\lambda<0$ for attractive or focusing interaction, and $\Omega=\mathbb{R}^d$ or $\Omega\subset\mathbb{R}^d$ is a bounded domain with periodic boundary condition or homogeneous Dirichlet boundary condition or homogeneous Neumann boundary condition. The nonlinearity is given as [16,35,40]

$$f(\rho) := \rho^\alpha, \quad \rho\geq 0, \tag{1.2}$$

where $\rho := |\psi|^2$ is the density and the exponent $\alpha>-1$ is a real constant, which is different in diverse applications. Specifically, when $\alpha=1$, i.e., $f(\rho)=\rho$, it is the most popular NLSE with cubic nonlinearity and also called Gross–Pitaevskii equation (GPE), especially in BEC [35,38,40]; and when $\alpha=2$, it is related to the quintic Schrödinger equation, which is regarded as the mean field limit of a Boson gas with three-body interactions and also widely used in the study of optical lattices [18,36]. When $0<\alpha<1$ or $1<\alpha<2$, it is usually stated that the NLSE with semi-smooth (or fractional) nonlinearity, which has been adapted in different applications [13,15,23,29]. For the NLSE with smooth or semi-smooth nonlinearity, i.e., $\alpha>0$, the existence and uniqueness of the Cauchy problem as well as the finite time blow-up have been widely studied [16,40].

Recently, interests have been surged for the study of the NLSE (1.1) with singular nonlinearity (1.2), i.e., $\alpha\in(-1,0)$. In this case, the NLSE (1.1) can be formally obtained as the nonrelativistic limit of the nonlinear Dirac equation with singular (or fractional) nonlinearity [30,31], which was proposed as a model of strong interaction of particles and it recovered the MIT bag model [19,24]. When $\alpha<0$ in (1.2), the nonlinearity $f(\rho)$ has a singularity at the origin and it is also called sublinear Schrödinger equation for the case $\alpha\in(-1/2,0)$ in the mathematical literature [4,27]. The study of the NLSE with singular nonlinearity is much more complicated in both analytical and numerical aspects. In recent years, dispersive PDEs with singular nonlinearity have attracted much attention, e.g., the existence of standing waves for nonlinear Dirac fields has been proven and the solution is of class C^1 when $-1/3<\alpha<0$, while $|\nabla\psi|$ is infinite on some sphere $\{|x|=R\}$ for $-1<\alpha<-1/3$ [5]. Since the nonlinear Schrödinger equation is the nonrelativistic limit of the nonlinear Dirac equation, it is also an interesting and challenging problem to study the nonlinear Schrödinger equation with such a singular nonlinearity. In this paper, we