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An Extended Fourier Pseudospectral Method for the Gross-Pitaevskii Equation with Low Regularity Potential

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Abstract. We propose and analyze an extended Fourier pseudospectral (eFP) method for the spatial discretization of the Gross-Pitaevskii equation with low regularity potential by treating the potential in an extended window for its discrete Fourier transform. The proposed eFP method maintains optimal convergence rates with respect to the regularity of the exact solution even if the potential is of low regularity and enjoys similar computational cost as the standard Fourier pseudospectral method, and thus it is both efficient and accurate. Furthermore, similar to the Fourier spectral/pseudospectral methods, the eFP method can be easily coupled with different popular temporal integrators including finite difference methods, time-splitting methods and exponential-type integrators. Numerical results are presented to validate our optimal error estimates and to demonstrate that they are sharp as well as to show its efficiency in practical computations.

AMS subject classifications: 35Q55, 65M15, 65M70, 81Q05
Key words: Gross-Pitaevskii equation, low regularity potential, extended Fourier pseudospectral method, time-splitting method, optimal error bound.

1. Introduction

The Gross-Pitaevskii equation (GPE), as a particular case of the nonlinear Schrödinger equation (NLSE) with cubic nonlinearity, is derived from the mean-field approximation of many-body problems in quantum physics and chemistry, which is widely adopted in modeling and simulation of Bose-Einstein condensation [6, 20, 38]. In this paper, we consider the following time-dependent GPE [6, 20, 38]:

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

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where t is time, $\mathbf{x} \in \mathbb{R}^d$, $d = 1,2,3$ is the spatial coordinate, $\psi := \psi(\mathbf{x},t)$ is a complex-valued wave function, and $\Omega = \Pi_{i=1}^d (a_i, b_i) \subset \mathbb{R}^d$ is a bounded domain equipped with periodic boundary condition. Here, $V := V(\mathbf{x})$ is a time-independent real-valued potential and $\beta \in \mathbb{R}$ is a given parameter that characterizes the nonlinear interaction strength.

Usually, the potential V is a smooth function which is chosen as either the harmonic potential — e.g. $V(\mathbf{x}) = |\mathbf{x}|^2/2$, or an optical lattice potential — e.g. $V(\mathbf{x}) = \sum_{j=1}^d A_j \cos(L_j x_j)$ in d-dimensions with A_j, L_j, $j = 1,\ldots,d$ being some given real-valued constants. For the GPE (1.1) with sufficiently smooth potential, many accurate and efficient temporal discretizations have been proposed and analyzed in last two decades, including the finite difference time domain (FDTD) method [1, 5–7], the exponential wave integrator (EWI) [8, 17, 25], the time-splitting method [5, 6, 9, 10, 12, 14, 19, 28, 29], and the low regularity integrator (LRI) [2, 4, 16, 27, 30–32, 34]. Generally, these temporal discretizations are followed by a spatial discretization, such as finite difference methods, finite element methods or Fourier spectral/pseudospectral methods, to obtain a full discretization for the GPE (1.1). Among them, the time-splitting Fourier pseudospectral (TSFP) method is the most popular one due to its efficient implementation and spectral accuracy in space as well as the preservation of many dynamical properties of the GPE (1.1) in the fully discretized level [5, 6].

On the contrary, in many physics applications, low regularity potential is also widely incorporated into the GPE. Typical examples include the square-well potential or step potential [21, 33, 36], which are discontinuous; narrow potential barriers [22, 23] and power-law potential [15, 26], which may have large or even unbounded derivatives; and the random potential or disorder potential in the study of Anderson localization [35, 40], which could be very rough. Some of them in one dimension (1D) and two dimensions (2D) are plotted in Fig. 1.

When considering the GPE with low regularity potential, most of the aforementioned full-discretization methods are still applicable. However, their performance may significantly deviate from the smooth cases, leading to possible order reduction in both time and space. Recently, much attention has been paid to the error analysis of those methods for

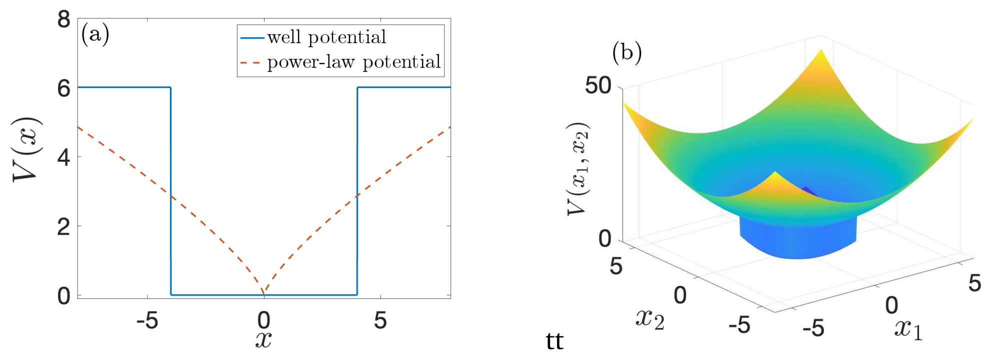

Figure 1: Examples of low regularity potential: (a) square-well potential and power-law potential with order 0.75 in 1D, and (b) square-well potential combined with a harmonic potential in 2D.