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Time-splitting finite difference method with the wavelet-adaptive grids for semiclassical Gross–Pitaevskii equation in supercritical case

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ABSTRACT

The Gross–Pitaevskii equation is the model equation of the single-particle wave function in a Bose–Einstein condensation. A computation difficulty of the Gross–Pitaevskii equation comes from the semiclassical problem in supercritical case. In this paper, we apply a diffeomorphism to transform the original one-dimensional Gross–Pitaevskii equation into a modified equation. The adaptive grids are constructed through the interpolating wavelet method. Then, we use the time-splitting finite difference method with the wavelet-adaptive grids to solve the modified Gross–Pitaevskii equation, where the approximation to the second-order derivative is given by the Lagrange interpolation method. At last, the numerical results are given. It is shown that the obtained time-splitting finite difference method with the wavelet-adaptive grids is very efficient for solving the one-dimensional semiclassical Gross–Pitaevskii equation in supercritical case and it is suitable to deal with the local high oscillation of the solution.

1. Introduction

Consider the one-dimensional Gross–Pitaevskii equation (GPE)

$$i\hbar\frac{\partial}{\partial t}\psi(t,x) = -\frac{\hbar^2}{2}\frac{\partial^2}{\partial x^2}\psi + V\psi + \lambda\hbar^r|\psi|^{2\sigma}\psi, \quad (t,x)\in\mathbb{R}_+\times\mathbb{R} \tag{1}$$

with the wave function $\psi = \psi(t,x)$ depending on the time t and the spatial variable x, where i is the imaginary unit, $\hbar > 0$, $\sigma > 0$, λ and r are real constants. The potential $V = V(x)$ is a real-valued function and $V \in C^2(\mathbb{R})$. In this paper, we mainly consider the semiclassical problem in supercritical case (cf. [3,4,15,20]), i.e. $0 < \hbar \ll 1$, $r < 1 + \sigma/2$. The GPE belongs to the nonlinear Schrödinger equation (NLSE). And for mathematical properties about NLSE, ones can refer to [1,3–5,11].

Let $q, p \in \mathbb{R}$ be the solution of the Hamiltonian equation

$$\begin{cases} q'(t) = p(t), \\ p'(t) = -V'\big(q(t)\big) \end{cases} \tag{2}$$

with the initial value

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$$q(0) = \int_{-\infty}^{+\infty} x\left|\psi(0,x)\right|^2 \mathrm{d}x,$$

$$p(0) = \int_{-\infty}^{+\infty} -i\hbar\psi(0,x)\frac{\partial}{\partial x}\psi(0,x)\,\mathrm{d}x,$$

and $S(t)$ be the classical action integral

$$S(t) = \int_0^t \left(\frac{1}{2}\left|p(\tau)\right|^2 - V\left(q(\tau)\right)\right)\mathrm{d}\tau. \tag{3}$$

Define the unitary operator (cf. [4])

$$\mathcal{T}_{q,p}^{\hbar} : L^2(\mathbb{R}) \to L^2(\mathbb{R})$$
$$f(x) \mapsto \hbar^{-\frac{1}{4}} f\left(\frac{x-q}{\sqrt{\hbar}}\right) e^{\frac{i}{\hbar}p(x-q)}. \tag{4}$$

Then, we obtain the modified GPE

$$i\frac{\partial}{\partial t}u(t,x) = -\frac{1}{2}\frac{\partial^2}{\partial x^2}u + Wu + \omega|u|^{2\sigma}u \tag{5}$$

with the diffeomorphism

$$\psi = e^{\frac{i}{\hbar}S(t)/}\mathcal{T}_{q(t),p(t)}^{\hbar}u, \tag{6}$$

where $\omega = \lambda\hbar^{r-1-\sigma/2}$ and $W = W(t,x)$ is the quadratic remainder of $V(x)$

$$W(t,x) = \frac{1}{\hbar}\left(V\left(q(t)+\sqrt{\hbar}x\right) - V\left(q(t)\right) - \sqrt{\hbar}V'\left(q(t)\right)x\right).$$

And the position average of the state $u(t,x)$, i.e. $\int_{-\infty}^{+\infty} x|u(t,x)|^2\,\mathrm{d}x$, is close to the original point within a finite interval $[0,T)$. For the numerical approach to Eq. (5), there are some difficulties when the nonlinear term is too large, i.e. $|\omega| \gg 1$, since the wave function $u(t,x)$ has the property of local high oscillation.

In this paper, our purpose is to give an efficient numerical method for the GPE (5) with large nonlinear term satisfying

$$W(t,0) \equiv 0, \qquad \frac{\partial}{\partial x}W(t,x)\Big|_{x=0} \equiv 0,$$
$$\int_{-\infty}^{+\infty} x\left|u(0,x)\right|^2\mathrm{d}x = -i\int_{-\infty}^{+\infty}\overline{u(0,x)}\frac{\partial}{\partial x}u(0,x)\,\mathrm{d}x = 0. \tag{7}$$

Then, the numerical solution of the original GPE (1) can be obtained from the transformation (6). For the numerical method of the Schrödinger equations, the spectral and pseudospectral methods (cf. [1,2,14,21]) are of high accuracy. However, the highly oscillatory problem needs a large number of spectral basis functions for approximating the solutions, and this brings the expensive computational cost. The finite difference methods (cf. [1,7,17,20,25]) have the sparse matrix structure, and they are suitable for the computation with large number of grid points. The wavelet method is also an efficient method for solving the partial differential equations including the Schrödinger equations (cf. [12,26]). Here, we only consider the compactly supported interpolating wavelets (cf. [8,9,24]). The advantage of such wavelets is manifest to the case of the weak regularity in a local area since the corresponding function $\Phi(x)$ have the compact support, and the function space $\mathcal{V}_0 = \mathrm{span}\{\Phi(\cdot-k)\}_{k\in\mathbb{Z}}$ contains all polynomials of fixed degree. Moreover, the interpolation property of such wavelets makes it more simple for computation. In this paper, we use the wavelet method to construct the wavelet-adaptive grid (cf. [18,19]). Then, we solve the GPE (5) by the time-splitting finite difference (TSFD) method (cf. [1,25]) with the wavelet-adaptive grids. As an effective method for solving GPE (5), the TSFD method is more accurate than forward Euler finite difference method and less time cost than the Crank–Nicolson finite difference method (cf. [1,7]). For handling the local high oscillation of the wave function $u(t,x)$, the equidistant grids need too many points for approximating $u(t,x)$, and the wavelet-adaptive method can reduce a lot of grid points. Therefore, the computational cost is much less than that of the finite difference method with the equidistant grids.

In Section 2, we briefly introduce the decomposition and the reconstruction of interpolating wavelets. Then, we give the method to construct the wavelet-adaptive grids.