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An improved semi-Lagrangian time splitting spectral method for the semi-classical Schrödinger equation with vector potentials using NUFFT

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ABSTRACT

In this paper, we propose a new time splitting Fourier spectral method for the semi-classical Schrödinger equation with vector potentials. Compared with the results in [21], our method achieves spectral accuracy in space by interpolating the Fourier series via the NonUniform Fast Fourier Transform (NUFFT) algorithm in the convection step. The NUFFT algorithm helps maintain high spatial accuracy of Fourier method, and at the same time improve the efficiency from $O(N^2)$ (of direct computation) to $O(N \log N)$ operations, where N is the total number of grid points. The kinetic step and potential step are solved by analytical solution with pseudo-spectral approximation, and, therefore, we obtain spectral accuracy in space for the whole method. We prove that the method is unconditionally stable, and we show improved error estimates for both the wave function and physical observables, which agree with the results in [3] for vanishing potential cases and are superior to those in [21]. Extensive one and two dimensional numerical studies are presented to verify the properties of the proposed method, and simulations of 3D problems are demonstrated to show its potential for future practical applications.

1. Introduction

Quantum effects play a significant role in many scientific and engineering areas, such as theoretical chemistry, solid-state mechanics and quantum optics, and the mathematical analysis and numerical simulation of Schrödinger equations are of fundamental importance. This type of equations form a canonical class of dispersive PDEs, i.e., equations where waves of different wavelengths propagate at different phase velocities. Whenever the magnetic field is considered, we need to incorporate the vector potentials in the Schrödinger equation.

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In this paper, we consider the semi-classical Schrödinger equation with vector potentials, which has the form

$$i\varepsilon\partial_t u^\varepsilon = \frac{1}{2}\left(-i\varepsilon\nabla_x - \mathbf{A}(x)\right)^2 u^\varepsilon + V(x)u^\varepsilon, \quad t\in\mathbb{R}^+, \quad x\in\mathbb{R}^3, \tag{1.1}$$

$$u^\varepsilon(x,0) = u_0(x), \quad x\in\mathbb{R}^3, \tag{1.2}$$

where $u^\varepsilon(x,t)$ is the complex-valued wave function, $V(x)\in\mathbb{R}$ is the scalar potential and $\mathbf{A}(x)\in\mathbb{R}^3$ is the vector potential. The scalar potential and the vector potential are introduced to mathematically describe the electromagnetic field, i.e., the electric field $\mathbf{E}(x)\in\mathbb{R}^3$ and the magnetic field $\mathbf{B}(x)\in\mathbb{R}^3$ given as follows

$$\mathbf{E} = -\nabla V(x), \qquad \mathbf{B} = \nabla\times\mathbf{A}(x). \tag{1.3}$$

The Schrödinger equation (1.1) above can be derived from the equation in the absence of the vector potential by local gauge transformation (see [28]). The quantum dynamics in the presence of the external electromagnetic field results in many far-reaching consequences in quantum mechanics, such as Landau levels, Zeeman effect and superconductivity. In the aspect of analysis, the Hamiltonian has different features in spectral and scattering properties (see [1]). Numerically, it gives new challenges as well, especially in the semi-classical regime. The presence of the vector potential introduces a convection term in the Schrödinger equation and in the meanwhile effectively modifies the scalar potential (see [21]).

In fact, one can simplify the potential description by imposing one more condition, namely, specifying the gauge. The electric field $\mathbf{E}(x)\in\mathbb{R}^3$ and magnetic field $\mathbf{B}(x)\in\mathbb{R}^3$ stay invariant in different gauges. One natural choice is, $\nabla_x\cdot\mathbf{A}=0$, which is the so-called Coulomb gauge. In this gauge, the vector potential and the canonical momentum operator commute, $[\mathbf{A},\ -i\varepsilon\nabla_x]=0$, so that the modified "kinetic" part of the Schrödinger equation (1.1) can be simplified as follows

$$\frac{1}{2}(-i\varepsilon\nabla_x - \mathbf{A})^2 u^\varepsilon = -\frac{\varepsilon^2}{2}\Delta_x u^\varepsilon + i\varepsilon\mathbf{A}\cdot\nabla_x u^\varepsilon + \frac{1}{2}|\mathbf{A}|^2 u^\varepsilon. \tag{1.4}$$

In the Schrödinger equation, the wave function acts as an auxiliary quantity used to compute macroscopic physical quantities (physical observables) such as the position density

$$n(x,t) = |u^\varepsilon(x,t)|^2, \tag{1.5}$$

and the modified current density

$$\mathbf{J}(x,t) = \frac{1}{2}\left(\overline{u^\varepsilon}\left(-i\varepsilon\nabla_x - \mathbf{A}\right)u^\varepsilon - u^\varepsilon\left(-i\varepsilon\nabla_x - \mathbf{A}\right)\overline{u^\varepsilon}\right), \tag{1.6}$$

where $\bar{f}$ denotes the complex conjugate of f. Actually, we have the following mass conservation equation

$$\frac{\partial}{\partial t}n + \nabla_x\cdot\mathbf{J} = 0. \tag{1.7}$$

We remark that n and $\mathbf{J}$ are gauge invariant quantities. Another two important physical quantities are the *mass*

$$m(t) := \|u^\varepsilon(x,t)\|_{L^2}^2 = \int_{\mathbb{R}^3} n(t,x)dx, \tag{1.8}$$

and *the energy*

$$\mathcal{E}(t) := \frac{1}{2}\|(-i\varepsilon\nabla - \mathbf{A})u^\varepsilon\|_{L^2}^2 + \langle u^\varepsilon, Vu^\varepsilon\rangle, \tag{1.9}$$

where $\langle f,g\rangle \equiv \int_{\mathbb{R}^d} f(x)\overline{g(x)}\,dx$ is the standard inner product. For $u^\varepsilon\in C(\mathbb{R}_t; L^2(\mathbb{R}^d)\cap\mathcal{S}(\mathbb{R}^d))$, these quantities are conserved through dynamics. We refer the readers to appendixes for detailed proofs.

In the semi-classical regime, namely $\varepsilon\ll 1$, the wave function u^ε is highly oscillatory both in space and time on the scale $O(\varepsilon)$, therefore it does not converge in the strong sense as $\varepsilon\to 0$. When $\varepsilon\ll 1$, several approximate methods other than directly solving the Schrödinger equation have been proposed, such as the level set method and the moment closure method based on the WKB analysis and the Wigner transform, see, for example, [9,18,16,17]. The Gaussian beam method (or the Gaussian wave packet approach) is another important one, which allows accurate computation around caustics and captures phase information (see, for example, [14,23,25,19,24,32]) with $O(\varepsilon^{1/2})$ model error. To improve the approximation accuracy, higher order Gaussian beam methods were introduced with an error $C_k(T)\varepsilon^{k/2}$ (see [31,20]). However, it has been shown in [22,33] that, for fixed ε, higher order Gaussian beam methods may not be a practical way to reduce the error. Whereas, the Hagedorn wave packets, studied by Hagedorn [13], analyzed and implemented as a computational tool in [13, 11,33,10], can effectively reduce the error for all $\varepsilon\in(0,1]$. In [33], Zhou has extended this method to the vector potential case and provided a rigorous proof for the higher order convergence with the Galerkin approximation. Recently, Russo and Smereka in [26,27] proposed a new approach based on the so-called Gaussian Wave packet transform, which is another worthy alternative.