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The Gaussian Wave Packet Transform for the Semi-Classical Schrödinger Equation with Vector Potentials

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The paper is dedicated to the memory of Professor Peter Smereka.

Abstract. In this paper, we reformulate the semi-classical Schrödinger equation in the presence of electromagnetic field by the Gaussian wave packet transform. With this approach, the highly oscillatory Schrödinger equation is equivalently transformed into another Schrödinger type wave equation, the w equation, which is essentially not oscillatory and thus requires much less computational effort. We propose two numerical methods to solve the w equation, where the Hamiltonian is either divided into the kinetic, the potential and the convection part, or into the kinetic and the potential-convection part. The convection, or the potential-convection part is treated by a semi-Lagrangian method, while the kinetic part is solved by the Fourier spectral method. The numerical methods are proved to be unconditionally stable, spectrally accurate in space and second order accurate in time, and in principle they can be extended to higher order schemes in time. Various one dimensional and multidimensional numerical tests are provided to justify the properties of the proposed methods.

AMS subject classifications: 65M70, 35Q41, 74Q10, 65Z05

Key words: Semi-classical Schrödinger equation, Gaussian wave packets, splitting methods, Fourier-spectral methods.

1 Introduction

In this paper, we propose an efficient approach for the semi-classical Schrödinger equation with external electromagnetic fields. This approach is a natural but worthy extension of the Gaussian Wave Packet Transform developed in [47, 48] to the cases where

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the Hamiltonians include vector potentials. With this formulation, the highly oscillatory Schrödinger equation is transformed into another Schrödinger type wave equation, which is much smoother and, as a consequence, requires much less computational effort. This problem is challenging for various reasons, and has many important applications in physics and chemistry (see [9,10,25,29]).

Consider the dimensionless Schrödinger equation for a charged particle, with a small (scaled) Planck constant ε,

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

$$\psi^\varepsilon(\mathbf{x},0) = \psi_0(\mathbf{x}), \quad \mathbf{x}\in\mathbb{R}^3, \tag{1.2}$$

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

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

For simplicity, we have assumed that the scalar and the vector potentials are time independent, but inclusion of the time dependence will not add intrinsic challenges to the current problem.

The quantum Hamiltonian in (1.1) is reminiscent of the classical Hamiltonian (see [26])

$$H(\boldsymbol{q},\boldsymbol{p}) = \frac{1}{2}(\boldsymbol{p} - \boldsymbol{A}(\boldsymbol{q}))^2 + V(\boldsymbol{q}).$$

This is the Schrödinger equation for a charged quantum particle moving in an electromagnetic field, where no spin or relativistic effects are considered (see [10]). It also shows a connection between quantum mechanics and macroscopic scale effects (the classical electromagnetic fields in this context). Alternatively, Eq. (1.1) above can be derived from the free-particle Schrödinger equation by local gauge transformation (see [50]).

The quantum dynamics in the presence of external electromagnetic fields results in many far-reaching consequences in quantum mechanics, such as Landau levels, Zeeman effect and superconductivity (see, e.g., [10]). Mathematically, 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 [33]).

The electromagnetic field is introduced by the scalar potential $V(\mathbf{x})$ and the vector potential $\mathbf{A}(\mathbf{x})$. One can simplify the potential description by imposing one more condition, namely, specifying the gauge. In fact, for any choice of a scalar function of position $\lambda(\mathbf{x})\in\mathbb{R}$, the potentials can be changed as follows:

$$\mathbf{A}' = \mathbf{A} + \nabla_{\mathbf{x}}\lambda, \quad V' = V. \tag{1.4}$$