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# Semi-Eulerian and High Order Gaussian Beam Methods for the Schrödinger Equation in the Semiclassical Regime

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*To the memory of David Gottlieb*

**Abstract.** A novel Eulerian Gaussian beam method was developed in [8] to compute the Schrödinger equation efficiently in the semiclassical regime. In this paper, we introduce an efficient semi-Eulerian implementation of this method. The new algorithm inherits the essence of the Eulerian Gaussian beam method where the Hessian is computed through the derivatives of the complexified level set functions instead of solving the dynamic ray tracing equation. The difference lies in that, we solve the ray tracing equations to determine the centers of the beams and then compute quantities of interests only around these centers. This yields effectively a local level set implementation, and the beam summation can be carried out on the initial physical space instead of the phase plane. As a consequence, it reduces the computational cost and also avoids the delicate issue of beam summation around the caustics in the Eulerian Gaussian beam method. Moreover, the semi-Eulerian Gaussian beam method can be easily generalized to higher order Gaussian beam methods, which is the topic of the second part of this paper. Several numerical examples are provided to verify the accuracy and efficiency of both the first order and higher order semi-Eulerian methods.

**AMS subject classifications**: 81Q20, 65M99

**Key words**: Schrödinger equation, semi-Eulerian Gaussian beam method, high order methods.

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# 1 Introduction

The Schrödinger equation is the fundamental equation in quantum mechanics. The rescaled linear Schrödinger equation can be written as

$$i\varepsilon\frac{\partial\Psi^\varepsilon}{\partial t}+\frac{\varepsilon^2}{2}\Delta\Psi^\varepsilon-V(\boldsymbol{x})\Psi^\varepsilon=0,\qquad \boldsymbol{x}\in\mathbb{R}^n, \tag{1.1}$$

where $\Psi^\varepsilon(\boldsymbol{x},t)$ is the wave function, $V(\boldsymbol{x})$ is the potential, $\varepsilon$ is the re-scaled Plank constant that describes the ratio between quantum time/space scale and the macroscopic time/space scale. This scaling corresponds to the so-called semiclassical regime. In this paper, we consider (1.1) with the WKB-initial condition

$$\Psi^\varepsilon(0,\boldsymbol{x})=A_0(\boldsymbol{x})\exp\Big[\frac{iS_0(\boldsymbol{x})}{\varepsilon}\Big]. \tag{1.2}$$

The direct numerical simulation of (1.1)-(1.2) has the difficulty that when $\varepsilon$ is small the wave function $\Psi^\varepsilon(\boldsymbol{x},t)$ becomes oscillatory of wave length $\mathcal{O}(\varepsilon)$. The best direct numerical solver so far is the time splitting spectral method which requires a mesh size of $\mathcal{O}(\varepsilon)$ [1]. Gaussian beam methods are asymptotic methods for such high frequency waves which allow numerical meshes to be $\mathcal{O}(\sqrt{\varepsilon})$, and they outperform the classical geometric optics method in that the Gaussian beam approximations are accurate even around caustics. While the classical Gaussian beam methods are in the Lagrangian framework [2–6, 16, 17], there have been very recent efforts in developing Eulerian Gaussian beam methods [8, 11, 12]. The error analysis on these Eulerian methods and their higher order extension were performed in [13, 14].

For more recent works in Gaussian beam methods the readers are also referred to [15, 19, 20].

We first summarize the Eulerian Gaussian beam method proposed in [8]. Consider the ansatz

$$\varphi^\varepsilon_{eu}(t,\boldsymbol{x},\boldsymbol{y},\boldsymbol{p})=A(t,\boldsymbol{y},\boldsymbol{p})\exp\Big[\frac{iT(t,\boldsymbol{x},\boldsymbol{y},\boldsymbol{p})}{\varepsilon}\Big], \tag{1.3}$$

where

$$T(t,\boldsymbol{x},\boldsymbol{y},\boldsymbol{p})=S(t,\boldsymbol{y},\boldsymbol{p})+\boldsymbol{p}\cdot(\boldsymbol{x}-\boldsymbol{y})+\frac{1}{2}(\boldsymbol{x}-\boldsymbol{y})^\top M(t,\boldsymbol{y},\boldsymbol{p})(\boldsymbol{x}-\boldsymbol{y}).$$

Here $(\boldsymbol{y},\boldsymbol{p})$ is defined by the following Hamiltonian system

$$\frac{\mathrm{d}\boldsymbol{y}}{\mathrm{d}t}=\boldsymbol{p}, \tag{1.4a}$$

$$\frac{\mathrm{d}\boldsymbol{p}}{\mathrm{d}t}=-\nabla_y V. \tag{1.4b}$$