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# THE GAUSSIAN BEAM METHODS FOR SCHRÖDINGER-POISSON EQUATIONS *

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**Abstract**

As an important model in quantum semiconductor devices, the Schrödinger-Poisson equations have generated widespread interests in both analysis and numerical simulations in recent years. In this paper, we present Gaussian beam methods for the numerical simulation of the one-dimensional Schrodinger-Poisson equations. The Gaussian beam methods for high frequency waves outperform the geometrical optics method in that the former are accurate even around caustics. The purposes of the paper are first to develop the Gaussian beam methods, based on our previous methods for the linear Schrödinger equation, for the Schrödinger-Poisson equations, and then check their validity for this weakly-nonlinear system.

*Mathematics subject classification:* 81Q20, 65M99
*Key words:* Schrödinger-Poisson equations, Gaussian beam methods, Vlasov-Poisson equations.

## 1. Introduction

The main purpose of this paper is to extend our Gaussian beam method [22], developed for the linear Schrödinger equation, to the one-dimensional nonlinear Schrödinger-Poisson equations

$$i\varepsilon\partial_t\Psi^\varepsilon = -\frac{\varepsilon^2}{2}\partial_{xx}\Psi^\varepsilon + V^\varepsilon\Psi^\varepsilon, \quad x\in\mathbb{R},\ t\geq 0, \tag{1.1}$$

$$\partial_{xx}V^\varepsilon = b(x) - c\left|\Psi^\varepsilon(t,x)\right|^2, \quad E^\varepsilon = \partial_x V^\varepsilon, \tag{1.2}$$

subject to the WKB initial condition

$$\Psi^\varepsilon(0,x) = A_0(x)e^{iS_0(x)/\varepsilon}. \tag{1.3}$$

Here $\Psi^\varepsilon = \Psi^\varepsilon(t,x)$ is the highly oscillatory wave function of wave length $\mathcal{O}(\varepsilon)$ (in the so-called semiclassical regime where the re-scaled Plank constant $\varepsilon$ is small). The electric potential $V^\varepsilon =$

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$V^\varepsilon(t,x)$ interacts with the wave function $\Psi^\varepsilon$ in a self-consistent way through the Schrödinger equation (1.1) and the Poisson equation (1.2). In the poisson equation (1.2), $b(x) \geq 0$ denotes the fixed positive charged background. The constant $c$ could be $\pm 1$, corresponding to focusing ('+') or defocusing ('-') potential respectively.

The Schrödinger-Poisson equations are a mean-field model for the linear $N$-particle Schrödinger equation with Coulomb potential [6,7,13], which is based on the Pauli's exclusion principle and the molecular chaos assumption. It is widely used in quantum semiconductor devices modeling [36] and the quantum transport theory [1,2].

The direct simulation of the Schrödinger-Poisson equations is expensive since the wave length $O(\varepsilon)$ is extremely small in the semiclassical regime. The standard time-splitting spectral method [3,4,42] and its adaptive version [5] need the mesh size to be of $\mathcal{O}(\varepsilon)$ and the time step to be of $\mathcal{O}(1)$ to capture the correct physical observables. The finite difference methods [34,35] are even worse since the mesh size and the time step are restricted to be $\mathcal{O}(\varepsilon)$.

One efficient alternative approach is to study the semiclassical limit of the Schrödinger-Poisson equations. When taking the rescaled Planck constant $\varepsilon \to 0$ , one can derive the Vlasov-Poisson equations [28,33,49] in the phase space

$$\partial_t f + \xi \partial_x f - \partial_x V \partial_\xi f = 0 \qquad x, \xi \in \mathbb{R},\ t \geq 0, \tag{1.4}$$

$$\partial_{xx} V = b(x) - c \int_{-\infty}^{\infty} f(t,x,\xi) \mathrm{d}\xi, \quad E = \partial_x V, \tag{1.5}$$

or the Euler-Poisson equations in the physical space [30]

$$\partial_t \rho + \partial_x (\rho u) = 0, \qquad x \in \mathbb{R},\ t \geq 0, \tag{1.6}$$

$$\partial_t (\rho u) + \partial_x (\rho u^2) = -\rho \partial_x V, \tag{1.7}$$

$$\partial_{xx} V = b(x) - c\rho. \tag{1.8}$$

There are many papers discussing mathematical analysis and numerical methods for those equations [8, 11, 12, 24, 37], such as the existence and uniqueness of suitable weak solution to Vlasov-Poisson equations [9,19,29,32,50] and numerical methods for capturing the multi-valued solutions to the Euler-Poisson equations [14, 27, 31].

A well-known drawback to the semiclassical approach is that it can not give accurate solutions around caustics. The Gaussian beam methods, developed for the high frequency linear waves [22, 23, 25, 26, 39, 40, 44, 46, 47] and also in the setting of quantum mechanics [15–17], on the other hand, are efficient asymptotic methods that give accurate solutions even around caustics ([45]). The key idea of the Gaussian beam methods is to complexify the phase function $S(t,x)$ off the beam center. Moreover, the imaginary part of $S(t,x)$ should be chosen delicately so that the solution decays exponentially. In this paper, we extend the Gaussian beam methods, proposed previously by the authors [22] for the linear Schrödinger equation, to the weakly nonlinear Schrödinger-Poisson equation (1.1)-(1.2). The original Gaussian beam methods were developed for linear high frequency waves, based on the linear superposition principle. It is of great mathematical and numerical interests to see if the methods can be extended to (at least weakly-) nonlinear problems. In this paper, we propose a class of Gaussian beam methods, in both Lagrangian and Eulerian frameworks, for the Schrödinger-Poisson equations, and check their validity for this weakly nonlinear system.

Our numerical studies show that the Gaussian beam methods can indeed be extended to this one-dimensional, weakly nonlinear system. Indeed, convergent results can be observed, even around caustics, for both the focusing and defocusing cases, when $\varepsilon \to 0$.