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Coupling of Gaussian Beam and Finite Difference Solvers for Semiclassical Schrödinger Equations

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Abstract. In the semiclassical regime, solutions to the time-dependent Schrödinger equation for molecular dynamics are highly oscillatory. The number of grid points required for resolving the oscillations may become very large even for simple model problems, making solution on a grid intractable. Asymptotic methods like Gaussian beams can resolve the oscillations with little effort and yield good approximations when the atomic nuclei are heavy and the potential is smooth. However, when the potential has variations on a small length-scale, quantum phenomena become important. Then asymptotic methods are less accurate. The two classes of methods perform well in different parameter regimes. This opens for hybrid methods, using Gaussian beams where we can and finite differences where we have to. We propose a new method for treating the coupling between the finite difference method and Gaussian beams. The new method reduces the needed amount of overlap regions considerably compared to previous methods, which improves the efficiency.

AMS subject classifications: 35Q41, 41A60, 65M06

Key words: Gaussian beams, semiclassical Schrödinger equation, hybrid methods.

1 Introduction

We consider the dynamics of atomic nuclei, which is decoupled from the electron dynamics through the Born–Oppenheimer approximation [30]. The atoms may be part of a single molecule, or of the reactants and products of a chemical reaction. Our model is the

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time-dependent Schrödinger equation (TDSE) in semiclassical scaling,

$$\mathrm{i}\varepsilon u_t = -\frac{\varepsilon^2}{2}\Delta u + Vu, \quad x \in \mathbb{R}^n, \quad t > 0, \tag{1.1a}$$

$$u(x,0) = u_0(x). \tag{1.1b}$$

The wave function $u = u(x,t)$ contains all retrievable information about the system. In particular, the squared modulus $|u(x,t)|^2$ is the probability density of the nuclei being located at the coordinates x at time t. The probability distribution for other properties, such as momentum and energy, can be extracted by applying operators to the wave function. The Hamiltonian $-(\varepsilon^2/2)\Delta + V$ is the operator for the total energy of the molecular system, and its two terms correspond to the kinetic and potential energies, respectively. The scaling parameter ε is the reciprocal square root of some characteristic mass for the problem. For heavier particles, and thus smaller ε, the problem behaves more classically. The limit $\varepsilon \to 0$ is called the semiclassical limit. The range of interesting ε is between 1 and 10^{-3}, corresponding to the masses of an electron and an uranium atom, respectively. In this paper we focus on semiclassical problems, i.e., problems with heavy particles. Such problems typically feature wave packets of width $\mathcal{O}(\sqrt{\varepsilon})$ and with wavelength $\mathcal{O}(\varepsilon)$, i.e., localised highly oscillatory solutions.

Solving highly oscillatory problems on a grid is often prohibitively expensive due to the vast number of grid points required for resolving the oscillations. This difficulty is not specific to the Schrödinger equation but common to all high frequency wave propagation problems. When resolving the oscillations on a grid becomes unfeasible one has to resort to something else, commonly asymptotic methods. Such methods have been studied in the fields of acoustics, seismology and electromagnetics [6, 15] as well as in quantum dynamics [13]. Asymptotic methods have modelling errors which are dependent on some problem parameter. For high frequency wave propagation problems the modelling error typically decays in the high frequency limit. This is the case for the method of Gaussian beams [1, 5, 27, 28], which we will consider in this work. A Gaussian beam is a complex-valued basis function with Gaussian profile which is propagated along a classical trajectory. Its phase exhibits oscillations with wave length of order ε, and if the potential V is a polynomial of at most second order Gaussian beams solve the TDSE exactly. By adding higher order terms to the amplitude and phase, higher order Gaussian beams can be constructed. Error estimates, in terms of the parameter ε, for more general potentials and Gaussian beams of arbitrary order were shown in [21]. In parallel to their development in the applied mathematics community, Gaussian beams were discovered by chemical physicists [8] motivated by the observation that if the potential is a quadratic polynomial, a Gaussian wave function will stay Gaussian for all time.

Gaussian beams perform well for short wave lengths, i.e., for small ε. The model assumption is that the features of the potential V have a length scale which is long compared to the width of a beam. In applications this is not always valid, the particle masses and the potential are problem parameters beyond our control. In this paper we focus on the situation where the potential is smooth and slowly varying in most of the domain,