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Original article

Time-dependent simulations of quantum waveguides using a time-splitting spectral method

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Abstract

The electron flow through quantum waveguides is modeled by the time-dependent Schrödinger equation with absorbing boundary conditions, which are realized by a negative imaginary potential. The Schrödinger equation is discretized by a time-splitting spectral method, and the quantum waveguides are fed by a mono-energetic incoming plane wave pulse. The resulting algorithm is extremely efficient due to the Fast Fourier Transform implementation of the spectral scheme. Numerical convergence rates for a one-dimensional scattering problem are calculated. The transmission rates of a two-dimensional T-stub quantum waveguide and a single-branch coupler are numerically computed. Moreover, the transient behavior of a three-dimensional T-stub waveguide is simulated.

MSC: 65M70; 35Q40; 37N20

Keywords: Schrödinger equation; Absorbing boundary conditions; Quantum transistor; Three-dimensional dynamical simulations

1. Introduction

Nanoscale quantum electronics is a promising research field for devising new device classes with a high degree of functionality. The electron transport in these devices can be considered to be ballistic at low temperatures. Then the electrical properties depend on quantum interferences, controlled by the bias voltage applied to the gate contacts. These devices may be used as nanoscale electronic switches, quantum interference transistors, multiplexers, etc. [10,35,39]. They are made of different semiconductor materials in such a way that the electrons are confined to small channels or waveguides. Due to the strong confinement of the electron gas to one or two space dimensions, the ballistic quantum transport may be modeled by the one-dimensional or two-dimensional Schrödinger equation. Since there are quantum effects which can be only explained in a three-dimensional model [37], also three-dimensional simulations are of interest.

In this paper, the electron transport in quantum waveguides is modeled by the time-dependent Schrödinger equation with open boundary conditions, which is suitable for ballistic transport. An alternative approach consists in the solution of the nonequilibrium Green's function equations (coupled selfconsistently with the Poisson equation), see, e.g., [36,40].

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Although the open boundary Schrödinger and non-equilibrium Green's functions approaches can be considered to be formally equivalent, their numerical treatment is different [30]. The dynamical behavior of the electrons in a quantum waveguide has been also described by Wigner function models [38]. The disadvantage of Wigner models is its high dimensionality, requiring to solve a six-dimensional problem in three-dimensional devices.

We discretize the Schrödinger equation by employing a time-splitting spectral method. More precisely, the Schrödinger equation is split into the free Schrödinger equation and an ordinary differential equation for the electric potential (see Section 2). The latter equation can be solved explicitly, whereas the former one is approximated by a spectral method [8,27]. There are several time-splitting strategies such as the Trotter and Strang splitting; see [17] for the corresponding error estimates. These methods are unconditionally stable, mass conservative, and gauge invariant [8]. Another advantage of the spectral method is that the discrete set of equations can be solved very efficiently by using the Fast Fourier Transform. In fact, the complexity of the full algorithm for one time step is of the order $\mathcal{O}(M \log M)$, where $M = M_1 \cdots M_d$ and M_j is the number of grid points in the j-th direction (see Section 2).

For the open boundary problem it is necessary to devise appropriate absorbing boundary conditions at the interface between the leads and the active device domain in order to avoid unphysical reflections at the boundary. In the literature, there are several ways of deriving absorbing or transparent boundary conditions (TBC). Analytic TBC are nonlocal in time, and their numerical implementation requires some care (see the review [1] and references therein). Moreover, inadequate discretizations may introduce strong reflections at the boundary [12].

In the quantum transmitting boundary method, the contact region along the leads is replaced by outgoing waveguide modes with known transmitting characteristics [20,30]. This method needs to sum up a large number of modes of the incident, reflected, and transmitted waves from each terminal, and therefore, its implementation is rather complex.

Another method is to introduce perfectly matched layers, first developed for the Maxwell equations [9]. The idea is to enlarge the computational domain by an artificial damping layer of finite width, where a modified equation has to be solved. The method has been applied to the Schrödinger equation in [11,26].

A different idea has been presented in [34]. The (periodic) wave function is decomposed periodically in time into a family of coherent states. In contrast to perfectly matched layer methods, the phase-space filter method of [34] filters only those regions of the phase space containing outgoing waves. However, like for perfectly matched layer methods, it is not easy to treat waves with low kinetic energy.

In the context of finite-difference discretizations such as the Crank–Nicolson method, discrete TBC have been derived [3]. They yield unconditionally stable numerical schemes which are completely reflection-free at the boundary [6]. Discrete TBC include the discrete convolution of the unknown function with a given kernel, and hence, its numerical computation is rather involved. The evaluation of discrete TBC can be significantly accelerated by approximating the kernel by a finite sum of exponentials that decay with respect to time [6]. The limit of vanishing spatial approximation parameters in the discrete TBC coincides with the temporally semi-discrete TBC of Schmidt and Deuflhard [32] and of Lubich and Schädle [21,22,31]. For more references on TBC, we refer to [1,41].

Our aim is to develop a *fast, easy-to-implement numerical scheme* for the open Schrödinger problem in up to three space dimensions. Therefore, in order to reduce the computational cost, we have chosen to model absorbing boundary conditions by the simple imaginary absorbing potential method. Negative imaginary potentials have been proposed to damp the wave function before it reaches the boundary of the computational domain [14,19,23,25]. In [25] criteria for selecting the optimal height and width of such potentials are investigated. It turns out that for low-energy waves, the computational domain has to be large compared to the physical domain, thus increasing the computational cost. However, due to the low complexity of the time-splitting spectral scheme, the overall complexity is still low, and three-dimensional simulations of quantum transistors are possible on modern standard PCs within a few hours of computing time (see Section 3).

Surprisingly, there are only few results in the literature on dynamical simulations of quantum devices in two and three space dimensions. In fact, most of the numerical results (in three dimensions) concern the stationary Schrödinger equation, see e.g. [11,30,33]. Transient simulations are typically performed in one or two space dimensions only, see e.g. [7,34] for Schrödinger simulations and [24] for Wigner simulations. In [15], the time-dependent Schrödinger equation is numerically solved in three space dimensions, but no devices have been simulated. In this paper, we present dynamical simulations of a three-dimensional quantum device.

Our work is organized as follows. In Section 2, we detail the time-splitting spectral method, the choice of the negative imaginary potential, and the injection of a continuously incoming mono-energetic plane wave pulse. Section 3 is devoted to the numerical examples. First, we perform a numerical test in one space dimension to compute numerical