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Original Article

A comparison of approaches for the solution of the Wigner equation

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Abstract

As nowadays semiconductor devices are characterized by active lengths on the nanometer scale, it is important to use models including fully the quantum mechanical effects. In this paper we focus on the Wigner equation, a convenient reformulation of the Schrödinger equation in terms of a phase-space, and present a Monte Carlo technique to solve it, based on signed particles. Then we adapt the concept of potential decomposition, widely utilized to simplify the numerical treatment of the Wigner equation, to our method. Both approaches are compared to the direct solution of the Schrödinger equation. We show that excellent agreement is reached with our Monte Carlo technique which is also computationally efficient. The numerical experiment chosen for the comparisons consists of a Gaussian wave packet tunneling through a realistic source-to-drain potential profile. This is a technologically relevant situation for today's semiconductor devices for which quantum mechanical effects are prominent.

Keywords: Wigner equation; Monte Carlo; Electrostatic potential decomposition; Schrödinger equation; Full quantum transport

1. Introduction

The continuous scaling of semiconductor devices is nowadays at a point, where active lengths are of the order of only a few tens of nanometers. Effects such as particle tunneling through source-to-drain potential profiles are now highly relevant and cannot be ignored. They must be included in simulations to achieve reliable, predictive results. From this perspective, only full quantum models are capable of describing the appropriate physics. A well-known model is the Wigner equation, an equivalent phase-space reformulation of the Schrödinger equation [23].

Despite the numerical difficulties, there has been a high interest around the Wigner formalism. Efforts towards the simulation of this model started several decades ago and were based on finite difference discretization methods [13]. Serious problems were introduced by the treatment of the diffusion term $(\hbar\mathbf{k})/m^* \cdot \nabla_{\mathbf{x}} f_W$. Indeed, the Wigner quasi-distribution function $f_W(\mathbf{x}, \mathbf{k}, t)$ oscillates very rapidly in the phase-space (with both positive and negative values). This can eventually cause problems in the calculation of the derivatives by means of finite difference methods [6].

Recently, two new approaches to solve the Wigner equation, based on Monte Carlo (MC) techniques, have been developed. They both avoid the problem of evaluating the diffusion term, since they use the integral characteristics

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of the Liouville operator, which are Newtonian trajectories. The first model [20–22,12] is an ensemble MC technique based on the concept of quantum affinity, a real number having the meaning of a stochastic weight (ranging in the set $[-\infty;1]$) similar (but not equal) to what happens in MC methods for the statistical enhancement of Boltzmann transport simulations [7,11], which is calculated according to the Wigner potential [12]. The method has proved to be reliable and applicable to several technologically relevant situations such as the simulation of one-dimensional (1D) resonant tunneling diodes. Despite its success, the method can hardly be applied to multi-dimensional simulations due to the demand of significant computational resources. In fact, the number of particle states in the ensemble increases during the simulation according to the complexity of the problem [12]. The second model [19], based on the concept of signed particles [8], is time-dependent, can take into account general initial and boundary conditions (BCs) and, to some phenomenological extent, can include the effects of lattice vibrations [17] (one should note that open BCs in the Wigner formalism still represent an open problem [14], in this paper we use absorbing BCs only which are in agreement with [3]). By exploiting some of the tenets of quantum mechanics, such as indistinguishability of particles and energy quantization, along with the classical notions of trajectories, ensembles and signed particle generation, it is possible to depict a MC approach to the Wigner equation, which is time-dependent and multi-dimensional [10,18,17].

Finally, a concept shown to be very successful and useful for the simulation of nanometer scaled semiconductor devices is the decomposition of the potential profile [4]. This method consists in separating the full potential acting on the domain in two parts, a smooth (classical) component and a rapidly varying (quantum) component. This allows the inclusion of quantum corrections in precedently implemented Monte Carlo simulators. However this concept is challenged by recently developed multi-dimensional Wigner MC methods [18].

In this paper we utilize the signed particle Wigner MC method (full WMC) [19] and simulate the evolution of a Gaussian wave packet moving in a pre-calculated potential profile corresponding to a 1D $n^+ - n - n^+$ diode. Then, we adapt the potential decomposition [4] to our MC method and apply it to the same numerical experiment. Finally, these approaches are compared to the time-dependent Schrödinger equation. An excellent quantitative agreement is demonstrated between the full WMC and the solutions of the Schrödinger equation.

2. The Monte Carlo approach to solving the Wigner equation

The Wigner equation is an intuitive formulation of quantum mechanics in terms of a quasi distribution function $f_W = f_W(x, k, t)$ defined over a phase-space. It reads [9]:

$$\frac{\partial f_W}{\partial t} + \frac{1}{\hbar}\nabla_k \epsilon(k) \cdot \nabla_x f_W = Q[f_W] \tag{1}$$

with

$$Q[f_W](x, k, t) = \int dk' V_W(x, k - k', t) f_W(x, k', t) \tag{2}$$

and

$$V_W(x, k, t) = \frac{1}{i\hbar 2\pi} \int dx' e^{-ik \cdot x'} \left(V\left(x + \frac{x'}{2}, t\right) - V\left(x - \frac{x'}{2}, t\right)\right) \tag{3}$$

(known as the Wigner potential). Here the function $V = V(x, t)$ is the (eventually time-dependent) electrostatic potential defined over the spatial domain.

Now, it is possible to reformulate the Wigner equation over a semi-discrete phase-space. Indeed, by introducing the quantity $\Delta k = \pi/L_C$ (where L_C is a cut-off length, sometimes know as the coherence length), the k-space can be expressed as a set of multiples $k = m\Delta k$ (with m an integer). The semi-discrete Wigner equation reads

$$\frac{\partial f_W}{\partial t} + \frac{\hbar}{m^*} m\Delta k \cdot \nabla_x f_W = \sum_{m'=-\infty}^{+\infty} V_W(x, m') f_W(x, m - m') \tag{4}$$