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A quantum energy transport model for semiconductor device simulation

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ABSTRACT

This paper describes numerical methods for a quantum energy transport (QET) model in semiconductors, which is derived by using a diffusion scaling in the quantum hydrodynamic (QHD) model. We newly drive a four-moments QET model similar with a classical ET model. Space discretization is performed by a new set of unknown variables. Numerical stability and convergence are obtained by developing numerical schemes and an iterative solution method with a relaxation method. Numerical simulations of electron transport in a scaled MOSFET device are discussed. The QET model allows simulations of quantum confinement transport, and nonlocal and hot-carrier effects in scaled MOSFETs.

1. Introduction

The semiconductor devices are scaled down into the nanoscale regime to achieve high circuit performance in the future integrated system. The performance of nanoscale semiconductor devices primarily relies on carrier transport properties in the short channels. Quantum energy transport (QET) models have been developed to understand such physical phenomena in scaled semiconductor devices. A full QET model has been derived from the collisional Wigner–Boltzmann equations using the entropy minimization principle [1]. Numerical simulations using this model, however, have not been performed [2]. Simplified QET models have been proposed as the energy transport extension of the quantum drift diffusion (QDD) model with Fourier law closure and numerically investigated [3,4]. In Ref. [4], the carrier temperature in the current density is further approximated by the lattice temperature to bring the model into a self-adjoint form.

In this paper, we develop numerical methods for a QET model derived from a quantum hydrodynamic (QHD) model. To overcome the difficulties associated with the Fourier law closure, we newly derive a four-moments QET model similar with a classical energy transport (ET) model [5]. The numerical stability is achieved by developing numerical schemes and an iterative solution method in terms of a new set of variables. Numerical results in a scaled MOSFET are demonstrated.

The paper is organized as follows: In Section 2, a four-moments QET model is derived from the QHD model. In Section 3, we present nonlinear discretization schemes and an iterative solution method to solve the QET system. In Section 4, numerical simulations of electron transport in a scaled MOSFET are discussed. Some conclusions are addressed in Section 5.

2. 4 Moments quantum energy transport model

The QET models are obtained by using a diffusion scaling in the quantum hydrodynamic equations, similar as in the classical hydrodynamic model [5]. The QHD model has been derived from the collisional Wigner-Boltzmann equations, assuming

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Fourier law closure [6]. For classical hydrodynamic simulations, the closure relation based on the four-moments of the Boltzmann equation has been discussed [7–9], and the four-moments ET models are developed for simulations of thin body MOSFETs [5,10]. In this work, we derive a four-moments QET model from four moments equations derived from the collisional Wigner–Boltzmann equation.

For simplicity, we consider only the case of electrons. The four moment equations have the same form as the classical hydrodynamic equations [7],

$$\partial_t n + \nabla \cdot (n\mathbf{v}) = nC_n, \tag{1}$$

$$\partial_t (n\mathbf{p}) + \nabla \cdot (nU) - n\mathbf{F}_E = nC_p, \tag{2}$$

$$\partial_t (nw) + \nabla \cdot (n\mathbf{S}) - n\mathbf{v} \cdot \mathbf{F}_E = nC_\epsilon, \tag{3}$$

$$\nabla \cdot (nR) - n(wI + U) \cdot \mathbf{F}_E = nC_{p\epsilon}, \tag{4}$$

where n, $\mathbf{p}$, and w are the electron density, momentum, and kinetic energy, respectively. $\mathbf{v}, U, \mathbf{S}$ and R are the velocity, second moment tensor, energy flow, and fourth moment tensor, respectively. I is the identity tensor. $F_E = -qE$, where E is the electric field. C_n, C_p, C_ϵ, and $C_{p\epsilon}$ are the electron generation rate, the production of crystal momentum, the energy production, and the production of the energy flux, respectively. (1), (2), (3), and (4) represent conservation of particles, momentum, energy, and energy flux, respectively. By assuming parabolic bands, we give the following closure relations for $\mathbf{p}$ and U as

$$\mathbf{p} = m\mathbf{v}, \tag{5}$$

$$U_{ij} = m v_i v_j - \frac{P_{ij}}{n}, \tag{6}$$

where m is an effective mass. The quantum correction to the stress tensor P_{ij} was proposed by Ancona and Iafrate [11], and the quantum correction to the energy density $W = nw$ was first derived by Wigner [12], which are given by

$$P_{ij} = -nkT_n \delta_{ij} + \frac{\hbar^2}{12m} n \frac{\partial^2}{\partial x_i \partial x_j} \log n + O(\hbar^4), \tag{7}$$

$$W = \frac{1}{2} mn v^2 + \frac{3}{2} nkT_n - \frac{\hbar^2}{24m} n \frac{\partial^2}{\partial x_k^2} \log n + O(\hbar^4), \tag{8}$$

where T_n and $\hbar$ are the electron temperature and Plank's constant, respectively.

For the collision terms, we employ a macroscopic relaxation time approximation to drive a QET model as follows:

$$C_n = 0, \tag{9}$$

$$C_p = -\frac{p}{\tau_p}, \tag{10}$$

$$C_\epsilon = -\frac{w - w_0}{\tau_\epsilon}, \tag{11}$$

where τ_p and τ_ϵ are the momentum and energy relaxation times, respectively. Substituting (5)–(7) into (1) and (2), we obtain moment equations for conservation of electron number and momentum

$$\frac{\partial n}{\partial t} + \frac{\partial}{\partial x_i}(n v_i) = 0, \tag{12}$$

$$\frac{\partial}{\partial t}(mn v_i) + \frac{\partial}{\partial x_j}\left(mn v_i v_j + knT_n - \frac{\hbar^2}{12m} n \frac{\partial^2}{\partial x_i \partial x_j} \log n \right) = -n \frac{\partial V}{\partial x_i} - \frac{mn v_i}{\tau_p}. \tag{13}$$

We further get the following relation:

$$\frac{\partial}{\partial x_i} n \frac{\partial^2}{\partial x_i \partial x_j} \log n = 2n \frac{\partial}{\partial x_j} \frac{1}{\sqrt{n}} \frac{\partial^2}{\partial x_i^2} \sqrt{n}. \tag{14}$$

With the relation (14), the quantum correction term in (13) is written as

$$-\frac{\hbar^2}{12m} \frac{\partial}{\partial x_i} n \frac{\partial^2}{\partial x_i \partial x_j} \log n = -\frac{\hbar^2 n}{6m} \frac{\partial}{\partial x_i} \left(\frac{1}{\sqrt{n}} \frac{\partial^2}{\partial x_j^2} \sqrt{n} \right) = -qn \frac{\partial}{\partial x_i} \gamma_n, \tag{15}$$

where the term

$$\gamma_n = \frac{\hbar^2}{6mq} \frac{1}{\sqrt{n}} \frac{\partial^2}{\partial x_j^2} \sqrt{n} \tag{16}$$