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NANOSCALE TRANSPORT DESCRIPTION VIA QHD SIMULATION

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Abstract
A key concession in nanoscale device modeling is the derivation of transport models able to depict the quantum effects and, at the same time, to be straightforward in computer codes. In this paper, we propose a model for ballistic transport in heterostructure devices within Quantum Hydrodynamic (QHD). The model is numerical implemented using a finite-difference discretization and tested in the case of resonant tunneling diode due to availability of experimental data. Genuine QHD model is a frame in development of a quantum photovoltaic device simulator.
Keywords: ballistic transport, Quantum Hydrodynamic, finite-difference.

1. Introduction

The viscous quantum hydrodynamic equations for semiconductors with constant temperature are numerically studied. The model consists of the one-dimensional Euler equations for the electron density and current density, including a quantum correction and viscous terms, coupled to the Poisson equation for the electrostatic potential. The numerical technique used is a central finite difference method.

Quantum semiconductor devices, like superlatices or resonant tunneling diodes [1], are becoming of increasing importance in state-of-the-art semiconductor modeling. These devices rely on quantum tunneling of charge carriers through potential barriers. The objective of this paper is to discretize the viscous quantum hydrodynamic equations in one space dimension in order to emphasize the behavior of the solutions.

2. Mathematical model

The equations for electron density $n(x,t)$ and current density $J(x,t)$ are [2]:

$$\frac{\partial n}{\partial t}+\frac{1}{q}divJ=\nu\Delta n \qquad (1)$$

$$\frac{\partial J}{\partial t}+div\left(\frac{J\otimes J}{n}\right)+T\nabla n-n\nabla\left(V+V_{ext}\right)-\frac{\varepsilon^2}{2}n\nabla\left(\frac{\Delta\sqrt{n}}{\sqrt{n}}\right)=-\frac{J}{\tau}+\nu\Delta J \qquad (2)$$

and Poisson equation for the electrostatic potential $V(x,t)$

$$\lambda^2 \Delta V = n - C(x) \tag{3}$$

The term $n\nabla V_{ext}$ models heterogeneous semiconductor materials [3].

These equations are scaled by introducing characteristic length L and the characteristic time τ_0 and define the characteristic density , voltage and current density, respectively, by

$$C^* = \sup|C|, \quad V^* = \frac{k_B T_0}{q}, \quad J^* = \frac{q k_B T_0 C^* \tau_0}{Lm} \frac{L}{i} \tag{4}$$

where i is the mean free path defined by $i^2 = k_B T_0 \tau_0^2 / m$. The scaled parameters are

$$\varepsilon^2 = \frac{1}{6}\left(\frac{L_b}{L}\right)^2, \quad \nu = \frac{1}{6}\left(\frac{L_b}{L}\right)^2 \frac{L}{i}\frac{t^*}{\tau_0}, \quad T = 1 + \frac{1}{\sqrt{18\pi}} \frac{\Omega\hbar}{k_B T_0} \frac{L_b}{i}, \quad \lambda^2 = \frac{\varepsilon_s k_B T_0}{q^2 L^2 C^*} \tag{5}$$

and $L_b = h / \sqrt{2mk_B T_0}$ is the de Broglie length.

The values of the parameters which we employ for the numerical simulations are: elementary charge $q = 1.6 \cdot 10^{-19} C$, effective electron mass $m = 0.063 \cdot 9.1 \cdot 10^{-31} kg$, Boltzmann constant $k_B = 1.38 \cdot 10^{-23} J/K$, Planck constant $h = 6.62 \cdot 10^{-34} Js$, semiconductor permittivity $\varepsilon_s = 12.9 \cdot 8.85 \cdot 10^{-12} As/Vm$, lattice temperature $T_0 = 77K$ and momentum relaxation time $\tau_0 = 0.9 \cdot 10^{-12} s$. The characteristic length and density are

$$L = 125nm, \quad C^* = 10^{24} m^{-3} \tag{6}$$

The viscous quantum hydrodynamic equations (1)-(3) in the one dimensional interval $\Omega = (0,1)$, are discretized using central finite differences.

The boundary conditions are like in [4], which express that the total charge $C - n$ vanishes at the interval boundary. For current density we take Neumann boundary condition $\partial J / \partial x = 0$. The boundary conditions for the electric potential are 0 and *U,* where *U* is the applied potential.

At each time step, after solving (1)-(2), the Poisson equation (3) is solved using the new value for n_j. The stationary solution is computed as the long time limit of the transient solution. The time step control is done heuristically, and the transient computations are stopped when the changes of the current density at selected points are smaller than a certain tolerance. At applied voltage $U = 0$, the initial conditions for (1)-(3) may be chosen as $n(x,0) = C(x)$ and $J(x,0) = 0$. The obtained solution at the applied voltage U is used as initial data for (1)-(2) with an applied voltage $U + \Delta U$.

3. Numerical simulations

3.1Simulation of a ballistic diode

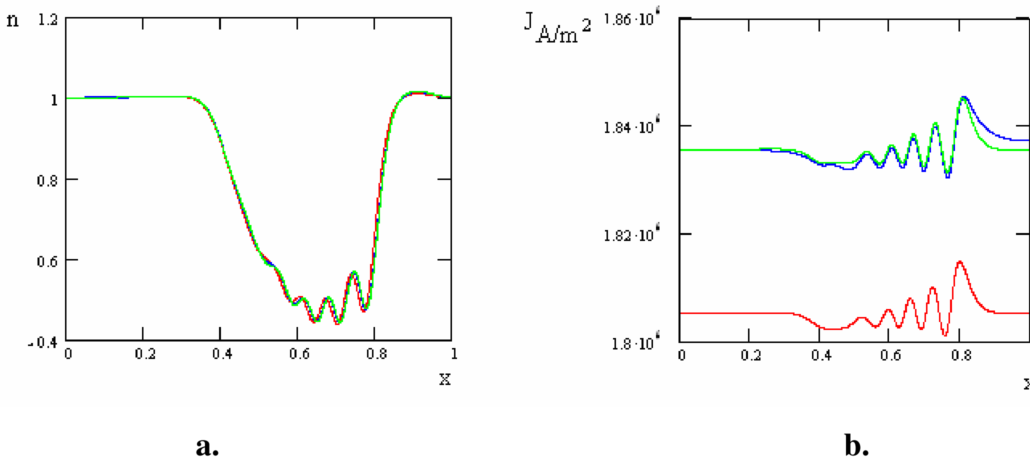
The scaled parameters are

$$\varepsilon = 0.00289 \qquad \lambda = 0.1 \qquad \tau = 0.125 \tag{7}$$

And the doping profile

$$C(x) = 1 + 0.45(\tanh(1000x - 600) - \tanh(1000x - 400)), \qquad x \in (0,1) \tag{8}$$

In Figure 1a we present the electron density for an applied voltage $U = 0.06V$. The particle density oscillates as already point out in [5]. The current density is not constant in the viscous model like in Figure 1b.



a. **b.**

Figure 1: a. Electron density versus position of the viscous quantum hydrodynamic model; b. Current density versus position for applied voltage U=0.06V

3.2 Simulation of a resonant tunneling diode

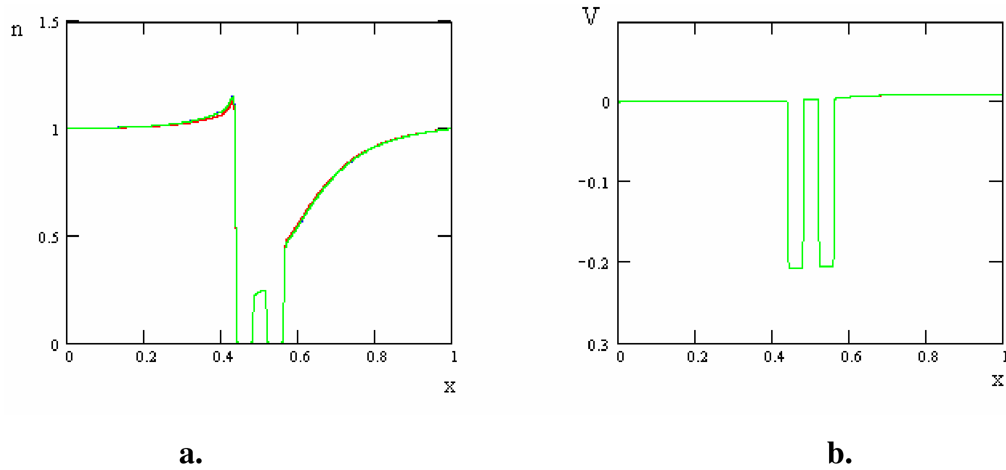
The tunneling diode consists of highly doped *GaGe* regions near the contacts and a lightly doped middle region of $50nm$ length. The middle region contains a quantum well of $5nm$ length sandwiched between two $5nm$ *AlGaAs* barriers. This resonant barrier structure is itself sandwiched between two $5nm$ *GaAs* spacer layers. The physical effect of the barriers can be modeled by an additional step function V_{ext} added to the electrostatic potential. The device length is $L = 125nm$ and the doping profile is

$$C(x) = \begin{cases} 5 \cdot 10^{21} m^{-3}, x \in [50nm, 75nm] \\ 10^{24}, else \end{cases} \tag{9}$$

The potential V_{ext} is taken as in [3]:

$$V_{ext} = \begin{cases} -0.209V, x \in [55nm, 60nm] \cup [65nm, 70nm] \\ 0, else \end{cases} \tag{10}$$

We take in the simulations 4000 grid points and a time step $10^{-5}\,ps$. Typically the equilibrium is reached in 10-20ps.



a. **b.**

Figure 2: a. Electron density versus position; b. Electrostatic potential versus position for $U = 0.02V$

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