Physica D 243 (2013) 1–13

Contents lists available at SciVerse ScienceDirect

Physica D

journal homepage: www.elsevier.com/locate/physd

Steady states and interface transmission conditions for heterogeneous quantum–classical 1-D hydrodynamic model of semiconductor devices

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ARTICLE INFO

Article history:
Received 23 October 2010
Received in revised form
15 May 2012
Accepted 25 May 2012
Available online 25 August 2012
Communicated by S. Kai

Keywords:
Mathematical models for semiconductors
Hybrid models for semiconductors
Quantum hydrodynamical models
Transmission conditions

ABSTRACT

We study a hybrid model linking the quantum hydrodynamics equation with classical hydrodynamics deriving the transmission conditions between the two PDE systems modeling the quantum and the classical dynamics. These conditions are derived under the assumption of constant scaled temperature and assuming a current jump across the interface between the classical and the quantum region. In Section 2.2 we shall give a heuristic and physically plausible explanation of this assumption.

Because of this fact we produce not a weak solution on the whole device domain, but a piecewise smooth solution.

1. Introduction

The recent growth of the microelectronic industry caused an increasing interest in the mathematical model for semiconductor devices. Since the invention in 1947 of the first bipolar point-contact transistor by Bardeen, Brattain, and Shockley (Nobel Prize in Physics 1956), many different devices have been designed. The ongoing progress of industrial semiconductor device technologies permits us to fabricate devices which employ quantum phenomena in their operation e.g. resonant tunneling diodes, quantum well lasers and nanowires. The drift–diffusion equation, introduced by van Roosbroeck in 1950, does not take into account these quantum effects, whereas the Schrödinger equation perfectly describes macroscopic variables like charge density and current density; nevertheless the numerical treatment of this equation is very expensive compared to the macroscopic model. Recently the quantum hydrodynamic equation (QHD) has been used in order to describe the modern quantum device. In one space dimension the (scaled) equations for the charge density n and for the current density J read:

$$n_t + J_x = 0$$
$$J_t + \left(\frac{J^2}{n} + nT\right)_x - nV_x - \delta^2 \left(n \left(\ln n\right)_{xx}\right)_x = -\frac{J}{\tau}.$$

Generally these equations are coupled with Poisson's equation:

$$\lambda^2 V_{xx} = n - C(x).$$

Formally, if $\delta = 0$, we get the classical hydrodynamic model (HD). For $\delta > 0$, the quantum correction term

$$\delta^2 \left(n \left(\ln n\right)_{xx}\right)_x = -2\delta^2 n \left(\frac{\sqrt{n}_{xx}}{\sqrt{n}}\right)_x \tag{1}$$

is the so-called Bohm potential.

Remark 1. In our approach we shall ignore the collision terms J/τ in the quantum part of the device, since the dynamics are dominated by the tunnel phenomena, but we will keep it in the classical one.

The QHD model is derived in different ways by the Wigner–Boltzmann equation [1] and from the Schrödinger equation and it has been analyzed from different points of view [2–10]. For example in [2] the authors prove the existence and the uniqueness of a steady state solution for QHD in the interval (0, 1) by using a linear pressure functional whereas in [3] the authors show that the QHD equation is equivalent to a non-standard integral differential equation and solve it. In [4] the authors analyze a multi-dimensional quantum hydrodynamical model for semiconductors which is simplified under the assumption that the pressure P is a known function of the density ρ. Generally the quantum effects are important in a limited region, e.g. around the double barrier in resonant tunneling diodes, whereas the rest of the device is well described by classical models. For this reason the

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doi:10.1016/j.physd.2012.08.012

hybrid strategy has been introduced. In [5] the authors consider a one-dimensional coupled stationary Schrödinger drift-diffusion without collision, in order to link quantum zone and classical zone supposing that the current density is continuous. In [6] the author discusses the transmission conditions between a classical transport model described by the Boltzmann equation and a quantum model described by a set of Schrödinger equations. It is known that, from the numerical point of view, the Schrödinger equation is very difficult to treat and the drift–diffusion equations do not provide good results in modeling modern semiconductor devices. Mathematical analysis of models described by the systems of quantum hydrodynamics can be found in [7,8]. The analytical methods to deal with heterogeneous domains are outlined in [9].

In this paper we will study a hybrid model linking the classical hydrodynamic model and the quantum hydrodynamic one, in order to get a method through which we can simplify the analysis of the modern complex device. The advantage of this type of model is to use a quantum (more complicated) equation just in a reduced zone of the device domain. For this reason, as a toy model, we consider a device domain $\Omega = [-1, a]$, which is divided into a classical zone $\Omega_c = [-1, 0]$ and a quantum zone $\Omega_q = [0, a]$. In the physical case $a \ll 1$, but we assume $a = 1$ in order to simplify the mathematical calculations, this does not produce loss of generality, since the final goal of this paper is the derivation of a compatible set of transmission conditions that do not depend on the quantum domain length. Moreover the assumption $a = 1$ will be justified in Section 2.1, where we show the scaling of the equations. It is very important to remark that our model does not produce a weak solution on the whole device-domain, but we only obtain a piecewise solution. In other words we consider separately quantum and classical systems in two different regions of our device and we link them by a given set of transmission conditions.

From now on the index q defines the quantum quantity whereas the index c denotes the classical objects. In the first region we work by using the classical hydrodynamic equation whereas in the second one we will use the quantum equation.

Unfortunately information is not available at the interface point, since it is impossible to take experimental measures in this point. We use the following assumptions:

A1. The charge density n is a continuous function in Ω, and in particular, at the interface point $x = 0$, i.e.:

$$n_c(0) = n_q(0). \tag{2}$$

A2. The current density is constant in Ω_c and in Ω_q, where we have, respectively, $J = J_c$ and $J = J_q$, but J has a finite jump at $x = 0$ namely

$$J_c \neq J_q, \tag{3}$$

therefore the continuity equation $n_t + J_x = 0$ will be valid, separately, in Ω_c and in Ω_q, but not in the whole Ω.

Here is the outline of the paper. Sections 2, 3, 5 and 6 contain the core of the mathematical physical model and of the mathematical tools. Specifically, in Section 2 we derive our model (by using scaling arguments) and a consistent set of transmission conditions.

In Section 3 we prove the existence of solutions to the problem

$$\left(\frac{J_q^2}{n_q} + n_q T\right)_x - n_q V_x - \delta^2 \left(n_q \left(\ln n_q\right)_{xx}\right)_x = 0 \tag{4}$$

coupled with the Poisson equation

$$\lambda^2 V_{xx} = n - C(x). \tag{5}$$

Here $n, V, J_c, J_q, T, \lambda$ are the electron density, classical electron current density, quantum electron current density, electrical potential, scaled electron temperature and scaled electrical permeability, respectively. Moreover $C(x) \in L^2(\Omega)$ is the doping profile describing the fixed charge background ions in the semiconductor crystal. We suppose J_c and J_q are (positive) constants, respectively, in Ω_c and Ω_q. We consider (4) coupled with the following set of boundary conditions

$$n_q(0) = n_c(0), \qquad n_q(1) = n_1, \qquad n_{qx}(0) = n_{qx}(-1) = 0,$$
$$V_q(1) + \delta^2 n_{q,xx}(1) = P, \tag{6}$$

for a given J_q and for a fixed value of the constant P. Note that *a priori* we do not know the correct value for $n_q(0)$, and, at the first step, we work, using a certain value $n_{q,0}(0)$ of $n_q(0)$, such that

$$C^- \le n_{q,0}(0) \le C^+ \tag{7}$$

where C^- and C^+ will be defined in Theorem 4. Afterwards, when the solution $n_{q,0}(x)$ is known, we compute $J_{c,1}$ using the potential jump condition (24). Then in Section 5, we will solve the classical hydrodynamical problem

$$\left(\frac{J_c^2}{n_c} + n_c T\right)_x - n_c V_x = -\frac{J_c}{\tau_c}, \tag{8}$$

coupled with (5) and with

$$n_{c,1}(-1) = 1, \qquad n_{c,x}(0) = 0, \qquad V_c(0) = 0 \tag{9}$$

where τ_c is the classical relaxation time. This allows us to calculate $n_{c,1}(0)$, since by (2) we have

$$n_{c,1}(0) = n_{q,1}(0). \tag{10}$$

Remark 2. We assume $V(0) = 0$, as condition for the electrical potential, because this choice simplifies the calculation. From the physical point of view it looks more reasonable to assume $V(-1) = V_{-1}$, we can ride out this problem assuming at every step (in our numerical interaction) $V_{c,k}(-1) = V_{c,k} - 1$ such that $V_{c,k}(0) = 0$.

To close this iterative procedure we need to show that the map

$$Y : n_c(0) \to n_q(0). \tag{11}$$

has a fixed point.

Then, in Section 6 we will prove the existence of a fixed point for Y by proving that the auxiliary map

$$\widetilde{Y} : (J_{c,k}^2/n_{c,k}^2(0)) \to (J_{c,k+1}^2/n_{c,k+1}^2(0)). \tag{12}$$

is contractive and we need to show that this implies (11).

In Section 4 we discuss the subsonic solution of the classical problem, whereas in Section 7 we test our model by using a simple devices.

The model presented in this paper allows us to produce numerical simulations that are quite realistic and very close to the ones obtained in [2]. However, it is still important to go on with modeling hypotheses that are less confined from the physical point of view for the temperature that here is constant at the interface point. We are going on with this analysis and some results for a new model including this effect will be developed in a forthcoming paper.

Please cite this article in press as: F. Di Michele, et al., Steady states and interface transmission conditions for heterogeneous quantum–classical 1-D hydrodynamic model of semiconductor devices, Physica D (2012), doi:10.1016/j.physd.2012.08.012