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A Note on Current-Voltage Characteristics from the Quantum Hydrodynamic Equations for Semiconductors

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Abstract—The quantum hydrodynamic model is primary used for the simulation of resonant tunneling diodes. The current-voltage characteristics of these diodes show negative differential resistance (NDR) effects. For two simplified one-dimensional quantum models derived by means of asymptotic analysis, explicit formulas of the current-voltage characteristics are given. It turns out that not only the quantum correction term but also the convection term are mathematically responsible for the NDR effects. This observation is confirmed by numerical simulations of the full isothermal quantum hydrodynamic model.

Keywords—Quantum hydrodynamics, Quantum drift-diffusion model, Asymptotic analysis, Numerical solution.

1. INTRODUCTION

For ultra-small electronic devices in which quantum effects are present, the mathematical semiconductor models have to incorporate the quantum mechanical phenomena. Recently, various so-called quantum hydrodynamic models were used in semiconductor simulations of tunneling diodes [1,2]. These models are macroscopic models describing the electron flow in semiconductor crystals, in terms of macroscopic variables like the electron density and the electron current density. They are dispersively regularized versions of the classical hydrodynamic equations, where the (scaled) Planck constant plays the role of the dispersivity. The quantum hydrodynamic equations can be derived from a many-particle Schrödinger-Poisson system [3] or from the Wigner equation via the moment method [1].

The primary application of the quantum hydrodynamic model is the simulation of quantum devices that depend on particle tunneling through potential barriers, like resonant tunneling diodes. One-dimensional simulations of tunneling diodes show negative differential resistance in the current-voltage characteristic (see [1,2]). In this note, we make evident that not only the quantum correction but also the convection term are mathematically responsible for these effects. If the convection term is neglected in the model, no negative differential resistance appears.

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The stationary isothermal quantum hydrodynamic equations in one space dimension read:

$$\frac{1}{q}\left(\frac{J^2}{n}\right)_x + \frac{qkT}{m}n_x - \frac{q^2}{m}n\left(V + V_{\text{ext}}\right)_x - \frac{q\hbar^2}{2m^2}n\left(\frac{(\sqrt{n})_{xx}}{\sqrt{n}}\right)_x = -\frac{J}{\tau}, \tag{1.1}$$

$$J_x = 0, \qquad \varepsilon_s V_{xx} = q(n - C), \qquad \text{in } \Omega. \tag{1.2}$$

Here, n denotes the electron density, J the electron current density, and V the electric potential. The external potential $V_{\text{ext}}(x)$ modelling (interior) quantum wells, and the doping profile $C(x)$ modelling background "ions" are given functions. The physical constants are the elementary charge q, the Boltzmann constant k, and the reduced Planck constant $\hbar$. We assume that the temperature T, the effective mass of the electrons m, the relaxation time τ, and the semiconductor permittivity ε_s are constant. The relaxation time is given by the expression $\tau = \iota/v_o$, where ι is the mean free path of the particles and $v_o = \sqrt{kT/m}$ is the characteristic velocity of the electrons. Finally, the semiconductor domain is the interval $\Omega = (0, L) \subset \mathbb{R}$, $L > 0$ being the device length.

In this paper, we consider the following different cases of the order of magnitude of the device length (for the details, see Section 2).

(i) If the device length is much larger than the mean free path, the convection term in (1.1) can be neglected and we get the so-called *quantum drift-diffusion model.*

(ii) If the device length is much smaller than the mean free path and the de Broglie length $L_b = \hbar/\sqrt{2mkT}$, the convection and quantum terms dominate the remaining terms in (1.1) and we get a *reduced quantum model.*

(iii) In the case where the device length is of the same order as the mean free path, we obtain, after an appropriate scaling, a dimensionless version of (1.1),(1.2), the *full quantum model*, where no term is neglected.

We choose the following boundary conditions. The electron density n, the electric potential V, and the velocity potential S (defined by $S_x = J/n$) are prescribed on the boundary $x = 0, L$. In the numerical simulations of Section 4, we also use Dirichlet boundary conditions for n and V and homogeneous Neumann boundary conditions for n as in [1]. The parameter $U = V(L) - V(0)$ is called the applied voltage. We are interested in the properties of the current-voltage characteristic $J = J(U)$.

We summarize the main results of this note.

(a) The current-voltage characteristic of the reduced quantum model is

$$J(U) = \sqrt{2}\delta_o \sin\frac{U}{\sqrt{2}\delta_o}, \qquad \text{for } 0 \le U < \sqrt{2}\delta_o\pi,$$

where $\delta_o > 0$ is some constant. Thus, we get negative differential resistance, i.e., $\frac{dJ}{dU} < 0$, in some interval.

(b) The current-voltage characteristic of the quantum drift-diffusion model for *constant* doping profile is given by

$$J(U) = U, \qquad \text{for } U \ge 0.$$

(c) Numerical simulations of a resonant tunneling diode using the full quantum model show effects of negative differential resistance. If the convection term is neglected (quantum drift-diffusion model), the current $J(U)$ increases monotonically with the applied voltage U.

In Section 2, we give the details of the scaling for the models (i)–(iii). The current-voltage curves for the quantum drift-diffusion and the reduced quantum model are computed in Section 3. Finally, Section 4 is devoted to the numerical simulation of the quantum drift-diffusion and the quantum hydrodynamic model.

2. SCALINGS

In this section, we scale appropriately the quantum hydrodynamic equations and we derive the quantum drift-diffusion and the reduced quantum model.

Let C_m be the maximal value of the doping profile, and recall that $\iota = \tau v_o$ and $L_b = \hbar/\sqrt{2mkT}$ are the mean free path and the de Broglie length, respectively, introduced in Section 1. Using the scaling (cf. [4])

$$n \to C_m n, \qquad C \to C_m C, \qquad x \to Lx,$$
$$V \to \frac{kT}{q} V, \qquad V_{\text{ext}} \to \frac{kT}{q} V_{\text{ext}}, \qquad J \to \frac{qkTC_m\tau}{Lm} J$$

in (1.1),(1.2), we get

$$\left(\frac{\iota}{L}\right)^2 \left(\frac{J^2}{n}\right)_x + n_x - n\left(V + V_{\text{ext}}\right)_x - \left(\frac{L_b}{L}\right)^2 n \left(\frac{\sqrt{n}_{xx}}{\sqrt{n}}\right)_x = -J, \tag{2.1}$$

$$J_x = 0, \qquad \lambda^2 V_{xx} = n - C, \qquad \text{in } \Omega = (0,1), \tag{2.2}$$

where $\lambda^2 = \varepsilon_s kT/q^2L^2C_m$ is the squared scaled Debye length. Notice that we have used the same notations for the scaled and unscaled variables.

2.1. The Full Quantum Hydrodynamic Model

Consider a device with the parameters (cf. [1])

$$T = 100\,\text{K}, \qquad \tau = 10^{-12}\,\text{s}, \qquad L = 0.1\,\mu\text{m}.$$

Then the free mean path is $\iota = 150\,\text{nm}$, and we get $\iota/L \approx 1$. The parameter $\delta = L_b/L \ll 1$ (here $\delta \approx 0.08$) is called the (scaled) Planck constant.

The equations (2.1),(2.2) can be formulated as an elliptic system. Indeed, assume that the density n is positive. Then, defining the velocity potential S (up to an additional constant) by $S_x = J/n$, dividing (2.1) by n and integrating, we find

$$\frac{1}{2}S_x^2 + \ln(n) - V - V_{\text{ext}} - \delta^2 n \left(\frac{\sqrt{n}_{xx}}{\sqrt{n}}\right)_x + S = 0.$$

The integration constant can be assumed to be zero by choosing a reference point for the electric potential. Setting $w = \sqrt{n}$, the equations (2.1),(2.2) can be written as

$$\delta^2 w_{xx} = w\left(\frac{1}{2}S_x^2 + \ln\left(w^2\right) - V - V_{\text{ext}} + S\right), \tag{2.3}$$

$$\left(w^2 S_x\right)_x = 0, \qquad \lambda^2 V_{xx} = w^2 - C. \tag{2.4}$$

The boundary data are assumed to be the superposition of the thermal equilibrium functions and the applied potential $\tilde{U}(0) = 0$, $\tilde{U}(1) = U$, which implies (fixing here the constant for S; cf. [5])

$$w = \sqrt{C}, \quad S = \tilde{U}, \quad V = \ln(C) + \tilde{U}, \qquad \text{on } \partial\Omega.$$

In the following, we assume that we are modelling devices with an n^+nn^+ structure (see Section 4) such that $C(0) = C(1) = 1$ holds. Hence, we impose the boundary conditions

$$w(0) = w(1) = 1, \qquad S(0) = V(0) = 0, \qquad S(1) = V(1) = U. \tag{2.5}$$

In the simulation of tunneling devices, other boundary conditions for (2.1),(2.2) are also used (see, e.g., [1]):

$$n(0) = n(1) = 1, \qquad n_x(0) = n_x(1) = 0, \qquad V(0) = 0, \qquad V(1) = U. \tag{2.6}$$

The system (2.3)–(2.5) is studied in [5]. It is shown that for sufficiently small $|U|$, there exists a solution (w, S, V) to (2.3)–(2.5) with strictly positive w. Therefore, the problems (2.3),(2.4) and (2.1),(2.2) are equivalent.

2.2. The Quantum Drift-Diffusion Model

In a quantum device with the data

$$T = 100\,\mathrm{K}, \qquad \tau = 10^{-13}\,\mathrm{s}, \qquad L = 0.1\,\mu\mathrm{m},$$

(τ corresponds to a low-field mobility in GaAs; see [1]) the mean free path is equal to $\iota = 15\,\mathrm{nm}$. Thus, the parameter $\varepsilon = \iota/L$ is small compared to one. Letting formally $\varepsilon \to 0$ in (2.1), we get the equation

$$n_x - n\,(V + V_{\mathrm{ext}})_x - \delta^2 n \left(\frac{\sqrt{n}_{xx}}{\sqrt{n}}\right)_x = -J,$$

or, as in Section 2.1,

$$\delta^2 w_{xx} = w\left(\ln\left(w^2\right) - V - V_{\mathrm{ext}} + S\right), \tag{2.7}$$

$$\left(w^2 S_x\right)_x = 0, \quad \lambda^2 V_{xx} = w^2 - C, \qquad \text{in } \Omega, \tag{2.8}$$

which, with the boundary conditions (2.5) or (2.6), is referred to as the quantum drift-diffusion equations. They are motivated in [6] and mathematically analyzed in [7].

2.3. The Reduced Quantum Model

For ultra-small devices with data

$$T = 1\,\mathrm{K}, \qquad \tau = 10^{-11}\,\mathrm{s}, \qquad L = 20\,\mathrm{nm},$$

(cf. [8]) the mean free path $\iota = 150\,\mathrm{nm}$ and the de Broglie length $L_b = 80\,\mathrm{nm}$ are much larger than the device length. Then $\varepsilon = L/\iota$ and $\varepsilon_b = L/L_b$ are "small" parameters. Thus, letting formally $\varepsilon \to 0$ and $\varepsilon_b \to 0$ such that $\varepsilon/\varepsilon_b \to \delta_o^2 > 0$, we obtain the reduced model equations

$$\delta_o^2 w_{xx} = \frac{1}{2} w S_x^2, \qquad \left(w^2 S_x\right)_x = 0, \tag{2.9}$$

with the boundary conditions (2.5) for w and S. For such ultra-small devices, we expect that quantum boundary effects may occur so that the boundary conditions (2.5) are only approximately satisfied.

3. ANALYTICAL CURRENT-VOLTAGE CHARACTERISTICS

In this section, we compute explicit solutions for the reduced quantum model and the quantum drift-diffusion model, from which the current-voltage characteristics can be derived. The current $J = J(U)$ is defined by $J = w^2 S_x \in \mathbb{R}$ (see (2.4)). Let $V_{\mathrm{ext}} = 0$ in Ω.

PROPOSITION 3.1. *For the reduced quantum model (2.5),(2.9), it holds* $J(U) = \sqrt{2}\delta_o \sin(U/\sqrt{2}\delta_o)$ *for all* $0 \le U < \sqrt{2}\delta_o \pi$.

PROOF. Let $\sigma = U/\sqrt{2}\delta_o$. A computation shows that the functions

$$w(x) = \left((1-2x)^2 + 2(1+\cos\sigma)x(1-x)\right)^{1/2},$$

$$S(x) = \sqrt{2}\delta_o \arccos \frac{1-(1-\cos\sigma)x}{w(x)}, \qquad x \in (0,1),$$

solve (2.5),(2.9), and that $J(U) = w(x)^2 S_x(x) = \sqrt{2}\delta_o \sin\sigma$ for $\sigma \in [0,\pi)$. ∎

For applied voltages near the limit value $U = \sqrt{2}\delta_o\pi$, the so-called valley current can be very small (compared to the peak current $\sqrt{2}\delta_o$). We expect that the diffusion term in (1.1) (and hence, a nonvanishing temperature) leads to a positive current for the full model. Physical experiments show that the valley current can be very small (compared to the peak current) and decreases as the temperature decreases [8].

PROPOSITION 3.2. *Let $C(x) = 1$ for $x \in (0,1)$. Then, for the quantum drift-diffusion model, it holds $J(U) = U$ for all $U \geq 0$.*

PROOF. The functions $w(x) = 1$, $S(x) = V(x) = Ux$, $x \in (0,1)$, solve (2.7), (2.8), and (2.5). Thus $J(U) = w^2 S_x = U$. ∎

Clearly, the equations with constant doping profile do not model a diode. However, in the next section we present a numerical example for a tunneling diode, where a similar behavior of the current-voltage curve as in Proposition 3.2 can be observed.

4. NUMERICAL CURRENT-VOLTAGE CHARACTERISTICS

We present a numerical simulation of a resonant tunneling diode. The experiments were performed employing the general purpose two-point-boundary-value-problem solver Colsys/Colnew, which uses piecewise polynomial collocation at Gaussian points [9]. The scaled parameters and functions for the diode are as follows. The doping profile is given by $C(x) = 1$ for $x < 0.3$ and $x > 0.7$, and $C(x) = 0.1$ for $0.3 < x < 0.7$. The external potential is $V_{\text{ext}}(x) = 1$ for $0.4 < x < 0.45$ and $0.55 < x < 0.6$, $V_{\text{ext}}(x) = 0$ for $x < 0.4$ and $x > 0.6$, and $V_{\text{ext}}(x)$ is a quadratic polynomial in $(0.45, 0.55)$ defined by $V_{\text{ext}}(0.45) = V_{\text{ext}}(0.55) = 1$ and $V_{\text{ext}}(0.5) = 0$. Furthermore, $\delta = 0.5$ and $\lambda = 0.1$ (see [10]). These values correspond to the unscaled parameters $L = 0.11\,\mu\text{m}$, $T = 4\,\text{K}$, $\tau = 10^{-12}\,\text{s}$, and $C_m = 1.8 \cdot 10^{15}\,\text{cm}^{-3}$.

In Figure 1, the current-voltage curves for the full quantum hydrodynamic model (QHD) and the quantum drift-diffusion model (QDD) for the above parameters and boundary conditions (2.6) are shown. The characteristic for the quantum hydrodynamic equations show negative differential resistance in some region, whereas the curve for the quantum drift-diffusion model is nearly linear. This means that if the convection term in (1.1) is neglected, the negative differential resistance disappears.

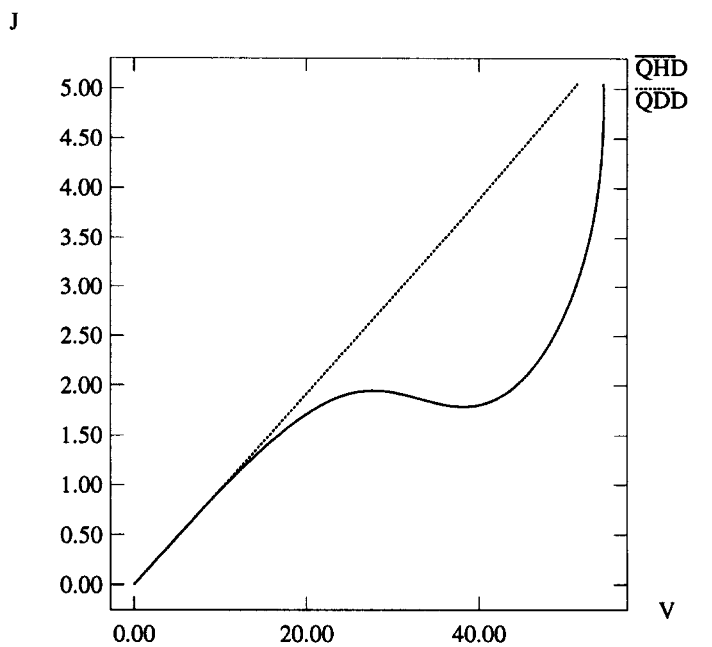

Figure 1. Current-voltage characteristics of a tunneling diode (J in $250\,\text{Acm}^{-2}$, U in $0.4\,\text{mV}$).

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