Nonlinear Problems in Quantum Semiconductor Modeling

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Abstract

A model hierarchy of macroscopic models for quantum semiconductors is presented. Furthermore, a review on recent results obtained for two classes of these macroscopic models: the quantum hydrodynamic and the quantum drift-diffusion equations is given. In particular, the existence of solutions and their qualitative behavior is studied and a numerical scheme for the quantum drift-diffusion model is derived. Finally, this scheme is applied to the transient simulation of a resonant tunneling diode.

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1 A model hierarchy

For ultra-small semiconductor devices in which quantum effects are present, the corresponding mathematical models have to incorporate the quantum mechanical phenomena. Roughly speaking, these models can be divided into two classes: microscopic and macroscopic quantum models.

Microscopic models include quantum kinetic equations, like the Wigner equation and the Wigner-(Poisson-)Fokker-Planck model, and Schrödinger-Poisson systems [6,24]. For semiconductor applications, these models have to be considered on bounded domains such that adequate boundary conditions have to

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be devised. Due to the intrinsic nonlinearity of quantum mechanics, it is far from being trivial to impose physically correct boundary conditions that are also numerically tractable [3]. Moreover, the numerical simulation of Wigner-Poisson-Fokker-Planck models is quite expensive [30], and higher dimensional Wigner simulations are even not feasible.

Macroscopic quantum models have the advantage that macroscopic quantities, like electron density or current density, can be prescribed at the boundary of the semiconductor domain. Moreover, the numerical part seems to be easier than for the microscopic models. The *(full) quantum hydrodynamic model* can be derived from the Wigner-Boltzmann equation using a moment method [11,13] or from the many-particle Schrödinger equation [15]. It governs the evolution of the electron density n, the electron current density J, the energy density E, and the electrostatic potential V. Assuming that the typical time scale is given by the momentum relaxation time constant τ_p and using the scaling as in [17], we obtain the following scaled equations:

$$\partial_t n - \varepsilon^2 \mathrm{div}\, J = 0, \tag{1}$$

$$\partial_t J - \varepsilon^2 \mathrm{div}\left(\frac{J \otimes J}{n}\right) - \nabla(nT) + n\nabla(V+Q) = C_J, \tag{2}$$

$$\partial_t E - \mathrm{div}\left(\varepsilon^2 \frac{J|J|^2}{2n^2} + \frac{5}{2}TJ + \kappa\nabla T\right) = -J\cdot\nabla(V+Q) + C_E, \tag{3}$$

$$\lambda^2 \Delta V = n - C(x), \tag{4}$$

where the ik-th component of the tensor product $J\otimes J$ equals J_iJ_k. The term $Q = \delta^2\Delta\sqrt{n}/\sqrt{n}$ is the Bohm quantum correction, T denotes the electron temperature, the energy density is given by

$$E = n\left(\frac{|J|^2}{2n^2} + \frac{3}{2}\frac{T}{\varepsilon^2} - \frac{\delta^2}{12}\Delta\log(n)\right),$$

and

$$C_J = -J, \quad C_E = -\frac{\tau_p}{\tau_w}\left(\frac{|J|^2}{2n} + \frac{3}{2}\frac{n(T-T_0)}{\varepsilon^2}\right)$$

are the momentum and energy relaxation terms, respectively. The scaled parameters are the ratio of the mean free path and the typical device length ε, the scaled Planck constant δ (the ratio of the de Broglie length and the device length), the Debye length λ, the energy relaxation time constant τ_w, and the ambient temperature T_0. The doping profile $C(x)$ models fixed background charges. The heat conduction term $-\kappa\nabla T$ comes from the closure condition. Eqs. (1)-(4) are considered in a bounded domain with appropriate initial and boundary conditions for n, J, and E [11].

To be more precise, from the (collisionless) Wigner equation or the Schrödinger-Poisson system, a quantum hydrodynamic model *without* relaxation terms can be derived. The above expressions are obtained by *assuming* that the collision operator in the Wigner-Boltzmann equation is such that the corresponding moments equal C_J and C_E, respectively [13]. The quantum correction to the energy density was first derived by Wigner [38]. The hydrodynamic formulation of quantum systems has been used already by Madelung in 1927 [23].

In special situations, simpler hydrodynamic models can be (formally) derived. For instance, assuming that the temperature only depends on the particle density via $T = T(n) = n^\gamma$ with $\gamma \geq 1$, one obtains the (isothermal or isentropic) *quantum hydrodynamic model* consisting of the equations (1), (2), and (4).

Assuming that both τ_p/τ_w and ε are small parameters, rescaling the time via $t \to t/\varepsilon^2$, and performing the formal limit $\tau_p/\tau_w \to 0$ and $\varepsilon \to 0$ such that $\varepsilon^2\tau_w/\tau_p \to \tau_0$, we obtain the *quantum energy-transport equations*:

$$\partial_t n - \operatorname{div} J = 0, \qquad J = \nabla(nT) - n\nabla(V+Q),$$
$$\partial_t \left(\frac{3}{2}nT\right) - \operatorname{div}\left(\frac{5}{2}TJ + \kappa\nabla T\right) = -J\cdot\nabla(V+Q) - \frac{3}{2}\frac{n(T-T_0)}{\tau_0},$$

If the relaxation time τ_0 is very small (compared to one), the electron temperature relaxes to T_0 and we get the *quantum drift-diffusion model*:

$$\partial_t n - \operatorname{div} J = 0, \qquad J = T_0\nabla n - n\nabla V - \delta^2 n\nabla\Big(\frac{\Delta\sqrt{n}}{\sqrt{n}}\Big). \tag{5}$$

This model can also be derived from the full quantum hydrodynamic equations (1)-(3) after rescaling the time via $t \to t/\varepsilon^2$ and letting formally $\varepsilon \to 0$ (keeping τ_p/τ_w fixed). The above models are considered in a bounded domain $\Omega \subset \mathbb{R}^d$ ($d \geq 1$) with appropriate initial and boundary conditions (see below).

Finally, we notice that related macroscopic quantum models has been derived, for instance "smoothed" quantum hydrodynamic models [12] or low and high field quantum diffusion equations [4].

We obtain the following hierarchy of macroscopic semiconductor models:

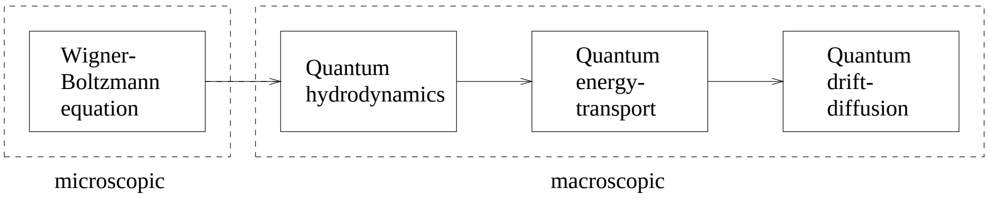

Fig. 1. Hierarchy of quantum semiconductor models.

In Section 2 we present analytical results on the quantum hydrodynamic equations. Section 3 is concerned with numerical results for the quantum drift-diffusion model. Finally, in Section 4 we give some open problems.

2 The quantum hydrodynamic model

In this section we study analytically the stationary isothermal quantum hydrodynamic equations. The main difficulty is the treatment of the third-order differential operator. We assume a potential flow formulation $J = n\nabla S$ with the quantum quasi-Fermi potential (or velocity potential) S. Then, using $\mathrm{div}\,(J \otimes J/n) = \frac{1}{2}n\nabla|\nabla S|^2$ and assuming $n > 0$ in Ω, we can divide the stationary version of Eq. (2) with $T = T_0$ by n, integrate and set $w = \sqrt{n}$ to obtain the following set of equations:

$$\delta^2 \Delta w = w(\tfrac{\varepsilon^2}{2}|\nabla S|^2 + T_0 \ln(w^2) - V + S), \tag{6}$$

$$\mathrm{div}\,(w^2 \nabla S) = 0, \tag{7}$$

$$\lambda^2 \Delta V = w^2 - C \qquad \text{in } \Omega. \tag{8}$$

The integration constant can be assumed to be zero by choosing a reference point for the electrostatic potential. We assume that the boundary data are the superposition of the thermal equilibrium functions and the applied potential and that no quantum effects occur on the boundary. This gives (see [18] for details)

$$w = w_0, \quad S = S_0, \quad V = V_0 \qquad \text{on } \partial\Omega \tag{9}$$

with $w_0 = \sqrt{C}$, $S_0 = U$, $V_0 = T_0 \ln(C) + U$, U being the applied potential. Clearly, mixed Dirichlet-Neumann boundary conditions are physically more realistic than pure Dirichlet conditions. However, we need to impose the boundary conditions (9) for technical reasons, since mixed boundary conditions exclude regularity of solutions.

In the analysis of (6)-(8), two main difficulties arise. The elliptic equation (6) is, a priori, of degenerate type with a non-standard (since non-local) degeneracy. We will show, however, that the solution w is strictly positive and therefore, (7) becomes strictly elliptic. Another difficulty comes from the term $|\nabla S|^2$ on the right hand side of (7), stemming from the convective term in (2).

The following assumptions are needed:

(A1) $\Omega \subset \mathbb{R}^d$ $(d \geq 1)$ is a bounded domain with boundary $\partial\Omega \in C^{1,1}$.
(A2) $w_0 \in W^{2,p}(\Omega)$ for $p > d/2$, $\inf_{\partial\Omega} w_0 > 0$; $S_0 \in C^{1,\gamma}(\overline{\Omega})$ with $\gamma = 2 - d/p$; $V_0 \in H^1(\Omega) \cap L^\infty(\Omega)$; $C \in L^\infty(\Omega)$.

The constants ε, δ, λ, and T_0 are assumed to be positive. We can prove the following result:

Theorem 1. *Let (A1)-(A2) hold. Then there exists $\eta > 0$ such that if*

$$(\varepsilon^2/T_0)\|S_0\|_{C^{1,\gamma}(\overline{\Omega})} \leq \eta, \tag{10}$$

there exists a solution (w, S, V) *of (6)-(9) satisfying, for some* $\underline{w} > 0$,

$$w \in W^{2,p}(\Omega),\ S \in C^{1,\gamma}(\overline{\Omega}),\ V \in H^1(\Omega) \cap L^\infty(\Omega), \quad w(x) \geq \underline{w} > 0 \ \textit{in}\ \Omega.$$

It is possible to prove existence of solutions for the isentropic case (i.e. $T(n) = n^\gamma$ with $\gamma > 1$; see [18]). The condition (10) in Theorem 1 means that existence of solutions holds if the mean free path is much smaller than the device length or if the electric energy (which is related to S_0) is much smaller than the thermal energy (which is related to T_0).

Condition (10) comes from the following consideration: If the density w is small (compared to one) in some region, we cannot control the convective term $\varepsilon^2|\nabla S|^2$. However, if w is small then the term $T_0 \ln(w)$ becomes very negative, and there is hope to control the convective term. This is indeed possible if T_0 is large enough or if εS_0 is small enough in some norm. The proof of Theorem 1 uses a truncation method, maximum principle arguments and elliptic estimates and can be found in [18,19].

We can also understand the condition (10) in a different way. For this let us consider the one-dimensional equations, where J is a given constant and $\varepsilon = 1$:

$$-\delta^2 \left(n(\ln n)_{xx}\right)_x + \left(\frac{J^2}{n} + T_0 n\right)_x - nV_x = -\frac{J}{\tau_0}, \tag{11}$$

$$\lambda^2 V_{xx} = n - C \quad \text{in } \Omega = (0,1), \tag{12}$$

$$n(0) = n_0, \quad n(1) = n_1, \quad n_x(0) = n_x(1) = 0, \quad V(0) = V_0, \tag{13}$$

where n_0, $n_1 > 0$, $V_0 \in \mathbb{R}$ and $C \in L^2(\Omega)$. Notice that here, we use different boundary conditions employed in numerical computations [11]. We can prove the following result [16,19]:

Theorem 2. *Under the above assumptions there exist* $\underline{n}$, $J_0 > 0$ *such that for all* $0 < J \leq J_0$ *there exists a solution* $(n, V) \in H^4(\Omega) \times H^2(\Omega)$ *to (11)-(13) satisfying*

$$n(x) \geq \underline{n} > 0 \quad \textit{and} \quad J/n(x) < \sqrt{T_0} \qquad \textit{for all}\ x \in \Omega.$$

In the case of the hydrodynamic model (i.e. $\delta = 0$ in Eq. (11)) the condition $J/n < \sqrt{T_0}$ means that the flow is subsonic. In this sense we have proven the existence of "subsonic" solutions to the quantum system (11)-(13).

For the proof we use the technique of exponential variables. More precisely, we divide Eq. (11) by n, take the derivative with respect to x and use the Poisson equation to obtain a fourth-order equation for n. Then using $n = e^u$ as a new variable we obtain a fourth-order equation for u with the corresponding boundary conditions. First we prove existence of weak H^2 solutions to a truncated version of this equation. Since $H^2(\Omega)$ injects continuously into $L^\infty(\Omega)$, we obtain an L^∞ solution u. The L^∞ bound for u can be controlled for sufficiently small $J > 0$, and the truncation parameter can be removed.

Since $u \in L^\infty(\Omega)$, we conclude the existence of a positive lower bound for $n = \ln(u)$. Notice that this yields positivity *without* the use of a maximum principle (which generally does not hold for fourth-order equations).

Remark. In the case of special boundary conditions, the system (11)-(12) with $T = T(n) = n^\gamma$ and $\gamma > 2$ has no weak solution if J is large enough. However, adding a so-called ultra-diffusive term in (11) gives the existence of solutions for all $J > 0$ [10]. For an existence result for the model (11) we also refer to [40]. Non-uniqueness of classical solutions for particular initial data has been shown in [34].

Another result concerns the semi-classical limit $\delta \to 0$. It is shown in [16] that for sufficiently small $J > 0$, the solution of the problem (11)-(12) converges, as $\delta \to 0$, to the solution of the hydrodynamic problem ($\delta = 0$). Moreover, adding an ultra-diffusive term in (11), the limit $\delta \to 0$ can be performed for all $J > 0$ [9]. The semi-classical limit for the multi-dimensional model (with $J = 0$) has been performed in [14,33].

The steady-state quantum hydrodynamic model in one dimension has been numerically solved in [16] using the general-purpose solver Colsys. Resonant tunneling diodes has been numerically simulated in [29] and the numerical behavior of the solutions in the semi-classical limit has been examined in [25].

The single-particle Schrödinger equation is equivalent to the (pressureless) quantum hydrodynamic model without relaxation terms. In this case the quantum hydrodynamic model is usually referred to as the Madelung equations [23]. In the physical literature, the hydrodynamic analogy to the Schrödinger equation has been employed in numerical simulations since the 1970s [35,36]. For instance, particle methods [31,35] and finite element methods are used [7,8]. In particular, hysteresis phenomena in the current-voltage characteristics has been numerically discovered [8].

3 The quantum drift-diffusion model

In this section we derive an implicit semi-discretization of the transient quantum drift-diffusion equations (4)-(5) in Ω together with the initial and boundary conditions

$$n = n_D, \quad V = V_D, \quad \Delta\sqrt{n} = 0 \quad \text{on } \Gamma_D, \tag{14}$$

$$J \cdot \nu = \nabla V \cdot \nu = \nabla\Big(\frac{\Delta\sqrt{n}}{\sqrt{n}}\Big) \cdot \nu = 0 \quad \text{on } \Gamma_N, \tag{15}$$

$$n(\cdot, 0) = n_0 \quad \text{in } \Omega, \tag{16}$$

where Ω satisfies (A1) and $\partial\Omega = \Gamma_D \cup \Gamma_N$, $\Gamma_D \cap \Gamma_N = \emptyset$, $\text{meas}_{d-1}(\Gamma_D) > 0$ and Γ_N is open in $\partial\Omega$. These conditions mean that there are no quantum effects on the Dirichlet boundary parts and that the normal components of the total current density, the quantum current density and the electric field vanish on the insulating boundary parts.

For the numerical discretization we introduce as in Section 2 the new variable $\rho = \sqrt{n}$ and write Eqs. (4)-(5) as

$$\partial_t(\rho^2) = \operatorname{div}(\rho^2 \nabla F), \quad -\delta^2 \frac{\Delta \rho}{\rho} + T_0 \ln(\rho^2) - V = F, \tag{17}$$

$$\lambda^2 \Delta V = \rho^2 - C \qquad \text{in } \Omega \times (0, \infty). \tag{18}$$

For the numerical treatment of (17)-(18) we employ a vertical line method and replace the transient problem by a sequence of elliptic problems.

Let $T > 0$ be given. We divide the time interval $[0, T]$ into N subintervals by introducing the temporal mesh $\{t_k : k = 0, \ldots, N\}$, where $t_k = k\tau$, $\tau > 0$ (to simplify). Now we discretize (17)-(18) in the following way: Set $\rho_0 = n_0^{1/2}$. For $k = 1, \ldots, N$ solve recursively the elliptic systems

$$\frac{1}{\tau}(\rho_k^2 - \rho_{k-1}^2) = \operatorname{div}(\rho_k^2 \nabla F_k), \quad -\delta^2 \frac{\Delta \rho_k}{\rho_k} + T_0 \ln(\rho_k^2) - V_k = F_k, \tag{19}$$

$$\lambda^2 \Delta V_k = \rho_k^2 - C \qquad \text{in } \Omega, \tag{20}$$

subject to the boundary conditions

$$\rho_k = \rho_D, \quad F_k = F_D, \quad V_k = V_D \qquad \text{on } \Gamma_D, \tag{21}$$

$$\nabla \rho_k \cdot \nu = \nabla F_k \cdot \nu = \nabla V_k \cdot \nu = 0 \qquad \text{on } \Gamma_N. \tag{22}$$

Then the approximate solution to (17)-(18) is given by $(\rho^{(\tau)}, F^{(\tau)}, V^{(\tau)})$, where $\rho^{(\tau)} = \rho_k$ on $(t_{k-1}, t_k]$, $k \geq 1$, etc. First we have to show solvability of the semi-discrete problem:

Theorem 3. *Assume $\rho_D \in H^2(\Omega)$, $\inf_{\partial\Omega} \rho_D > 0$, $V_D, F_D \in C^{2,\gamma}(\overline{\Omega})$ for $0 < \gamma < 1 - 2/d$, $F_D \leq -\overline{F}_D < 0$ in Ω, $\rho_0 \in H^2(\Omega)$, and $C^{0,\gamma}(\overline{\Omega})$. Furthermore, assume that Ω is a one-dimensional interval, $\partial\Omega = \Gamma_D$, and $\rho_{k-1} \in C^{0,\gamma}(\overline{\Omega})$ for some $k \in \{1, \ldots, N\}$. Then then there exists a solution (ρ_k, F_k, V_k) of the system (19)-(22), fulfilling $\rho_k, F_k, V_k \in C^{2,\gamma}(\overline{\Omega})$, and*

$$\rho_k \geq c_k > 0 \quad \text{in } \Omega.$$

Notice that we prove the positivity of the solution to a *fourth-order* equation. Since no maximum principle exists here, we use the technique of exponential variables as in Section 2, i.e. we define $\rho = e^u$. The restriction to one space dimension comes from the fact that we use $u - \ln(\rho_D)$ as a test function in the equation for u and that boundary integrals appear which can be estimated appropriately only in one space dimension [19,21] (also see [27]).

In order to prove the numerical convergence of the semi-discrete solutions $(\rho^{(\tau)}, F^{(\tau)}, V^{(\tau)})$ to a solution (ρ, F, V) of the continuous problem, a priori bounds are obtained using the discrete entropy (or free energy) of the system:

$$\eta_k = \frac{\delta^2}{2} \int\limits_\Omega |\nabla \rho_k|^2 dx + \int\limits_\Omega H(\rho_k^2) dx + \frac{\lambda^2}{2} \int\limits_\Omega |\nabla V_k|^2 dx - \int\limits_\Omega F_D \rho_k^2 dx,$$

where $H(s) = T_0 s(\ln(s) - 1) + T_0$, $s > 0$. This first yields uniform $L^\infty(0, T; H^1(\Omega))$ bounds on $\rho^{(\tau)}$ and $V^{(\tau)}$. Further estimates give even uniform $L^2(0, T; H^2(\Omega))$ bounds on $\rho^{(\tau)}$. Then it is possible to prove uniform bounds on the time derivative of the linear interpolation of the ρ_k and to use standard compactness arguments. These stability bounds are valid in *any* space dimension. For the convergence result, however, we need again the mono-dimensional assumption. We can prove:

Theorem 4. *Let the assumptions of Theorem 3 hold. Then there exists a subsequence of* $(\rho^{(\tau)}, F^{(\tau)}, V^{(\tau)})$ *(not relabeled) such that*

$$\begin{aligned}
\rho^{(\tau)} &\rightharpoonup \rho \qquad && \textit{weakly in } L^2(0, T; H^2(\Omega)), \\
\rho^{(\tau)} &\to \rho && \textit{strongly in } C^0(0, T; C^{0,\gamma}(\overline{\Omega})), \\
(\rho^{(\tau)})^2 F_x^{(\tau)} &\rightharpoonup J && \textit{weakly in } L^2(0, T; L^2(\Omega)), \\
V^{(\tau)} &\to V && \textit{strongly in } C^0(0, T; C^{2,\gamma}(\overline{\Omega})),
\end{aligned}$$

as $\tau \to 0$*, where* (ρ, J, V) *is a solution of (5) in a weak sense.*

Notice that since only $\rho \geq 0$ holds in Ω, the term $\Delta\sqrt{\rho}/\sqrt{n}$ has to be interpreted appropriately; see [21]. Clearly, Theorem 4 yields also global existence of weak solutions to the quantum drift-diffusion equations.

It is possible to prove that the order of convergence is one (and hence optimal) if ρ is regular enough [20].

The above numerical scheme is applied to the simulation of a resonant tunneling diode [11,22]. Their main characteristic is the appearance of negative differential resistance in the stationary current-voltage characteristic. The double barrier structure consists of a quantum well GaAs layer sandwiched between two $\mathrm{Al_xGa_{1-x}As}$ layers, each 5 nm thick. This resonant structure is itself sandwiched between two spacer layers of 5 nm thickness and supplemented with two contact GaAs layers, each 25 nm thick. The contact region ist highly doped with $C = 10^{18}\mathrm{cm}^{-3}$, while the channel is moderately doped with $C = 10^{15}\mathrm{cm}^{-3}$. The barrier height is assumed to be $B_{\max} = 0.4\mathrm{eV}$ and the relaxation time is fixed at $\tau_{\mathrm{relax}} \approx 10^{-12}\mathrm{s}$.

For the numerical simulation, we have used the vertical line method as above for the one-dimensional Eqs. (5). The potential V is replaced by $V + B$, where B is a step function modeling the barriers. The discretization in space was done using finite differences on a uniform grid with 300 points. The resulting nonlinear system is solved using Newton's method. The time step was initially set to 10^{-4} and adjusted heuristically during the evolution.

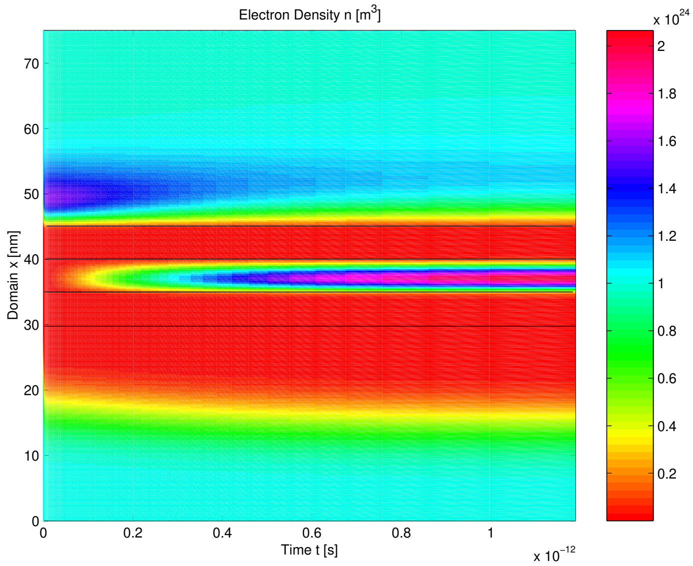

Fig. 2. Electron density versus time.

In Fig. 2 we present the computed transient electron density over a period corresponding to the relaxation time $\tau_{\text{relax}} = 10^{-12}$s for the applied voltage $U = 0.3$V. This voltage corresponds to the valley state in the (static) current-volatge characteristic (Fig. 3 left). Notice that the electrons move top-down in Fig. 2. After a short initial time layer in front of the first barrier, the electrons tunnel through this barrier and accumulate in the quantum well.

The transient current density is reported in Fig. 3 (right). During the evolution to the stationary state the current density oscillates. This oscillatory behavior was also noticed in [22], where the resonant tunneling diode was simulated using the Wigner-Poisson model. The steady state in Fig. 3 (right) is reached after 10^{-11}s, which is ten times the relaxation time.

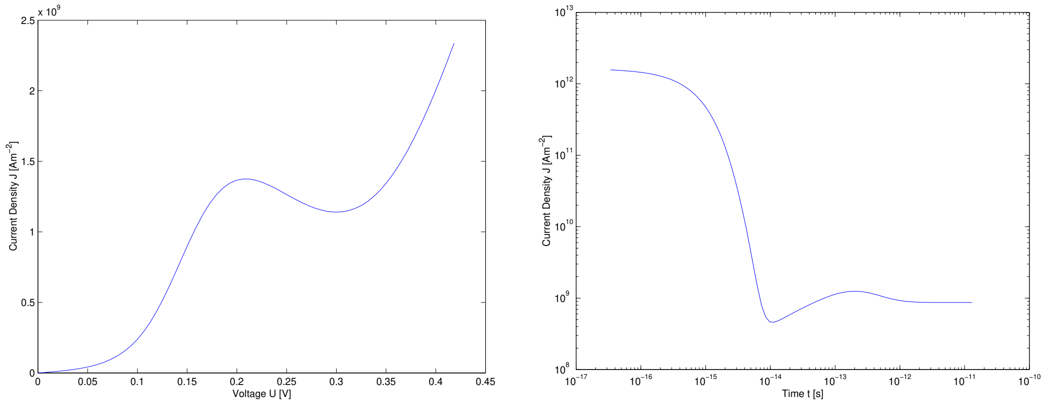

Fig. 3. *Left:* Current density versus applied voltage. *Right:* Current density versus time.

Remark. In [26] the stability of the linearized transient quantum drift-diffusion model has been proved. The stationary equations has been analyzed in [5]. There, the existence of weak solutions with positive particle density has been shown. Moreover, the semi-classical limit could be performed. A Gummel-type iteration method for the steady-state system has been proposed and analyzed in [28] and static current-voltage characteristics for a resonant tunneling diode has been computed.

The quantum drift-diffusion model is known in the physical literature as the density gradient model [2]. This model has been employed to study the carrier distribution in ultra-small MOSFET devices [1,32,37,39].

4 Open problems

The mathematical theory of macroscopic quantum models is far from being complete. Here, we mention some open problems useful for the understanding of these models.

- Existence of solutions to the full or isothermal transient quantum hydrodynamic equations (work in progress in collaboration with C. Mariani (Buenos Aires) and H. Teismann (Fargo, USA)).
- Rigorous derivation of the isothermal quantum hydrodynamic, quantum energy-transport and quantum drift-diffusion equations from the full quantum hydrodynamic model.
- Analysis and numerical approximation of the quantum energy-transport model and study of its range of validity compared to other models.
- Analysis of the current-voltage characteristics of the macroscopic quantum models and its hysteresis phenomena [8].
- Numerical comparison of the macroscopic quantum models (work in progress in collaboration with P. Pietra (Pavia) and R. Pinnau (Darmstadt)) and numerical comparison of macroscopic and microscopic quantum models.
- Numerical simulation of 2D MOS transistors with nano-scale oxide layer using various quantum models.

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