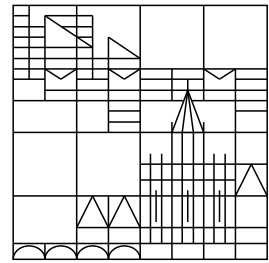


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# MACROSCOPIC MODELS FOR SEMICONDUCTOR DEVICES: A REVIEW

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**Abstract.** A model hierarchy for semiconductor devices is presented, in particular kinetic models (Boltzmann and quantum Boltzmann equations) and fluid dynamical models (hydrodynamic, energy-transport and drift-diffusion equations). Fluid dynamical models including quantum correction terms are also discussed. The links between the various models are given.

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## 1. INTRODUCTION

The numerical simulation of semiconductor devices becomes more and more important for the development of new industrial devices in order to reduce development cost and time. For an efficient numerical simulation models have to be used which are physically accurate in the corresponding field of application. Therefore, it is of great importance to possess a model hierarchy and the corresponding information where these models can be used. In this review article we present a model hierarchy and explain the links between the various models.

Roughly speaking, we can divide semiconductor models into two classes: kinetic models and quasi-hydrodynamic (fluid dynamical) models. For each of these classes we can consider (semi-) classical and quantum models (see Fig. 1). For instance, the Boltzmann and the quantum Boltzmann equation are kinetic equations, whereas the hydrodynamic, the energy-transport and the drift-diffusion equations are quasi-hydrodynamic models. Fluid dynamical models which take into account quantum effects are, for instance, the quantum

hydrodynamic, the quantum energy-transport and the quantum drift-diffusion equations. Other semiconductor models, for instance kinetic models, so-called SHE models or high-field models, can be found in the literature [34, 61, 163, 185, 186], but in this paper we only discuss the above mentioned models.

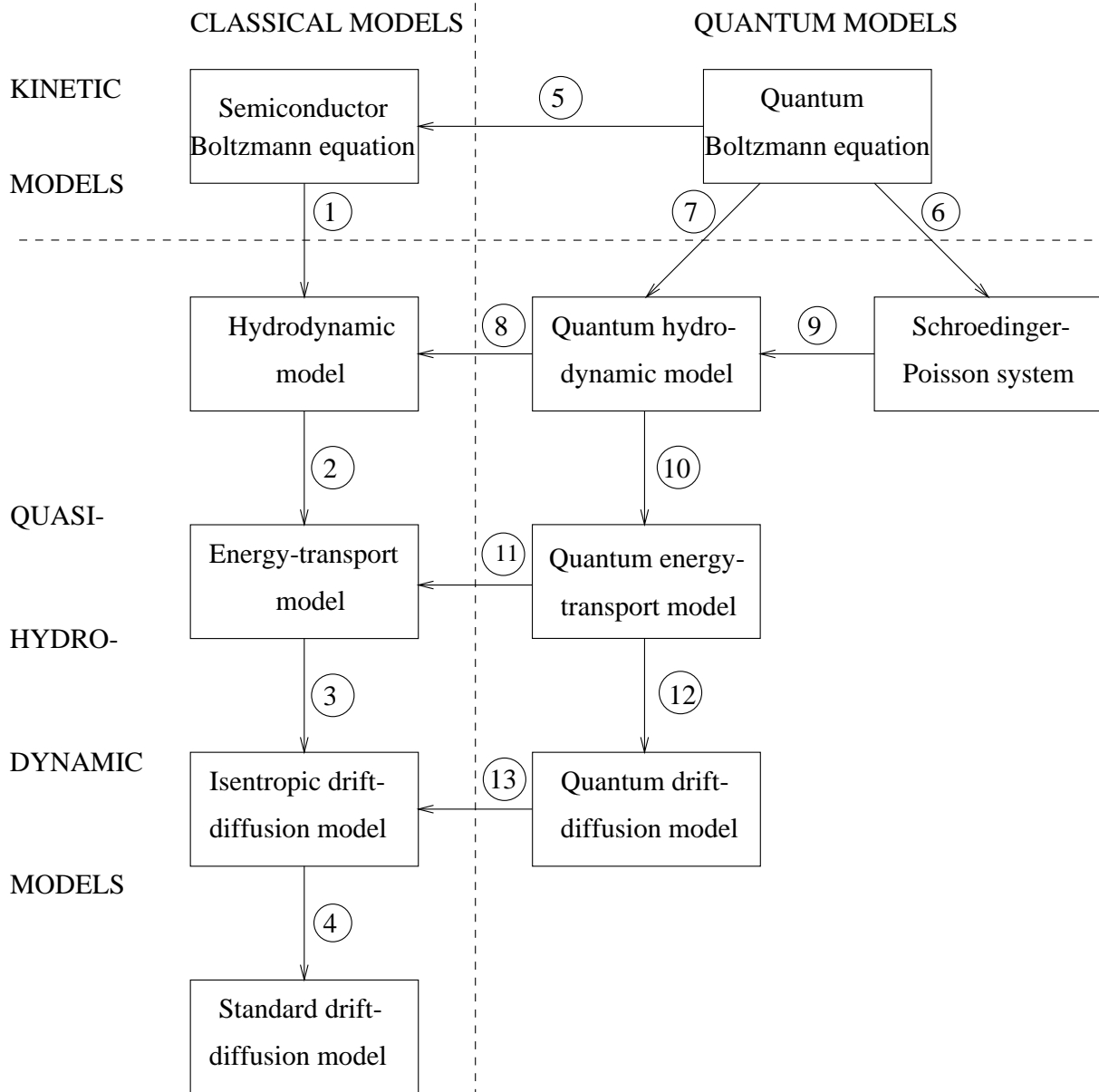


FIGURE 1. A hierarchy of semiconductor models.

## 2. THE BOLTZMANN EQUATION

The Boltzmann equation for semiconductors models the flow of charge carriers (e.g. electrons) in semiconductor crystals. It describes the temporal evolution of the phase space (position-momentum space) distribution function  $f = f(x, k, t)$ , where  $x \in \mathbb{R}^3$  is the position variable,  $k \in B$  is the wave vector,  $B$  denotes the Brillouin zone associated with the underlying crystal lattice [16], and  $t \geq 0$  is the time. The semi-classical Boltzmann equation reads [39, 163, 186]

$$(1) \quad \begin{aligned} \frac{\partial f}{\partial t} + v(k) \cdot \nabla_x f + \frac{q}{\hbar} \nabla_x V \cdot \nabla_k f &= Q(f), \quad x \in \mathbb{R}^3, k \in B, t > 0, \\ f(x, k, 0) &= f_I(x, k), \quad x \in \mathbb{R}^3, k \in B, \end{aligned}$$

subject to periodic boundary conditions on  $\partial B$ . Here, the physical constants are the elementary charge  $q$  and the reduced Planck constant  $\hbar$ ,  $v(k) = (1/\hbar)\nabla_k \varepsilon(k)$  is the mean electron velocity,  $\varepsilon(k)$  the energy-wave vector function, and  $V = V(x, t)$  is the electric potential. The collision operator  $Q(f)$  is supposed to model short range interactions of the electrons with crystal impurities, phonons, and electrons (see [163] for some examples). In the parabolic band approximation, the energy band function  $\varepsilon(k)$  can be written as

$$\varepsilon(k) = E_c + \frac{\hbar^2}{2m^*} |k|^2,$$

where  $E_c$  is the conduction band minimum energy and  $m^*$  is the effective electron mass. The electrostatic potential  $V$  is a given function or it is coupled selfconsistently to the Poisson equation

$$\varepsilon_s \Delta V = q(n - C(x)).$$

In this equation  $\varepsilon_s$  denotes the semiconductor permittivity and  $C = C(x)$  models fixed charged background ions (doping profile). The electron density  $n = n(x, t)$  is defined by

$$n = \int_B f dk.$$

The first result on the existence of solutions to the space homogeneous Boltzmann equation has been obtained by Carleman in 1932 [33]. The corresponding  $L^1$  theory has been developed by Arkeryd [12]. In [13] solutions close to a space homogeneous solution have been studied. DiPerna and Lions have proved the first general global existence result for the Boltzmann equation in 1987 [68] (also see the review article of Gérard [102]). Further results can be found in, e.g. [37, 38, 157, 184]. We refer to [14, 39, 166] for reviews of recent mathematical results. Numerically, the Boltzmann equation has been solved by Monte-Carlo methods [7, 8, 148] or deterministic particle methods [26, 27, 60, 175]. An overview of several numerical techniques is given in [215].

The numerical simulation of the Boltzmann equation (or the Boltzmann-Poisson system) requires a lot of computing power in real life applications. Therefore, simpler models which represent a reasonable compromise between the physical accuracy and computational efficiency have to be derived., e.g. fluid dynamical models. One of these fluid dynamical models are the hydrodynamic equations.

### 3. HYDRODYNAMIC MODELS

The hydrodynamic model is a system of hyperbolic-parabolic equations which can be derived from the Boltzmann equation by using a moment method (arrow 1 in Fig. 1). The idea of this method is to multiply the Boltzmann equation by 1,  $v$ , and  $\frac{1}{2}|v|^2$  and to integrate over the velocity space. This leads to a system of equations for the first moments of the distribution function. Making an ansatz for the distribution function, a closed system of equations can be obtained.

Assuming the parabolic band approximation (see above), we can identify  $v$  with  $k$  and we set  $B = \mathbb{R}^3$ . For the collision operator  $Q(f)$  a low density collision term is used which is linear in  $f$  [163]. The particle density, the current density, and the energy tensor, respectively, are defined (essentially) as the first moments of the distribution function  $f$ :

$$(2) \quad \begin{aligned} n &= \int_{\mathbb{R}^3} f(x, v, t) dv, \\ J_n &= -q \int_{\mathbb{R}^3} v f dv, \\ E &= \frac{m^*}{2} \text{tr} \int_{\mathbb{R}^3} v \otimes v f dv, \end{aligned}$$

where ‘tr’ is the trace of the tensor  $v \otimes v$  whose  $ij$ -th element is given by  $v_i v_j$ . As an ansatz for the moment method, the shifted Maxwellian

$$f(x, v, t) = n \left( \frac{m^*}{2\pi k_B T} \right)^{3/2} \exp \left( \frac{-m^* |v - u|^2}{2k_B T} \right)$$

can be used since this function belongs to the kernel of  $Q(f)$  [163]. The electron density  $n$ , the effective temperature  $T$  and the mean velocity  $u$  are the free parameters. After inserting the ansatz function, the Boltzmann equation is multiplied by a number of linearly independent functions of velocity and integrated over the velocity space. The result are partial differential equations for the time and space dependent parameters  $n$ ,  $T$ , and  $u$  (arrow 1):

$$(3) \quad \frac{\partial n}{\partial t} + \nabla \cdot (nu) = 0,$$

$$(4) \quad \frac{\partial u}{\partial t} + (\nabla \cdot u)u + \frac{k_B}{m^* n} \nabla(nT) - \frac{q}{m^*} \nabla V = C_u,$$

$$(5) \quad \frac{\partial T}{\partial t} + \frac{2}{3} T \nabla \cdot u + u \cdot \nabla T = C_T.$$

The terms on the right hand sides, stemming from the collision operator, are the relaxation terms. If they are omitted the system (3)-(5) represents the Euler equations of gas dynamics for a gas of charged particles in an electric field. For the moments (2) we get

$$J_n = -qnu, \quad E = n \left( \frac{m^*}{2} |u|^2 + \frac{3}{2} k_B T \right).$$

We rewrite the *hydrodynamic equations* (3)-(5) in the variables  $(n, J_n, E)$ :

$$(6) \quad \frac{\partial n}{\partial t} - \frac{1}{q} \operatorname{div} J_n = 0,$$

$$(7) \quad \frac{\partial J_n}{\partial t} - \frac{1}{q} \operatorname{div} \left( \frac{J_n \otimes J_n}{n} \right) - \frac{qk_B}{m^*} \nabla(nT) + \frac{q^2}{m^*} n \nabla V = C_J,$$

$$(8) \quad \frac{\partial E}{\partial t} - \operatorname{div} \left( \frac{m^*}{2q^3} \frac{J_n |J_n|^2}{n^2} + \frac{5}{2} \frac{k_B}{q} T J_n \right) = -J_n \cdot \nabla V + C_E.$$

These equations can be considered in the whole space with  $x \in \mathbb{R}^3$ ,  $t > 0$ , or in a bounded domain with appropriate boundary conditions [4, 205]. The relaxation terms are written in the relaxation time approximation as (see, e.g., [99])

$$(9) \quad C_J = -\frac{J_n}{\tau_p}, \quad C_E = -\frac{1}{\tau_w} \left( \frac{m^*}{2q^2} \frac{|J_n|^2}{n} + \frac{3}{2} n k_B (T - T_L) \right),$$

where  $\tau_p$ ,  $\tau_w$  are the momentum and energy relaxation times, respectively, and  $T_L$  is the lattice temperature.

In [25], where the model (3)-(5) for semiconductors has been introduced, an additional heat conduction term

$$-\operatorname{div}(\kappa \nabla T)$$

was added to the left hand side of (8). Here,  $\kappa > 0$  is called heat conductivity. In [193] this term was derived from a closure condition in the moment method. Using this heat conduction term, the equation (8) transforms into

$$(10) \quad \frac{\partial E}{\partial t} - \operatorname{div} \left( \frac{m^*}{2q^3} \frac{J_n |J_n|^2}{n^2} + \frac{5}{2} \frac{k_B}{q} T J_n + \kappa \nabla T \right) = -J_n \cdot \nabla V + C_E.$$

The derivation of the hydrodynamic model from the semiconductor Boltzmann equation has been investigated in, e.g., [7, 8, 193, 209]. The problem of the closure conditions in hydrodynamic equations has been addressed in [7, 9], using the maximum entropy principle (also see [171]).

There is a huge literature for the fluid dynamical limits, in particular Euler and Navier-Stokes equations, from the Boltzmann equation. The first rigorous result for the hydrodynamical limit was carried out by Caffisch [32] and generalized by Lachowicz [149]. The compressible Euler equations have been derived by Nishida [176] and Ukai and Asano [208] based on the work by Grad [104]. The Navier-Stokes equations are derived from the Boltzmann equation in [37, 62]. For new developments, we refer to the works of Levermore *et al.* [17, 18, 152].

Mathematically, the hydrodynamic equations form a quasilinear hyperbolic-parabolic system of balance laws. The solution can become discontinuous in finite time. We refer to [151] for general references on various shock waves phenomena. In the last years, many authors have been examined the existence of solutions to this or to the isentropic model.

The *isentropic* model consists of the first two equations (6), (7), where the temperature is assumed to depend only on the density:

$$T = T(n) = T_0 n^{\alpha-1}, \quad \alpha > 1, \quad T_0 > 0.$$

If  $\alpha = 1$  then  $T$  is constant, and the corresponding equations are called the *isothermal* hydrodynamic model. The existence of global weak entropy solutions to the transient isentropic model in one space dimension with zero electric field has been first proved by DiPerna [66, 67] for  $\alpha = 1 + 2/(2N + 1)$  where  $N \in \mathbb{N}$ ,  $N > 1$ , using compensated compactness techniques. Chen and Ding *et al.* [42, 43, 65] extended the existence result to  $1 < \alpha \leq 5/3$ , whereas P.L. Lions, Perthame and Tadmor [153, 154] gave a proof for all  $\alpha > 1$ . The isothermal case  $\alpha = 1$  has been considered by Matsumura and Nishida in [167]. The existence of global solutions to the time-dependent model including the Poisson equation has been proved in [50, 51, 187] for the isothermal case and in [122, 123, 160, 216, 223, 225] for the isentropic case. Degond and Markowich [58, 59], Gamba [83, 85] and Fang and Ito [73, 74] considered the stationary isentropic model in one and two space dimensions.

Existence of solutions of the full system of Eqs. (6), (7), (10) in one or several space dimensions has been studied in [5, 221] for the stationary problem and in [217, 220, 227] for the transient equations. For related results for Euler-Poisson systems with geometric structure, see [44, 47].

The numerical discretization and solution of the hydrodynamic model, by using Scharfetter-Gummel type methods (for subsonic transport) or streamline diffusion methods (for transonic flow), is studied in [49, 86, 120, 121, 194, 195]. Other numerical techniques, like the Nessyahu-Tadmor scheme or Gudonov scheme or (essentially non-oscillatory, ENO) shock-capturing algorithms, are used in [46, 76, 88, 119, 158, 191, 201, 223].

#### 4. ENERGY-TRANSPORT MODELS

In applications it turns out that the quotient  $\varepsilon^2 = \tau_p/\tau_w$  (see (9)) is very small compared to one. Using  $\varepsilon$  as a parameter in the diffusion time scaling

$$(11) \quad t \rightarrow t/\varepsilon, \quad J_n \rightarrow \varepsilon J_n, \quad \tau_w = \tau_0/\varepsilon, \quad \tau_p = \varepsilon \tau_0,$$

and letting  $\varepsilon \rightarrow 0$  in the equations (6), (7), and (10), assuming the Wiedemann-Franz law

$$(12) \quad \kappa = \kappa_0 \frac{\tau_p k_B^2}{m^*} n T, \quad \kappa_0 > 0,$$

we get the *energy-transport model* (arrow 2):

$$(13) \quad \frac{\partial n}{\partial t} - \frac{1}{q} \operatorname{div} J_n = 0,$$

$$(14) \quad \frac{\partial U}{\partial t} - \operatorname{div} J_w = -J_n \cdot \nabla V + W(n, T),$$

$$(15) \quad J_n = L_{11} \left( \frac{\nabla n}{n} - \frac{q \nabla V}{k_B T} \right) + \left( \frac{L_{12}}{k_B T} - \frac{3}{2} L_{11} \right) \frac{\nabla T}{T},$$

$$(16) \quad q J_w = L_{21} \left( \frac{\nabla n}{n} - \frac{q \nabla V}{k_B T} \right) + \left( \frac{L_{22}}{k_B T} - \frac{3}{2} L_{21} \right) \frac{\nabla T}{T}.$$

We refer to [99] for details and a justification of the asymptotic limit. Here,  $U = \frac{3}{2}k_B nT$  is the internal energy,  $W(n, T) = \frac{3}{2}nk_B(T - T_L)/\tau_0$  the energy relaxation term, and the diffusion matrix is given by

$$(17) \quad L = (L_{ij}) = \mu_0 n k_B T \begin{pmatrix} 1 & \frac{5}{2}k_B T \\ \frac{5}{2}k_B T & (\frac{25}{4} + \kappa_0)(k_B T)^2 \end{pmatrix},$$

with the mobility constant  $\mu_0 = q\tau_0/m^*$ . Usually, (13)-(16) are considered in a bounded domain subject to mixed Dirichlet-Neumann boundary conditions for  $n, T$  and initial conditions for  $n, U$  (see [55]). The energy-transport equations can be obtained formally from the hydrodynamic equations by neglecting all terms including  $|J_n|^2$ ,  $J_n \otimes J_n$ , and  $\partial_t J_n$  (see [193]).

The model (13)-(16) can also be derived directly from the Boltzmann equation in the diffusive limit, using the Hilbert expansion method [19, 20, 22, 101]. In this derivation, the dominant scattering mechanisms are assumed to be electron-electron and elastic electron-phonon scattering. The same diffusion equations as above are obtained, but the diffusion coefficients are different. One example is:

$$(18) \quad L = (L_{ij}) = \tilde{\mu}_0 n \begin{pmatrix} 1 & \frac{3}{2}k_B T \\ \frac{3}{2}k_B T & \frac{15}{4}(k_B T)^2 \end{pmatrix}.$$

In order to get this diffusion matrix, we assumed the parabolic band approximation, Boltzmann statistics and a special ansatz for the momentum relaxation time (see [57] for details). The corresponding model has been considered by Chen *et al.* [40]. Different momentum relaxation time approximations give different diffusion matrices [57]. Note that both diffusion matrices (17) and (18) are symmetric and positive definite. Related energy-transport models are derived in [61]. The derivation of the energy-transport model from the Boltzmann equation is explained in more detail in [19, 136].

In the physical and mathematical literature, the energy-transport equations are investigated numerically since several years. They are discretized by using extensions of the Scharfetter-Gummel scheme [10, 202, 203] or by using ENO schemes [118, 119] and solved by using the Gummel method [155, 213, 214] or the full Newton method [40]. The results are compared to Monte-Carlo simulations [40, 41, 178] or to hydrodynamic simulations [40, 203]. Recently, the equations are numerically solved by using mixed finite elements [57, 165] or by employing compact finite difference schemes [77].

Mathematically, however, the energy-transport equations are analyzed only recently. In [3] a stationary energy-transport system with very special diffusion coefficients (not being of the form (15)-(16)) has been investigated and the existence of solutions has been proved. Jerome [116] and Griepentrog [105] proved the existence of steady-state solutions of particular systems under restrictive conditions on the data. Some mathematical properties of the energy-transport equations are proved in [2, 24]. In [53, 56] the existence and uniqueness of steady-state solutions to the energy-transport system with general uniformly positive definite diffusion matrix have been shown, whereas in the papers [54, 55] the parabolic equations with general diffusion matrix are studied. The existence of global weak



solutions could be proved. The question of uniqueness of transient solutions is investigated in [135].

## 5. DRIFT-DIFFUSION MODELS

In gas dynamics, an ideal gas satisfies the gas law  $r = nT$ , where  $r$  denotes the pressure of the gas. In the isentropic case, the temperature (only) depends on the particle density. Then  $T(n) = T_0 n^{2/3}$  holds for particles without spin for adiabatic and hence for isentropic states [52]. Note that the physical unit of  $T_0$  is Kcm<sup>2</sup>. If the diffusion matrix is described by (17), we can rewrite the electron current density as

$$(19) \quad J_n = \mu_0(\nabla(nk_B T) - qn\nabla V),$$

and we get

$$(20) \quad J_n = \mu_0(k_B T_0 \nabla(n^{5/3}) - qn\nabla V).$$

This current relation together with the continuity and Poisson equation

$$(21) \quad \frac{\partial n}{\partial t} - \frac{1}{q} \operatorname{div} J_n = 0,$$

$$(22) \quad \varepsilon_s \Delta V = q(n - C(x)),$$

is called the *isentropic drift-diffusion model* (arrow 3). Mathematically, Eq. (21), together with (20), is a degenerate parabolic equation. Therefore, so-called *vacuum sets*  $\{x : n(x, t) = 0\}$  may occur locally. Physically, these sets can be interpreted as regions in which the particle density is very small compared to the reference density.

The electron density signify the number of electrons in the conduction band of the semiconductor crystal (per space unit). The motion of the holes, or defect electrons, at the top of the valence band also renders a contribution to the current flow in the crystal. The hole density is denoted by  $p$ , the hole current density by  $J_p$ . A positive charge  $+q$  is assigned to the holes. Therefore, the evolution of the hole density is described by the equations

$$(23) \quad \frac{\partial p}{\partial t} + \frac{1}{q} \operatorname{div} J_p = 0,$$

$$(24) \quad J_p = -\mu_0(k_B T_0 \nabla(p^{5/3}) + qp\nabla V),$$

where the Poisson equation now writes

$$(25) \quad \varepsilon_s \Delta V = q(n - p - C(x)).$$

The equations (20)-(21), (23)-(25) are called the *bipolar isentropic drift-diffusion model*. Usually, these equations are considered in a bounded domain with mixed Dirichlet-Neumann boundary conditions for  $n$ ,  $p$ ,  $V$  and initial conditions for  $n$ ,  $p$  [130].

There are several derivations of this model. One derivation starts from the hydrodynamic equations. Formally, we obtain (20) from (7) by assuming isentropic states and by neglecting  $\partial_t J_n$  and the convective term  $q^{-1} \operatorname{div}(J_n \otimes J_n/n)$ . More rigorously, the isentropic drift-diffusion model can be derived from the isentropic hydrodynamic equations in

the zero-relaxation-time limit [45, 112, 124, 125, 139, 140, 141, 159, 162, 172, 189]. Another derivation starts from the transport equations

$$(26) \quad J_n = q\mu_0 n \nabla \phi_n, \quad J_p = -q\mu_0 p \nabla \phi_p,$$

where the carrier densities are given by Fermi-Dirac statistics [28, 82, 130]:

$$n = N_c F_{1/2} \left( \frac{\mu_0}{D_0} \left( \phi_n + V - \frac{E_c}{q} \right) \right), \quad p = N_v F_{1/2} \left( \frac{\mu_0}{D_0} \left( \phi_p - V + \frac{E_v}{q} \right) \right).$$

Here,  $\phi_n$ ,  $\phi_p$  are the quasi-Fermi potentials,  $N_j$ ,  $E_j$  ( $j = c, v$ ) are physical constants, and  $F_{1/2}$  is the Fermi integral with index 1/2 [28]. The constant  $D_0 > 0$  is called diffusivity. In the high injection case  $F_{1/2}^{-1}(y)$  can be approximated by a constant times  $y^{2/3}$  so that  $\nabla \phi_n$  can be approximated by  $\nabla(\text{const.} n^{2/3} - V)$ , which gives the current expression (20). This derivation is mathematically justified in [130]. A different drift-diffusion model incorporating Fermi-Dirac statistics is derived in [103].

The time-dependent and the stationary isentropic drift-diffusion model are mathematically analyzed in [63, 64, 75, 126, 127, 129, 131, 132, 145, 164, 210]. The existence and uniqueness of solutions and their qualitative behavior have been studied. The model is numerically solved by using mixed finite elements [11, 128, 142].

In low injection situations, where Boltzmann statistics can be used, i.e.

$$n = N_c \exp \left( \frac{\mu_0}{D_0} \left( \phi_n + V - \frac{E_c}{q} \right) \right), \quad p = N_v \exp \left( \frac{\mu_0}{D_0} \left( \phi_p - V + \frac{E_v}{q} \right) \right),$$

we get from (26) the (bipolar) *standard drift-diffusion model* (arrow 4), consisting of the continuity equations (21), (23), the Poisson equation (25) and the current relations

$$(27) \quad J_n = \mu_0 (k_B T_0 \nabla n - qn \nabla V), \quad J_p = -\mu_0 (k_B T_0 \nabla p + qp \nabla V),$$

where the diffusivity is related to the mobility by the Einstein relation

$$D_0 = U_T \mu_0, \quad U_T = \frac{k_B T_0}{q}.$$

The physical unit of  $T_0$  is here K.

This set of equations was first proposed by Van Roosbroeck in 1950 [192]. The first computational solution was presented in 1964 by Gummel [106] and improved some years later by Scharfetter and Gummel [197]. The developed Scharfetter-Gummel scheme was interpreted as a mixed finite element method in [30, 31]. In the seventies mathematicians started to pay attention to the drift-diffusion model. Mock proved an existence and uniqueness result in 1974 [168]. In the eighties a large amount of papers can be found in the mathematical literature, where the drift-diffusion equations and variants of them are analyzed (see [115, 161, 163, 169] for an overview and references). The modeling aspects are summarized in [109, 200]. Also in the last years the isothermal drift-diffusion model (27) and its variants were the subject of various mathematical research both analytically (see, e.g., [1, 69, 70, 71, 72, 78, 80, 91, 137, 138, 140, 173, 174, 188, 198, 199, 212]) and numerically (see, e.g., [81, 100, 110, 111, 116, 117, 170, 196, 218]).

The standard drift-diffusion model can also be derived from other equations. For instance, assuming  $T = \text{const.}$  in the energy-transport model in the formulation (19) (for the electron current density), we directly get (27). Similar as for the isentropic drift-diffusion model, the standard drift-diffusion equations can be derived from the hydrodynamic model (6)-(8) (or the energy-transport model) in the zero-relaxation-time limit [99, 124]. Finally, the standard model can be obtained directly from the Boltzmann equation by using the Hilbert expansion method [163, 183].

More general drift-diffusion models than presented here have been derived; see, e.g., [34, 61, 103].

## 6. QUANTUM MODELS

For ultra-small electronic devices in which quantum effects are present, the mathematical semiconductor models have to incorporate the quantum mechanical phenomena. The *quantum Boltzmann equation* is a kinetic equation describing the evolution of the Wigner function  $w = w(x, v, t)$  [108]:

$$(28) \quad \frac{\partial w}{\partial t} + v \cdot \nabla_x w + \frac{q}{m^*} \theta_{\hbar}[V]w = Q_{\hbar}(w), \quad x, v \in \mathbb{R}^3, t > 0,$$

$$(29) \quad w(x, v, 0) = w_0(x, v), \quad x, v \in \mathbb{R}^3.$$

Here,  $Q_{\hbar}(w)$  is the collision operator and  $V$  is the effective potential given, in the case of Coulomb interactions, by the Poisson equation (22). The electron density and the current density, respectively, are defined by

$$n = \int_{\mathbb{R}^3} w(x, v, t) dv, \quad J_n = -q \int_{\mathbb{R}^3} v w(x, v, t) dv.$$

The operator  $\theta_{\hbar}[V]$  is a pseudo-differential operator with symbol

$$(\delta V)_{\hbar}(x, \eta, t) \stackrel{\text{def}}{=} \frac{im^*}{\hbar} \left( V\left(x + \frac{\hbar}{2m^*}\eta, t\right) - V\left(x - \frac{\hbar}{2m^*}\eta, t\right) \right),$$

i.e.  $\theta_{\hbar}[V]w$  is defined by

$$(\theta_{\hbar}[V]w)(x, v, t) = \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} (\delta V)_{\hbar}(x, \eta, t) w(x, v', t) e^{i(v-v') \cdot \eta} dv' d\eta$$

for appropriate functions  $w$ . For the mathematical setting of pseudo-differential operators we refer to [204, 206].

In the (semi-)classical limit  $\hbar \rightarrow 0$ , the collisionless quantum Boltzmann equation, which is called quantum Vlasov equation, becomes (for given  $V$ )

$$\frac{\partial w}{\partial t} + v \cdot \nabla_x w + \frac{q}{m^*} \nabla_x V \cdot \nabla_v w = 0,$$

which is similar to the Boltzmann equation (1) (arrow 5). We refer to [163, Ch. 1.4] for details on this limit. The quantum Vlasov equation is equivalent to a system of countable

many Schrödinger equations for the wave functions  $\psi_k$  (arrow 6):

$$(30) \quad i\hbar \frac{\partial \psi_k}{\partial t} = -\frac{\hbar^2}{2m^*} \Delta \psi_k - qV \psi_k, \quad x \in \mathbb{R}^3, \quad t > 0,$$

$$(31) \quad \psi_k(x, 0) = \psi_k^0(x), \quad x \in \mathbb{R}^3.$$

The existence of solutions to Schrödinger-Poisson systems has been shown in [35, 150]. The stationary equations have been studied in [21, 114, 146]. For the mathematical techniques, see [36].

From the quantum Boltzmann equation quantum fluid dynamical models can be obtained. Using a moment method, the *(full) quantum hydrodynamic model* can be derived (see [87, 95, 97, 98, 113], arrow 7):

$$(32) \quad \frac{\partial n}{\partial t} - \frac{1}{q} \operatorname{div} J_n = 0,$$

$$(33) \quad \frac{\partial J_n}{\partial t} - \frac{1}{q} \operatorname{div} \left( \frac{J_n \otimes J_n}{n} \right) - \frac{qk_B}{m^*} \nabla(nT) + \frac{q^2}{m^*} n \nabla(V + Q) = -\frac{J_n}{\tau_p},$$

$$(34) \quad \frac{\partial E}{\partial t} - \operatorname{div} \left( \frac{m^* J_n |J_n|^2}{2q^3 n^2} + \frac{5k_B}{2q} T J_n + \kappa \nabla T \right) = -J_n \cdot \nabla(V + Q) + C_E,$$

$$(35) \quad \varepsilon_s \Delta V = q(n - C(x)),$$

where  $E$  is the energy density given by

$$E = n \left( \frac{m^* |J_n|^2}{2q^2 n^2} + \frac{3}{2} k_B T - \frac{\hbar^2}{24m^*} \Delta \log(n) \right),$$

the term

$$Q = \frac{\hbar^2}{2qm^*} \frac{\Delta \sqrt{n}}{\sqrt{n}}$$

is the Bohm quantum correction, and  $C_E$  is the energy relaxation term defined in (9). The heat flux  $-\kappa \nabla T$  comes from the closure condition. The quantum correction to the energy density was first derived by Wigner [219]. The hydrodynamic formulation of quantum systems has been used already by Madelung in 1927 [156].

Eqs. (32)-(35) are considered in the whole space  $\mathbb{R}^3$  or in a bounded domain with initial conditions for  $n$ ,  $J_n$  and  $E$ . The question of appropriate boundary conditions is delicate; see [87, 134, 144] for some answers in special situations.

Assuming that the particle temperature  $T$  is given by the explicit expression  $T(n) = T_0 n^{\alpha-1}$  with  $\alpha \geq 1$ , we obtain the isentropic/isothermal version of the quantum hydrodynamic equations, where the energy equation can be dropped. In the formal classical limit  $\hbar \rightarrow 0$  we get the hydrodynamic equations (6)-(7) (arrow 8). This limit is justified in [93, 211] for the thermal equilibrium state and in [107] for ‘subsonic’ solutions.

The quantum hydrodynamic model without relaxation terms can also be derived from the system of countable Schrödinger equations (30)-(31) assuming a closure condition in the energy equation (arrow 9). We refer to [97, 98, 136] for details of this derivation.

The quantum hydrodynamic equations in the thermal equilibrium state  $J_n = 0$  are mathematically studied in [29, 93, 177, 211]. The existence and uniqueness of solutions to the stationary model are investigated in [84, 107, 134, 224]. For results on the transient equations, see [92, 94]. Gardner has used this model to simulate numerically resonant tunneling diodes [48, 87, 90], whereas Ferry and Zhou solved numerically a modified set of equations for the simulation of high electron mobility transistors (HEMT; [226]). The full quantum hydrodynamic equations are numerically solved in [179, 182]. A dispersive numerical method is developed in [96].

It is common to replace the potential  $V$  by  $V + B$ , where  $B$  is a discontinuous function modeling heterostructures. The disadvantage of the above model is that discontinuities  $V + B$  lead to difficulties in the numerical discretization of Eqs. (33), (34). Gardner and Ringhofer have derived in [89, 90] so-called “smooth” quantum hydrodynamic models where the quantum term involves a smoothed potential. More precisely, they get from the Bloch equation in the Born approximation the equations (32)-(35) in which the term

$$\nabla Q = \frac{\hbar^2}{4qm^*n} \operatorname{div} (n(\nabla \otimes \nabla) \log(n))$$

in the momentum and energy equation is replaced by

$$\frac{q\hbar^2}{4m^*n} \operatorname{div} \left( \frac{n}{k_B T} (\nabla \otimes \nabla) \bar{V} \right),$$

with the definition

$$\bar{V}(x, \beta) = \frac{1}{(\pi\beta^2)^{3/2}} \int_0^\beta (\beta')^2 B(\beta')^{3/2} \int_{\mathbb{R}^3} e^{-B(\beta')(x'-x)^2} V(x') dx' d\beta'.$$

Here,  $B(\beta') = 2m^*\beta/((\beta + \beta')(\beta - \beta')\hbar^2)$  and  $\beta = 1/k_B T$  is the inverse temperature [89]. Moreover, the energy density is now given by

$$E = n \left( \frac{m^*}{2q^2} \frac{|J_n|^2}{n^2} + \frac{3}{2} k_B T + \frac{\hbar^2}{8m^*} \frac{\Delta \bar{V}}{k_B T} \right).$$

The quantum hydrodynamic equations are obtained in the  $O(\hbar^2)$  approximation:

$$\begin{aligned} \bar{V} &= \frac{1}{3} V + O(\hbar^2), \\ \nabla \log(n) &= -\frac{1}{k_B T} \nabla V + O(\hbar^2), \end{aligned}$$

if  $n$  and  $J_n$  are varying very slowly such that  $n$  can be approximated by  $\exp(-V/k_B T)$  and  $T$  is nearly constant. Then

$$n(\nabla \otimes \nabla) \bar{V} = \frac{1}{3} k_B T n(\nabla \otimes \nabla) \log(n) + O(\hbar^2)$$

and we get Eq. (33), where the term  $n\nabla Q$  is replaced by  $(1/3)n\nabla Q$ . The factor  $1/3$  comes from the mixed quantum states (“thermal averaging”) and does not appear in the derivation from the Schrödinger-mixed quantum states formulation.

We can use a diffusion scaling in the full quantum hydrodynamic equations, similar as in the full hydrodynamic model, to obtain the so-called *quantum energy-transport model*. More precisely, we are using the scaling (11), assuming that  $\varepsilon^2 = \tau_p/\tau_w$  is a small parameter. Then, letting  $\varepsilon \rightarrow 0$  in the full hydrodynamic equations, we obtain (arrow 10)

$$\begin{aligned} \frac{\partial n}{\partial t} - \frac{1}{q} \operatorname{div} J_n &= 0, \\ J_n &= \mu_0(k_B \nabla(nT) - qn \nabla(V + Q)), \\ \frac{\partial E}{\partial t} - \operatorname{div} \left( \frac{5k_B}{2q} T J_n + \tilde{\kappa} \nabla T \right) &= -J_n \cdot \nabla(V + Q) - \frac{3}{2\tau_0} n(T - T_L), \end{aligned}$$

where  $\mu_0 = q\tau_0/m^*$  and  $\tilde{\kappa} = \kappa_0\mu_0q^{-1}k_B^2nT$ . The energy density becomes

$$E = \frac{3}{2}k_BnT - \frac{\hbar^2}{24m^*}n\Delta \log(n).$$

Clearly, we can write these equations in the form (13)-(16) with  $V$  replaced by  $V + Q$  and the diffusion matrix (17). Formally, in the limit  $\hbar \rightarrow 0$  we obtain the classical energy-transport equations (arrow 11). The quantum energy-transport equations are yet not studied, neither analytically nor numerically.

In the zero-relaxation-time limit the convective term in the isentropic quantum hydrodynamic model can be neglected [133, 180] and we obtain the *quantum drift-diffusion equations* (arrow 12):

$$\begin{aligned} \frac{\partial n}{\partial t} - \frac{1}{q} \operatorname{div} J_n &= 0, \\ J_n &= \mu_0(k_B T_0 \nabla(n^\alpha) - qn \nabla V) - \frac{\mu_0 \hbar^2}{2m^*} n \nabla \left( \frac{\Delta \sqrt{n}}{\sqrt{n}} \right), \end{aligned}$$

with the Poisson equation (22), considered in a bounded domain with an initial condition for  $n$ , mixed Dirichlet-Neumann boundary conditions for  $n$ ,  $V$  and an additional boundary condition for the quantum term (for instance, a homogeneous Dirichlet-Neumann condition for  $Q$ ; see [144]).

The quantum drift-diffusion model with  $\alpha = 1$  is used to describe the behavior of electrons in the vicinity of strong inversion layers near the gate oxide of MOSFET transistors [6] or as a quantum correction to the classical drift-diffusion equations [190, 207, 222]. Mathematically, the above equations form a fourth-order parabolic equation which has the important property that the non-negativity of the particle density is preserved [143, 144]. The stationary model has been analyzed in [23] and numerically solved in [181]. The transient equations are studied analytically and numerically in [143, 144]. In the classical limit  $\hbar \rightarrow 0$  we obtain (formally) the isentropic drift-diffusion equations (arrow 13).

Other approaches to the modeling of quantum semiconductors are, for instance, Wigner function methods [15, 147] and density matrix methods [79].

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