The modern computer and telecommunication industry relies heavily on the use of semiconductor devices. The reason for the rapid development and success in the semiconductor technology is due to the ongoing miniaturization of these devices. The microelectronics industry produces very miniaturized components with small characteristic length scale, like tunneling diodes, which have a length of only a few nanometers. In such components, quantum phenomena become no longer negligible, even sometimes predominant, and the physical phenomena have to be described by quantum mechanics equations.

Depending on the device structure, the transport of particles can be very different, due to several physical phenomena, like drift, diffusion, scattering, and quantum effects. An appropriate way to describe a large number of particles flowing through a device is a kinetic or fluid-dynamic type description. On the other hand, electrons are in a semiconductor crystal quantum object, for which a wave-like description using the Schrödinger equation seems to be necessary. Therefore, there are several mathematical models which are able to describe particular phenomena in particular devices.

Usually quantum effects can be described by microscopic models, like Schrödinger-Poisson or Wigner-Poisson system. The motion of semi-classical particles in semiconductors is described most accurately by the Boltzmann equation, the basic equation of kinetic theory of semiconductors. The equation takes into account the microscopic mechanism of carrier transport. Generally, for microscopic equations, the complexity of the collision term, together with the high number of independent variables, requires numerical simulations a lot of computation power.

Moreover, as semiconductor devices are modeled in bounded domain and the natural physical setting of microscopic models is based on an unbounded
position domain, it’s difficult to find for them appropriate boundary conditions.

Recently, macroscopic quantum equations have been developed and used in quantum devices simulations. These macroscopic models are referred to as fluid-dynamical models. To this class of equations belong the quantum drift diffusion (QDD) model and the quantum hydrodynamic (QHD) model.

There are advantages of a macroscopic description: first, better tractability from the numerical point of view; second, easier for macroscopic variables to find relevant boundary conditions.

Working on the analytical and numerical study of the above mentioned macroscopic models, I already showed well-posedness of a stationary QHD model and of the transient QDD in case of zero temperature and zero electric field in one space dimension and gave some numerical examples.

The main goals of my current research are:
(i) global existence in time of the QDD model,
(ii) global existence in time of the QHD model including specific diffusion effects due to particle scattering,
(iii) numerical approximation for the QHD model.

Macroscopic models are derived from kinetic equations via several methods. Since 1927, it is well known that there exists a fluid-dynamical formulation of the Schrödinger equation. By separating the real and the complex part of that equation, the electron density, the current density, and the electrostatic potential satisfy (formally) the pressureless quantum hydrodynamic model. If we consider a statistical mixture of particles, the computation of the averaged quantities leads to closure problems, which appear in the passage from kinetic to fluid-dynamic equations. In the literature, several closure conditions have been proposed, such as approximation near the thermal equilibrium or entropy minimization.

Concerning the quantum description of electrons-phonons interactions, some collision model has been derived. For example, Caldeira and Legget [6] derived a Wigner-Fokker-Planck equation in the large temperature limit

\[
\partial_t w + p \cdot \nabla_x w - \Theta[V]w = Q(w), \quad t > 0, \quad (x, p) \in \mathbb{R}^{2d},
\]

where \( w(x, p, t) \) is the Wigner function, \( (x, p) \) are the position-momentum variables, \( t \) is the time, \( \Theta[V] \) is a pseudo-differential operator applied to the electrostatic potential \( V \), and the collision operator has the following form

\[
Q(w) = \alpha \Delta_p w + \frac{1}{\tau} \text{div}_p (pw) + \beta \text{div}_x (\nabla_p w) + \nu \Delta_x w,
\]

with \( \alpha, \beta, \tau, \) and \( \nu \) positive constants.
Applying a moment method for this equation and using as closure condition an expansion of the thermal equilibrium Wigner distribution function, similar to that in [12], the resulting system is termed as **viscous QHD model**

\[
\begin{align*}
\partial_t n + \text{div} J &= \nu \Delta n, \quad \lambda^2 \Delta V = n - C(x), \\
\partial_t J + \text{div} \left( \frac{J \otimes J}{n} \right) - n \nabla V + T \nabla n - \frac{\varepsilon^2}{2} n \nabla \left( \frac{\Delta \sqrt{n}}{\sqrt{n}} \right) &= \nu \Delta J - \frac{J}{\tau},
\end{align*}
\]

where \( n(x,t) \) is the particle density, \( J(x,t) \) is the current density, and \( V(x,t) \) is the electrostatic potential. The function \( C(x) \) describes the concentration of fixed background charges. The physical constants are the (scaled) Planck constant \( \varepsilon \), the Debye length \( \lambda \), the (scaled) temperature \( T \), the positive constant \( \nu \) called **viscosity**, and the (scaled) momentum relaxation time \( \tau \). The symbol \( J \otimes J \) denotes the tensor with components \( J_i J_k \). The quantum term can be interpreted either as an internal self-potential, the so-called Bohm potential, \( \Delta \sqrt{n} / \sqrt{n} \), or as a non-diagonal pressure tensor, \( (\nabla \otimes \nabla) \log n \). The relaxation term \( J/\tau \) models interactions of the electrons with the phonons of the semiconductor crystal lattice. For vanishing scaled Planck constant \( \varepsilon = 0 \) the above equation is equal to the classical Euler momentum equation for charged particles.

Recently, another method [8] has been used in order to derive model (3)-(4) in case \( \nu = 0 \). This new approach starts from the scaled Wigner equation (1) with a collision operator of BGK type, i.e.,

\[
Q(w) = \frac{1}{\tau} (M[w] - w),
\]

where \( M[w] \) is the so-called quantum Maxwellian, defined as the minimizer of the quantum entropy, subject to the constraint that its moments are given. This method leads to an **inviscid** quantum hydrodynamic model (\( \nu = 0 \) in (3)-(4)).

Concerning the mathematical analysis of the inviscid QHD (\( \nu = 0 \)), many results are available ([20], [11], [18], [19]). The main difficulties in the analysis of systems like (3)-(4) are the mathematical treatment of the third order quantum term and the proof of positivity for the particle density. Generally, the maximum principle is not available for higher order differential equations and in this case other methods are required.

For the stationary case, it has been shown that there exists a weak solution in one and more space dimensions, with several choices of boundary conditions, if a subsonic-type condition for the current density, similar to the classical subsonic flow, is satisfied. Moreover, for special boundary conditions, it is proved that the model does not possess a weak solution if the current density is large enough.

In [15], we prove the existence of a stationary solution for (3)-(4), with \( \nu > 0 \), in one space dimension with Dirichlet-Neumann boundary conditions...
under a “weakly supersonic condition” flows. Indeed, the viscous terms regularize the model in such a way that classical solutions also exist in the transonic region, but a limitation on the effective current density is still needed.

The long-time asymptotics of (3)-(4) have been studied in [16]. In order to prove exponential convergence to the (unique) thermal equilibrium state as the time tends to infinity, the existence of global in time solutions has been required, but not proved. The rigorous proof of this part is one objective of my research.

Recently, from the collisional Wigner equation (1) with collision operator (2), through diffusion limit, the Quantum Drift Diffusion model has been formally derived [7]:

\begin{equation}
\begin{aligned}
\partial_t n + \text{div} J &= 0, \\
J + T \nabla n - n \nabla V - \frac{\varepsilon^2}{2} n \nabla \left( \frac{\Delta \sqrt{n}}{\sqrt{n}} \right) &= 0.
\end{aligned}
\end{equation}

The mathematical analysis and the numerical understanding in this model are now in a rather advanced state. The stationary problem has been solved in [3] and the thermal equilibrium problem in [27], and a generalized Gummel iteration for an efficient numerical treatment has been developed in [26].

Concerning the transient case, only partial results are known. The crucial problem in the analysis comes from the fourth-order nature of the system. In order to understand better the influence of the fourth order term, we studied a simplified model: setting vanishing temperature and zero electric fields in (6), the system can be rewritten as a fourth-order parabolic equation for the particle density. In one space dimension, assuming smooth nonvacuum solutions, the Bohm potential differential operator \((n (\sqrt{n})_{xx}/\sqrt{n})_x\) can be equivalently rewritten as \((n \log n)_{xx}\). The nonlinear fourth order parabolic problem

\begin{equation}
\begin{aligned}
\partial_t n + (n \log n)_{xx} &= 0, \\
n(0, x) &= n_I(x),
\end{aligned}
\end{equation}

arises also as a scaling limit in the study of interface fluctuations in a certain spin system (see [9]). The analytical result has been presented in [22] for a boundary value problem with homogeneous Dirichlet and Neumann boundary conditions \(n(0, t) = n(1, t) = 1, n_x(0, t) = n_x(1, t) = 0\). This kind of boundary condition follows from a physical consideration, such as charge neutrality at the boundary contacts. However, these assumptions may not hold for ultra-small semiconductor devices. In particular, the homogeneous Neumann boundary conditions may be questionable in very small devices (see [25]). Therefore, in [17], the problem is with more general non-homogeneous boundary conditions

\begin{equation}
\begin{aligned}
n(0, t) &= n_0, \\
n(1, t) &= n_1, \\
n_x(0, t) &= w_0, \\
n_x(1, t) &= w_1,
\end{aligned}
\end{equation}

is analyzed, where \(n_0, n_1 > 0, \) and \(w_0, w_1 \in \mathbb{R}\). Problem (7) has been studied in [10], also with periodic boundary conditions.
Recently, the Cauchy problem (7) has been solved [14] for any space dimension. The proof makes use of mass transportation techniques: the solution is computed solving a minimization problem (in the Wasserstein metric) over some appropriate space. The main advantage is that this method circumvents the problem of non-negativity or positivity for the density function. In fact, as the solution is the minimum of such energy functional over all nonnegative functions with the same $L^1$-norm as the function $n_I$, it is automatically nonnegative. We recall that this method is not useful in the case of Dirichlet-Neumann boundary conditions; in fact, these conditions do not imply conservation of mass, which is the basic property in mass transportation techniques.

References


