Multi-scale modeling of quantum semiconductor devices

Anton Arnold[1] and Ansgar Jüngel[2]

[1] Institut für Analysis und Scientific Computing, Technische Universität Wien,
Wiedner Hauptstr. 8, A-1040 Wien, Austria
[2] Institut für Mathematik, Universität Mainz, Staudingerweg 9, D-55099 Mainz,
Germany

`anton.arnold@tuwien.ac.at`, `juengel@mathematik.uni-mainz.de`

Summary. This review is concerned with three classes of quantum semiconductor equations: Schrödinger models, Wigner models, and fluid-type models. For each of these classes, some phenomena on various time and length scales are presented and the connections between micro-scale and macro-scale models are explained. We discuss Schrödinger-Poisson systems for the simulation of quantum waveguides and illustrate the importance of using open boundary conditions. We present Wigner-based semiconductor models and sketch their mathematical analysis. In particular we discuss the Wigner-Poisson-Focker-Planck system, which is the starting point of deriving subsequently the viscous quantum hydrodynamic model. Furthermore, a unified approach to derive macroscopic quantum equations is presented. Two classes of models are derived from a Wigner equation with elastic and inelastic collisions: quantum hydrodynamic equations and their variants, as well as quantum diffusion models.

1 Introduction

The modern computer and telecommunication industry relies heavily on the use of semiconductor devices. A very important fact of the success of these devices is that their size can be very small compared to previous electronic devices (like the tube transistor). While the characteristic length of the first semiconductor device (a germanium transistor) built by Bardeen, Brattain, and Shockley in 1947 was 20μm, the characteristic size has been decreased up to now to some deca-nanometers only. With decreasing device length quantum mechanical effects are becoming more and more important in actual devices. In fact, there are devices, for instance tunneling diodes or quantum wave guides, whose function is based on quantum effects. The development of such devices is usually supported by computer simulations to optimize the desired operating features. Now, in order to perform the numerical simulations, mathematical equations are needed that are both physically accurate and numerically solvable with low computational cost.

We wish to model the flow of electrons in a semiconductor crystal with the goal to predict macroscopically measurable quantities by means of computer simulations. Although the physical process is always the transport of charged particles in a solid crystal, we need to devise different mathematical models because of the wide range of operating conditions and the desired need of accuracy. Moreover, since in some cases we are not interested in all the available physical information, we also need simpler models which help to reduce the computational cost in the numerical simulations.

We shall discuss three model classes: Schrödinger, Wigner, and fluid-type models. Schrödinger models describe the purely ballistic transport of electrons and holes, and they are employed for simulations of quantum waveguides and nano-scale semiconductor heterostructures. As soon as scattering mechanisms (between electrons and phonons, e.g.) become important, one has to resort to Wigner function or the equivalent density matrix formalism. For practical applications Wigner functions have the advantage to allow for a rather simple, intuitive formulation of boundary conditions at device contacts or interfaces. On the other hand, the Wigner equation is posed in a high dimensional phase space which makes its numerical solution extremely costly. As a compromise, fluid-type models can provide a reasonable approximation and is hence often used. Since one only computes the measurable physical quantities in these fluid models, they are computationable cheap. Moreover, classical boundary conditions can also be employed here.

The multi-scale character in semiconductor device modeling becomes manifest in a hierarchy of models that differ in mathematical and numerical complexity and incorporate physical phenomena on various time and length scales. The microscopic models clearly include the highest amount of information, but they involve the highly oscilatory Schrödinger and Wigner functions. However, the macroscopic variables of interest for practitioners (like particle and current densities) are typically much smoother. Hence, it is very attractive (particularly with respect to reduce numerical costs) to settle for simplified macroscopic quantum transport models. Scaling limits allow to relate these models and to obtain important information for the range of validity (and the limitations) of the reduced macro-scale models. Starting from Wigner-Boltzmann-type equations it is indeed possible to obtain a unified derivation of quantum hydrodynamic and quantum diffusion models.

2 Microscopic picture I: Schrödinger models

This section is concerned with Schrödinger-Poisson models for semiconductor device simulations. Such models are only applicable in the ballistic regime, i.e. to devices or subregions of devices, where the quantum mechanical transport is the dominant phenomenon and scattering plays only a minor role.

As particular examples we name interferences in quantum waveguides, the tunneling through nano-scale semiconductor heterostructures (in a resonant tunneling diode, e.g.), and the ballistic transport along nano-size channels of MOSFETs. In all of these examples we are dealing with *open quantum systems*, refering to a model on a finite geometry along with *open boundaries* (this contrasts with the situation in §3.1, where we shall consider collisional open quantum systems). Here, the transport model (the Schrödinger equation, e.g.) is posed on a finite domain $\Omega \subset \mathbb{R}^d$ (d being the space dimension). At the device contacts or interfaces *open boundary conditions* are specified, such that an incoming current can be prescribed and outgoing electron waves will not be reflected at such boundaries.

2.1 Quantum waveguide simulations

In this subsection we discuss simulation models for quantum waveguides. These are novel electronic switches of nanoscale dimensions. They are made of several different layers of semiconductor materials such that the electron flow is confined to small channels or waveguides. Due to their sandwiched structure the relevant geometry for the electron current is essentially two dimensional. Figure 2.1 shows the example of a T-shaped *quantum interference transistor*. The actual structure can be realized as an etched layer of GaAs between two layers of doped AlGaAs (cf. [69]). Applying an external potential at the gate (i.e. above the shaded portion of the stub, the "allowed region" for the electrons, and hence the geometry (in particular the stub length) can be modified. This allows to control the current flow through such an electronic device. It makes it a switch, which resambles a transistor – but on a nano-scale. Such a device shows sharp peaks in conductance that are due to the presence of bound states in the stub (see Figures 2.2, 2.3). It is expected that these novel devices will operate at low power and high speed.

The electron transport through a quantum waveguide can be modeled in good approximation by a two dimensional, time dependent Schrödinger-Poisson system for the wave functions $\psi_\lambda(x,t)$, indexed by the energy variable $\lambda \in \Lambda \subset \mathbb{R}$. The (possibly time-dependent) spatial domain $\Omega \subset \mathbb{R}^2$ consists of (very long) leads and the active switching region (e.g. T-shaped as in Fig. 2.1). In typical applications electrons are continuously fed into the leads as plane waves ψ_λ^{pw}. The Schrödinger model now reads

$$i\frac{\partial \psi_\lambda}{\partial t} = -\frac{1}{2}\Delta\psi_\lambda + V(x,t)\psi_\lambda, \quad x \in \Omega,\ \lambda \in \Lambda,\ t > 0. \tag{2.1}$$

The potential $V = V_e + V_s$ consists of an external, applied potential V_e and the selfconsistent potential satisfying the Poisson equation with Dirichlet boundary conditions:

$$\begin{aligned} -\Delta V_s(x,t) = n(x,t) = \int_\Lambda |\psi_\lambda(x,t)|^2 g(\lambda)\, d\lambda, \quad x \in \Omega, \\ V_s = 0, \quad \text{on } \partial\Omega. \end{aligned} \tag{2.2}$$

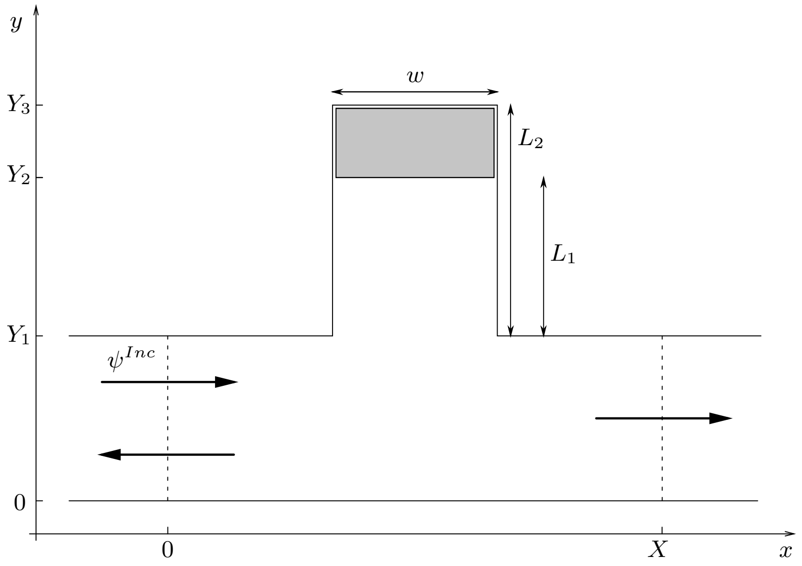

Fig. 2.1. T-shaped geometry $\Omega \subset \mathbb{R}^2$ of a quantum interference transistor with source and drain contacts to the left and right of the channel. Applying a gate voltage above the stub allows to modify the stub length from L_1 to L_2 and hence to switch the transistor between the on- and off-states.

Here, n is the spatial electron density and $g(\lambda)$ denotes the prescribed statistics of the injected waves (Fermi-Dirac, e.g.). In the simplest case (i.e. a 1D approximation) open or "transparent" boundary conditions at the contacts or interfaces take the form

$$\frac{\partial}{\partial\eta}(\psi_\lambda - \psi_\lambda^{pw}) = -e^{-i\pi/4}\sqrt{\partial_t}\,(\psi_\lambda - \psi_\lambda^{pw}),\ \lambda \in \Lambda, \tag{2.3}$$

where η denotes the unit outward normal vector at each interface. $\sqrt{\partial_t}$ is the fractional time derivative of order $\frac{1}{2}$, and it can be rewritten as a time-convolution of the boundary data with the kernel $t^{-3/2}$. For the derivation of the 2D-variant of such transparent boundary conditions and the mathematical analysis of this coupled model (2.1)-(2.3) we refer to [15, 7].

The discretization of such a model poses several big numerical challenges, both for stationary and for transient simulations: Firstly, the wave function is highly oscillatory for larger energies, while the macroscopic variables of interest (particle density n and potential V) are rather smooth. Secondly, solutions to (2.1)-(2.3) can exhibit sharp peaks in the curve of conductance versus injection energy (both in quantum waveguides and in resonant tunneling diodes). To cope with these two problems, WKB-type discretization schemes for the 1D stationary analogue of the above model and adaptive energy grids (for $\lambda \in \Lambda$) were devised in [16].

Thirdly, the numerical discretization of the transparent boundary condition (2.3) is very delicate in the time dependent case, as it may easily render the initial-boundary value problem unstable and introduce hugh spurious wave reflections. Based on a Crank-Nicolson finite difference discretization of the Schrödinger equation, unconditionally stable *discrete transparent boundary conditions* were developed in [5] for the one-dimensional and in [9, 11] for the two-dimensional problem. An extension of such discrete open boundary conditions for (multiband) kp-Schrödinger equations appearing in the simulation of quantum heterostructures were developed in [75].

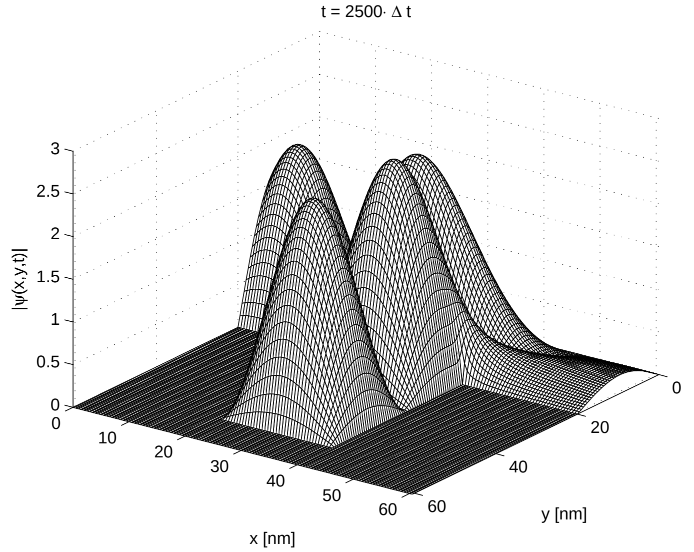

Fig. 2.2. Stationary Schrödinger wave function for T-shaped waveguide with short stub (i.e. $L_1 = 32$ nm) – "off state"

To close this subsection we present some first simulations of the electron flow through the T-shaped waveguide from Figure 2.1 with the dimensions $X = 60$ nm, $Y_1 = 20$ nm. These calculations are based on the linear Schrödinger equation for one wave function with $V \equiv 0$ and the injection of a mono-energetic plane wave with 130 meV, entering in the transparent boundary condition (2.3). The simulation was based on a compact forth order finite difference scheme ("Numerov scheme") and a Crank-Nicolson discretization in time [11].

Important device data for practitioners are the current-voltage (I-V) characteristics, the ratio between the on- and the (residual) off-current as well as the switching time between these two stationary states. Depending on the size and shape of the stub, the electron current is either reflected (off-state of the device, see Fig. 2.2) or it can flow through the device (on-state, see Fig. 2.3). Starting from the stationary state in Fig. 2.2, the swiching of the device was realized by an instantaneous extension of the stub length from $L_1 = 32$ nm to $L_2 = 40.5$ nm. After a transient phase the new steady state Fig. 2.3 is reached after about 4 ps.

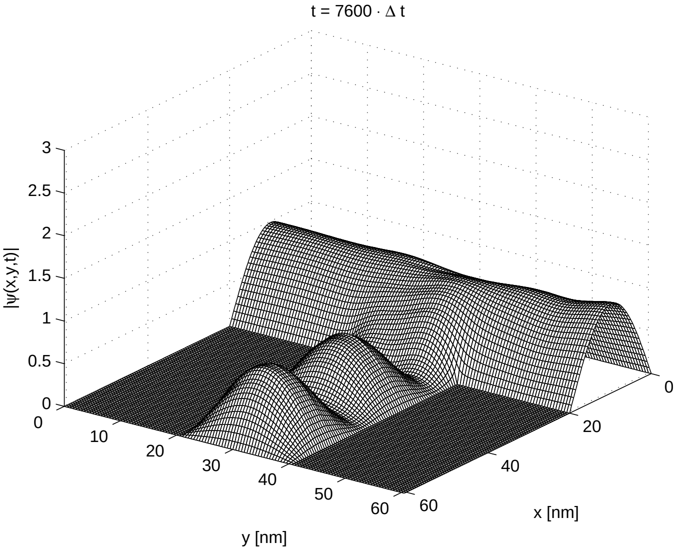

Fig. 2.3. Stationary Schrödinger wave function for T-shaped waveguide with long stub (i.e. $L_2 = 40.5$ nm) – "on state"

3 Microscopic picture II: Wigner models

In this section we shall present and discuss semiconductor models that are based on the quantum-kinetic Wigner formalism. As mentioned before there are two main reasons for using this framework in applications (indeed, mostly for time dependent problems): In contrast to Schrödinger models the Wigner picture allows to include the modeling of scattering phenomena in the form of a *quantum Boltzmann equation.* Secondly, this quantum-kinetic framework makes is easier to formulate reasonable boundary conditions at the device contacts, using guidance and inspiration from classical kinetic theory [33]. This approach makes indeed sense, as quantum effects are not important close to the (typically highly doped) contact regions.

The Wigner function $f = f(x, v, t)$ is one of several equivalent formalisms to describe the (mixed) state of a physical quantum system (cf. [74]). It is a real-valued quasi-distribution function in the position-momentum (x, p) phase space at time t. In collision-free regimes, the quantum equivalent of the Liouville equation of classical kinetic theory governs the time evolution of f. In the d-dimensional whole space it reads

$$\partial_t f + p \cdot \nabla_x f + \theta[V]f \; = \; 0, \quad t > 0, \quad (x, p) \in \mathbb{R}^{2d}, \tag{3.1}$$

where the (real-valued) potential $V = V(x)$ enters through the pseudo-differential operator $\theta[V]$ defined by

$$\begin{aligned}(\theta[V]f)(x, p, t) &= \frac{i}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} \delta V(x, \eta) \mathcal{F}_{p\to\eta} f(x, \eta, t) e^{ip\cdot\eta}\, d\eta \\ &= \frac{i}{(2\pi)^d} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \delta V(x, \eta) f(x, p', t) e^{i(p-p')\cdot\eta}\, dp'\, d\eta. \end{aligned} \tag{3.2}$$

Here, $\delta V(x, \eta) := \frac{1}{\varepsilon}\left[V(x + \frac{\varepsilon\eta}{2}) - V(x - \frac{\varepsilon\eta}{2})\right]$, and $\mathcal{F}_{p\to\eta} f$ denotes the Fourier transform of f with respect to p, and $\varepsilon > 0$ is the scaled Planck constant.

For semiconductor device simulations it is crucial to include the self-consistent potential. The electrostatic potential $V(x, t)$ is hence time-dependent and obtained as a solution to the Poisson equation

$$\varDelta_x V(x, t) = n(x, t) - C(x), \tag{3.3}$$

with the particle density

$$n(x, t) = \int_{\mathbb{R}^d} f(x, p, t)\, dp. \tag{3.4}$$

Here, $C(x)$ denotes the time-independent doping profile of the device, i.e. the spatial density of the doping ions implanted into the semiconductor crystal.

3.1 Wigner models for open quantum systems

Until now we only considered the ballistic and hence reversible quantum transport of the electrons in a one-particle (Hartree) approximation. Such purely ballistic models (either in the Wigner or Schrödinger framework - cf. §2) are useful semiconductor models for device lengths in the order of the electrons' mean free path. For larger devices, however, scattering phenomena between electrons and phonons (i.e. thermal vibrations of the crystal lattice) or among the electrons have to be taken into account. In this case an appropriate collision operator $Q(f)$ has to be added as a right hand side of (3.1). In contrast to §2 the term *open quantum system* refers here to the interaction of our considered electron ensemble with some 'environment' (an external phonon bath, e.g.) and not to the influence of the boundaries or contacts.

For the classical semiconductor Boltzmann equation excellent models for the most important collisional mechanisms have been derived (cf. [66]) and are incorporated into today's commercial simulation tools. In quantum kinetic theory, however, realistic and numerically usable collison models are much less developed. In contrast to classical kinetic theory, quantum collision operators are actually non-local in time (cf. the Levinson equation [61] as one possible model). However, since most of the current numerical simulations involve only local in time approximations, we shall confine our discussion to such collision operators. The three most used models are firstly relaxation time approximations of the form

$$Q(f) = \frac{f_0 - f}{\tau}, \tag{3.5}$$

with some appropriate steady state f_0 and the relaxation time $\tau > 0$ [58, 3]. Secondly, many applications (cf. [73, 39, 67]) use quantum Fokker-Planck models:

$$Q(f) = \beta \mathrm{div}_p(pf) + \sigma \Delta_p f + 2\gamma \mathrm{div}_p(\nabla_x f) + \alpha \Delta_x f, \tag{3.6}$$

(cf. [20, 23] for a derivation) with the friction parameter $\beta \geq 0$. The non-negative coefficients α, γ, σ constitute the phase-space diffusion matrix of the system. We remark that one would have $\alpha = \gamma = 0$ in the Fokker-Planck equation of classical mechanics [71].
As a third option, the Wigner equation (3.1) is often augmented by a semiclassical Boltzmann operator [59]. However, since this model is quantum mechanically not consistent, we shall not discuss it any further. Finally, we mention the quantum-BGK type models [27] that were recently introduced for deriving quantum hydrodynamics (cf. §4.2 for details).

At the end of this section we briefly list the numerical methods developed so far for Wigner function-based device simulations. Virtually all simulations were carried out for one dimensional resonant tunneling diodes. The earliest approaches were based on finite difference schemes for the relaxation-time Wigner-Poisson system [33, 58]. Spectral collocation methods were designed as an efficient alternative to discretize the non-local pseudo-differential operator $\theta[V]$ (cf. [70]). In [13] this approach was combined with an operator splitting between the transport term $p \cdot \nabla_x$ and $\theta[V]$ which has also been common practice for Boltzmann type equations. This mixed operator splitting/spectral collocation technique was recently extended to the Wigner-Fokker-Planck system in [29]. In [59] the classical Monte Carlo method was extended to Wigner models, and it has the potential to make multi-dimensional simulations feasible. Since the Wigner function takes both positive and negative values, novel algorithms for particle creation and annihilation had to be developed within this Monte Carlo approach.

3.2 Open quantum systems in Lindblad form

Since the Wigner function takes also negative values, it is a-priori not clear why the macroscopic particle density satisfies $n(x,t) := \int f(x,p,t)\,dp \geq 0 \;\forall x, t$. This physically important non-negativity is a consequence of the non-negativity of the density matrix (operator) that is associated with a Wigner function: Let $\widehat{\rho}$ be an operator on $L^2(\mathbb{R}^d)$ with integral kernel $\rho(x,x') = \rho \in L^2(\mathbb{R}^{2d})$, i.e.

$$(\widehat{\rho}\phi)(x) = \int_{\mathbb{R}^d} \rho(x,x')\phi(x')\,dx' \quad \forall \phi \in L^2(\mathbb{R}^d). \tag{3.7}$$

The Wigner transform of the density matrix $\widehat{\rho}$ is now defined as the following Wigner function f (cf. [74, 64]):

$$W(\widehat{\rho})(x,p) := f(x,p) = \frac{1}{(2\pi)^d}\int_{\mathbb{R}^d} \rho(x+\frac{\varepsilon}{2}\eta, x-\frac{\varepsilon}{2}\eta)e^{i\eta\cdot p}\,d\eta. \tag{3.8}$$

In terms of density matrices, a mixed quantum states is described as a positive trace class operator on $L^2(\mathbb{R}^d)$ (i.e. $\widehat{\rho} \in \mathcal{I}_1$, $\widehat{\rho} \geq 0$), mostly with the normalization $\mathrm{Tr}\widehat{\rho} = 1$, where Tr denotes the operator trace. The positivity of $\widehat{\rho}$ as an operator then implies pointwise positivity of the particle density

$$n(x) := \rho(x,x) \geq 0, \quad x \in \mathbb{R}^d, \tag{3.9}$$

and of the corresponding kinetic energy

$$E_{kin} := \frac{1}{2}\int_{\mathbb{R}^{2d}} |p|^2 f(x,p)\,dxdp = \frac{\varepsilon^2}{2}\mathrm{Tr}(-\Delta\widehat{\rho}) = \frac{\varepsilon^2}{2}\mathrm{Tr}(\sqrt{-\Delta}\widehat{\rho}\sqrt{-\Delta}) \geq 0. \tag{3.10}$$

The time evolution of a density matrix is given by the Heisenberg-von Neumann equation, obtained by applying the Wigner transform (3.7), (3.8) to the Wigner equation (3.1). It reads

$$\begin{aligned} &i\varepsilon\widehat{\rho}_t = H(t)\widehat{\rho} - \widehat{\rho}H(t), \quad t>0, \\ &\widehat{\rho}(t=0) = \widehat{\rho}_I, \end{aligned} \tag{3.11}$$

with the (possibly time dependent) Hamiltonian $H(t) = -\frac{\varepsilon^2}{2}\Delta + V(x,t)$. For an open quantum system the right hand side of (3.11) has to be augmented by a non-Hamiltonian term $iA(\widehat{\rho})$. It is well known from [63] that such quantum evolution equations preserve the positivity of $\widehat{\rho}(t)$ (more precisely, it is actually the complete positivity) if and only if the dissipative term $A(\widehat{\rho})$ satisfies the following structural condition. It must be possible to represent it in the so-called Lindblad form:

$$A(\widehat{\rho}) = \sum_{j\in J} L_j^* L_j \widehat{\rho} + \widehat{\rho} L_j^* L_j - 2L_j\widehat{\rho}L_j^*, \tag{3.12}$$

with some appropriate (but typically not uniquely defined) Lindblad operators L_j, and a finite or infinite index set $J \subset \mathbb{N}$. Furthermore, such models then preserve the mass of the system, i.e. $\mathrm{Tr}\,\widehat{\rho}(t) = \mathrm{Tr}\,\widehat{\rho}_I,\ t \geq 0$.

For the relaxation time Wigner equation we have $A(\widehat{\rho}) = \frac{\widehat{\rho}_0 - \widehat{\rho}}{\tau}$ with some steady state $\widehat{\rho}_0$. Under the natural assumption $\mathrm{Tr}\,\widehat{\rho}_I = \mathrm{Tr}\,\widehat{\rho}_0 = 1$, and if the relaxation time τ is constant, we have (cf. [4])

$$A(\widehat{\rho}) = \frac{1}{\tau}(\widehat{\rho}_0 \operatorname{Tr} \widehat{\rho} - \widehat{\rho} \operatorname{Tr} \widehat{\rho}_0) = \sum_{j,k \in \mathbb{N}} L_{jk}^* L_{jk} \widehat{\rho} + \widehat{\rho} L_{jk}^* L_{jk} - 2 L_{jk} \widehat{\rho} L_{jk}^*,$$

with the Lindblad operators $L_{jk} = \sqrt{\mu_k/\tau}\ |\varphi_k >< \varphi_j|$. Here, $(\mu_k, \varphi_k)_{k \in \mathbb{N}}$ denotes the eigenpairs of $\widehat{\rho}_0$. Hence, the relaxation time Wigner equation (possibly with a selfconsistent potential) is an admissible open quantum model in Lindblad form.

For the Wigner-Fokker-Planck (WFP) equation with $Q(f)$ from (3.6), the Lindblad condition (3.12) holds iff

$$\begin{pmatrix} \alpha & \gamma + \frac{i\varepsilon}{4}\beta \\ \gamma - \frac{i\varepsilon}{4}\beta & \sigma \end{pmatrix} \geq 0. \tag{3.13}$$

Under this assumption the WFP model is also quantum mechanically correct. Here, the Lindblad operators are linear combinations of x_j and ∂_{x_j} (cf. [10]).

3.3 Analysis of the Wigner-Poisson-Fokker-Planck system

In this section we will sketch the different approaches to the well-posedness analysis for the Cauchy problem of the Wigner-Poisson-Fokker-Planck (WPFP) system in three dimensions:

$$\begin{aligned} \partial_t f + p \cdot \nabla_x f + \theta[V]f &= \beta \operatorname{div}_p(pf) + \sigma \Delta_p f + 2\gamma \operatorname{div}_p(\nabla_x f) + \alpha \Delta_x f,\ t > 0, \\ f(x,p,t=0) &= f_I(x,p),\ (x,p) \in \mathbb{R}^6, \\ \Delta_x V(x,t) = n(x,t) &= \int_{\mathbb{R}^3} w(x,p,t)\, dp. \end{aligned} \tag{3.14}$$

For simplicity we set here all physical constants equal to 1, and we chose $C \equiv 0$ as this would not change the subsequent analysis. Also, the Lindblad condition (3.13) is assumed to hold in the sequel.

First we remark that the WPFP model cannot be writen as an equivalent system of countably many Schrödinger equations coupled to the Poisson equation (and this is typical for open quantum systems). Therefore, the approach of [19] employed in the well-posedness analysis of the (reversible) Wigner-Poisson system cannot be adapted to WPFP. Hence, there are two remaining frameworks for the analysis: the Wigner function and density matrix formalisms, which we shall both briefly discuss here.

On the quantum kinetic level there are two main analytic difficulties for the nonlinear WPFP system. Since the natural analytic setting for Wigner functions is $f(.,.,t) \in L^2(\mathbb{R}^6)$ we cannot expect that $f(x,.,t) \in L^1(\mathbb{R}^3)$ holds. Hence, the definition of the particle density by $n(x,t) = \int_{\mathbb{R}^3} f(x,p,t)\, dp$ is purely formal. The second key problem is the lack of usable a-priori estimates on the Wigner function which would be needed to prove global-in-time existence of WPFP-solutions: The only useful (and almost trivial) estimate is

$$||f(t)||_{L^2(\mathbb{R}^6)} \leq e^{\frac{3}{2}\beta t} ||f_I||_{L^2(\mathbb{R}^6)}, \quad t \geq 0. \tag{3.15}$$

The other physically obvious conservation laws

$$\int f(x,p,t)\,dxdp = const \qquad \text{(mass conservation)},$$

and a simple energy balance involving the kinetic energy $E_{kin} = \frac{1}{2}\int |p|^2 f(x,p,t)\,dxdp$ both include functionals of f that are, a-priori, not necessarily positive and hence not useable on the quantum kinetic level.

Dispersive effects in quantum kinetic equations. Both of the described analytic problems – proper definition of the particle density n (or, equivalently, the electric field $E = \nabla_x V$) and additional a-priori estimates – can be coped with by exploiting dispersive effects of the free-streaming operator jointly with the parabolic regularization of the Fokker-Planck term. Such dispersive techniques for kinetic equations were first developed for the Vlasov-Poisson system (cf. [68]) and then adapted to the Vlasov-Poisson-Fokker-Planck equation in [22]. In [6, 8] these tools were extended to quantum kinetic theory. They yield first of all an a-priori estimate for the field $E(t)$ in terms of $\|f(t)\|_{L^2(\mathbb{R}^6)}$ only (remember (3.15) !). This estimate allows a *novel definition* of the macroscopic quantities (namely, the self-consistent field, the potential, and the density), which, in contrast to the definition (3.3), (3.4) is now non-local in time. This way, no p-integrability of f is needed.

Next we illustrate these dispersive tools in some more detail. With $G(t) = G(x,p,x',p',t)$ denoting the Green's function of the linear part of (3.14) (cf. [72]), the (linear) WFP equation can be rewritten as

$$\begin{aligned} f(x,p,t) &= \iint G(t) f_I(x',p')dx'dp' \\ &\quad + \int_0^t \iint G(s)(\theta[V]f)(x',p',t-s)\,dx'dp'ds, \quad t \geq 0. \end{aligned} \tag{3.16}$$

According to the two terms on the r.h.s. we split the electric field

$$E(x,t) = \nabla_x V(x,t) = \frac{x}{4\pi|x|^3} * n(x,t)$$

into $E = E_0 + E_1$ with

$$E_0(x,t) = \frac{x}{4\pi|x|^3} *_x \iiint G(t) f_I(x',p')dx'dp'dp, \tag{3.17}$$

$$E_1(x,t) = \frac{x}{4\pi|x|^3} *_x \int_0^t \iiint G(s)(\theta[V]f)(x',p',t-s)\,dx'dp'dpds.$$

With some tricky reformulation this last equation can be rewritten as

$$\begin{aligned} &(E_1)_j(x,t) \\ &= \frac{1}{4\pi}\sum_{k=1}^{3} \frac{3x_jx_k - \delta_{jk}|x|^2}{|x|^5} *_x \int_0^t \frac{\vartheta(s)}{R(s)^{3/2}} \mathcal{N}\left(\frac{x}{\sqrt{R(s)}}\right) *_x F_k[f](x,t,s)\,ds, \end{aligned} \tag{3.18}$$

$j = 1, 2, 3$; with

$$
\begin{aligned}
F_k[f](x,t,s) &:= \int (\Gamma_k[E_0+E_1]f)\,(x-\vartheta(s)p, p, t-s)\,dp, \quad k=1,2,3,\\
\mathcal{N}(x) &:= (2\pi)^{-3/2}\exp\left(-\frac{|x|^2}{2}\right),\\
\vartheta(t) &:= \frac{1-e^{-\beta t}}{\beta}; \qquad \vartheta(t) \;:=\; t, \quad \text{if } \beta = 0,\\
R(t) &:= 2\alpha t + \sigma\left(\frac{4e^{-\beta t}-e^{-2\beta t}+2\beta t-3}{\beta^3}\right) + 4\gamma\left(\frac{e^{-\beta t}+\beta t-1}{\beta^2}\right),
\end{aligned}
$$

and the (vector valued) pseudo-differential operator $\Gamma[E]$ is related to $\theta[V]$ by

$$
\theta[V]f(x,p) \;=\; \operatorname{div}_p\left(\Gamma[\nabla_x V]f\right)(x,p).
$$

Notice that (3.18) is a closed equation (more precisely a linear Volterra integral equation of the second kind) for the self-consistent electric field $E_1 \in \mathbb{R}^3$, for any given Wigner trajectory $f \in \mathcal{C}([0,T]; L^2(\mathbb{R}^6))$.

These motivations lead to our new definition of the Hartree-potential:
Definition 3.1 (New definition of mean-field quantities) *To a Wigner trajectory* $f \in \mathcal{C}([0,T]; L^2(\mathbb{R}^6))$ *we associate*

- *the field* $E[f] := E_0 + E_1[f]$, *with* E_0 *given by (3.17), and* $E_1[f]$ *the unique solution of (3.18),*
- *the potential* $V[f] := V_0 + V_1[f]$ *with*

$$
V_0(x,t) := \frac{1}{4\pi}\sum_{i=1}^{3}\frac{x_i}{|x|^3} *_x (E_0)_i(x,t), \tag{3.19}
$$

$$
V_1[f](x,t) := \frac{1}{4\pi}\sum_{i=1}^{3}\frac{x_i}{|x|^3} *_x (E_1[f])_i(x,t), \tag{3.20}
$$

- *and the position density* $n[f] := \operatorname{div} E[f]$ *(at least in a distributional sense).*

In contrast to the standard definitions (3.3), (3.4), these new definitions are *non-local in time.* Also, the map $f \mapsto V[f]$ is now *non-linear.* For a given Wigner trajectory these two definitions clearly differ in general. However, they coincide if f is the solution of the WPFP system. These new definitions of the self-consistent field and potential have the advantage that they only require $f \in \mathcal{C}([0,T]; L^2(\mathbb{R}^6))$ and not $f(x,.,t) \in L^1(\mathbb{R}^3)$. If $f(t=0)$ only lies in $L^2(\mathbb{R}^6)$, the corresponding field and the potential will consequently only be defined for $t > 0$.

The equation (3.18) now easily yields the announced $\|E(t)\|_{L^2(\mathbb{R}^3)}$–estimate for $t \in (0,\infty)$ in terms of f_I and $\|f(t)\|_{L^2(\mathbb{R}^6)}$ only. The fixed-point map

$f \mapsto V[f] \mapsto \tilde{f}$ (where the last steps refers to solving the linear WFP equation (3.16) with given $V(t)$, $t \geq 0$) is now contractive in $\mathcal{C}([0,T]; L^2(\mathbb{R}^6))$ and it yields the global mild solution for the WPFP system (3.14).

Without going into details we briefly list alternative kinetic approaches for the WPFP system that were developed in the last few years: In [6] p-weighted L^2-spaces were used to make the definition of the particle density by $n = \int f\, dp$ meaningful. In [10, 21], instead, an L^1-setting is chosen with the same motivation. The pseudo-differential operator $\theta[V]$ is rewritten there as a convolution operator in the p-variable. We remark that such kinetic strategies are valuable as they can, possibly, be extended to the WPFP boundary value problems used for semiconductor device modeling.

The quantum Fokker-Planck system for density matrices. Using the Wigner transforms we first rewrite the WPFP system (3.14) for the integral kernel $\rho(x,x',t)$ from (3.7):

$$\begin{aligned}\rho_t = &-iH_x\rho + iH_{x'}\rho - \frac{\beta}{2}(x-x')\cdot(\nabla_x - \nabla_{x'})\rho \\ &+ \alpha|\nabla_x + \nabla_{x'}|^2\rho - \sigma|x-x'|^2\rho + 2i\gamma(x-x')\cdot(\nabla_x+\nabla_{x'})\rho,\end{aligned} \tag{3.21}$$

coupled to the Poisson equation for V, where $H_{x'}$ is a copy of the Hamiltonian $H = H_x = -\frac{1}{2}\Delta_x + V(x,t)$, but acting on the x'–variable. The corresponding density matrix $\widehat{\rho}$ then satisfies the evolution equation (3.11), augmented with a r.h.s. $iA(\widehat{\rho})$ in Lindblad form (3.12) and coupled to the Poisson equation.

For the whole space case the density matrix formalism provides the most elegant analytic setup. Motivated by the kinetic energy $E_{kin}(\widehat{\rho})$ defined in (3.10) we define the "energy space"

$$\mathcal{E} := \{\widehat{\rho} \in \mathcal{I}_1 \mid \sqrt{1-\Delta}\,\widehat{\rho}\sqrt{1-\Delta} \in \mathcal{I}_1\}.$$

For physical quantum states (i.e. $\widehat{\rho} \geq 0$) we then have

$$\|\widehat{\rho}\|_{\mathcal{E}} = \operatorname{Tr}\widehat{\rho} + E_{kin}(\widehat{\rho}).$$

The simple estimate

$$\|n\|_{L^1(\mathbb{R}^3)} \leq \|\widehat{\rho}\|_{\mathcal{I}_1}$$

gives a rigorous meaning (in L^1) to the definition of the particle density (3.9), and the Lieb-Thirring-type estimate (cf. [3, 64]) yields

$$\|n\|_{L^3(\mathbb{R}^3)} \leq C\|\widehat{\rho}\|_{\mathcal{E}}.$$

Therefore the nonlinearity $[V(x,t) - V(x',t)]\rho(x,x',t)$ in (3.21) is locally Lipschitz in $\mathcal{E}$. Since the linear part of (3.21) generates a mass conserving semigroup on $\mathcal{E}$, standard semigroup theory yields a unique local-in-time solution to (3.21). A-priori estimates on the mass $\operatorname{Tr}(\widehat{\rho})$ and the total energy $E_{tot}(\widehat{\rho}) = E_{kin}(\widehat{\rho}) + \frac{1}{2}\|\nabla_x V[\widehat{\rho}]\|^2_{L^2}$, due to the energy balance

$$\frac{d}{dt}E_{tot} = 3\sigma \operatorname{Tr} \widehat{\rho}_I - 2\beta E_{kin}(t) - \alpha \|n(t)\|_{L^2}^2,$$

then shows that there exists a unique global mild solution of (3.21) in $\mathcal{C}([0,\infty);\mathcal{E})$ (cf. [12]).

4 Macroscopic picture: fluid-type models

The aim of this section is to derive macroscopic quantum models from the following Wigner-Boltzmann equation for the distribution function $f(x,p,t)$:

$$\partial_t f + p \cdot \nabla_x f + \theta[V]f = Q(f), \quad f(x,p,0) = f_I(x,p), \quad (x,p) \in \mathbb{R}^{2d}, \ t > 0. \tag{4.1}$$

Here, (x,p) denotes the position-momentum variables of the phase space, $t > 0$ is the time, $d \geq 1$ the dimension, $Q(f)$ a collision operator, and $\theta[V]f$ is the pseudo-differential operator defined by (3.2). Notice that in the semi-classical limit $\varepsilon \to 0$, the term $\theta[V]f$ converges to $\nabla_x V \cdot \nabla_p f$ and thus, (4.1) reduces to the semi-classical Vlasov equation [66]. The electric potential $V = V(x,t)$ is selfconsistently coupled to the Wigner function f via Poisson's equation

$$\lambda_L^2 \Delta V = \int_{\mathbb{R}^d} f dp - C, \tag{4.2}$$

where λ_L is the scaled Debye length and $C = C(x)$ the doping concentration characterizing the semiconductor device [44].

In classical fluiddynamics, macroscopic models can be derived from the Boltzmann equation by using a moment method. The idea is to multiply the kinetic equation by some monomials $\kappa_i(p)$ and to integrate the equation over the momentum space. This yields the so-called *moment equations*. Usually, not all integrals can be expressed in terms of the moments (which is called the *closure problem*) and an additional procedure is necessary in order to close the equations. Depending on the number of moments which are taken, a variety of fluiddynamical models can be derived [14, 60]. The aim of this section is to mimic this procedure in the quantum case. Figure 4.1 shows the resulting models arising from special choices of the set of monomials. We will discuss these models in detail in the following subsections. For this, we need to specify the collision operator $Q(f)$ in (4.1). First we introduce in the following subsection the so-called quantum Maxwellian.

4.1 Definition of the quantum Maxwellian

In order to define the quantum Maxwellian, we use the Wigner transform $W(\widehat{\rho})$ of an integral operator $\widehat{\rho}$ on $L^2(\mathbb{R}^d)$ as defined in (3.7), (3.8). Its inverse W^{-1}, also called Weyl quantization, is defined as an operator on $L^2(\mathbb{R}^d)$:

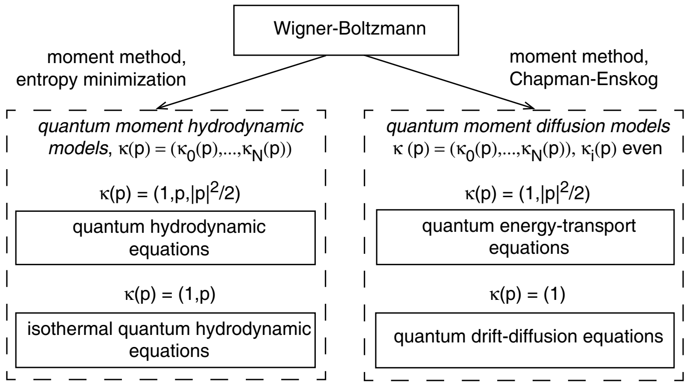

Fig. 4.1. Multiscale hierarchy of macroscopic quantum models.

$$(W^{-1}(f)\phi)(x) = \int_{\mathbb{R}^{2d}} f\Big(\frac{x+y}{2}\Big)\phi(y)e^{ip\cdot(x-y)/\varepsilon}dpdy \quad \text{for all } \phi \in L^2(\mathbb{R}^d).$$

With these definitions we are able to introduce as in [27] the *quantum exponential* and the *quantum logarithm* formally by $\operatorname{Exp} f = W(\exp W^{-1}(f))$ and $\operatorname{Log} f = W(\log W^{-1}(f))$, where exp and log are the operator exponential and logarithm, respectively.

Inspired by Levermore's moment method for the classical case [60], Degond and Ringhofer [27] have defined the quantum Maxwellian by using the entropy minimization principle. Let a quantum mechanical state be described by the Wigner function f solving (4.1). Then its *relative quantum (von Neumann) entropy* is given by

$$H(f) = \int_{\mathbb{R}^{2d}} f(x,p,\cdot)\Big((\operatorname{Log} f)(x,p,\cdot) - 1 + \frac{|p|^2}{2} + V(x,\cdot)\Big)dxdp.$$

Whereas the classical entropy is a function on the configuration space, the above quantum entropy at given time is a real number, underlining the nonlocal nature of quantum mechanics.

We define the *quantum Maxwellian* M_f for some given function $f(x,p,t)$ as the solution of the constrained minimization problem

$$H(M_f) = \min\left\{H(\hat{f}) : \int_{\mathbb{R}^d} \hat{f}(x,p,t)\kappa_i(p)dp = m_i(x,t) \text{ for all } x,\ t,\ i\right\}, \tag{4.3}$$

where $\kappa_i(p)$ are some monomials in p and $m_i(x,t)$ are the *moments* of f,

$$m_i(x,t) = \langle f(x,p,t)\kappa_i(p)\rangle, \quad i = 0,\ldots,N, \tag{4.4}$$

where we have used the notation $\langle g(p)\rangle = \int g(p)dp$ for functions $g(p)$. The formal solution of this minimization problem (if it exists) is given by $M_f = \operatorname{Exp}(\widetilde{\lambda}\cdot\kappa - \frac{1}{2}|p|^2 - V(x,\cdot))$, where $\kappa = (\kappa_0,\ldots,\kappa_N)$, and $\widetilde{\lambda} = (\widetilde{\lambda}_0,\ldots,\widetilde{\lambda}_N)$ are some Lagrange multipliers. If $\kappa_0(p) = 1$ and $\kappa_2(p) = \frac{1}{2}|p|^2$, setting $\lambda_0 = \widetilde{\lambda}_0 - V$, $\lambda_2 = \widetilde{\lambda}_2 - 1$ and $\lambda_i = \widetilde{\lambda}_i$ otherwise, we can write

$$M_f = \operatorname{Exp}(\lambda \cdot \kappa(p)). \tag{4.5}$$

4.2 Quantum moment hydrodynamic models

In this section we will derive the quantum moment hydrodynamic equations from the Wigner-Boltzmann equation (4.1) with dominant elastic scattering employing a moment method. For a special choice of the moments, the quantum hydrodynamic equations are obtained. If a Fokker-Planck approach is taken for the inelastic collision operator, viscous corrections to the quantum hydrodynamic model are derived.

General quantum moment hydrodynamics. Introducing the hydrodynamic scaling $x' = \alpha x$, $t' = \alpha t$, where $0 < \alpha \ll 1$ measures the typical energy gain or loss during an electron-phonon collision, the Wigner-Boltzmann equation for (f_α, V_α) becomes (omitting the primes)

$$\alpha \partial_t f_\alpha + \alpha(p \cdot \nabla_x f_\alpha + \theta[V_\alpha] f_\alpha) = Q(f_\alpha), \quad (x, p, t) \in \mathbb{R}^{2d} \times (0, \infty), \tag{4.6}$$

together with an initial condition for f_α and the Poisson equation (4.2) for V_α. The collision operator is assumed to split into two parts:

$$Q(f_\alpha) = Q_0(f_\alpha) + \alpha Q_1(f_\alpha),$$

where the first (dominant) part models elastic collisions and the second part models inelastic scattering processes. The operator Q_0 is supposed to satisfy the following properties:

$$\text{(i) If } Q_0(f) = 0 \text{ then } f = M_f, \quad \text{(ii) } \langle Q_0(f)\kappa(p)\rangle = 0, \tag{4.7}$$

where M_f is the quantum Maxwellian introduced in section 4.1 and $\kappa(p)$ is a vector of some monomials $\kappa_i(p)$. If $\kappa(p) = (1, p, |p|^2/2)$, condition (ii) expresses the conservation of mass, momentum, and energy, which is meaningful for elastic collisions. An example fulfilling conditions (i) and (ii) is the BGK-type operator [18] $Q_0(f) = (M_f - f)/\tau$ with the relaxation time $\tau > 0$. An example of an inelastic collision operator Q_1 will be given in the subsection "Viscous quantum hydrodynamic equations" below.

In the following we proceed similarly as in [27]. The *moment equations* are obtained by multiplying (4.6) by $\kappa(p)/\alpha$, integrating over the momentum space, and using condition (ii):

$$\partial_t \langle \kappa(p) f_\alpha \rangle + \operatorname{div}_x \langle \kappa(p) p f_\alpha \rangle + \langle \kappa(p) \theta[V_\alpha] f_\alpha \rangle = \langle \kappa(p) Q_1(f_\alpha) \rangle.$$

The second integral on the left-hand side of the moment equations cannot be expressed in terms of the moments; this is called the *closure problem*. We can solve this problem by letting $\alpha \to 0$. Indeed, the formal limit $\alpha \to 0$ in (4.6) gives $Q_0(f) = 0$ where $f = \lim_{\alpha\to 0} f_\alpha$. Hence, by condition (i), $f = M_f$. Then the formal limit $\alpha \to 0$ in the above moment equations yields

$$\partial_t m + \mathrm{div}_x \langle \kappa(p) p M_f \rangle + \langle \kappa(p) \theta[V] M_f \rangle = \langle \kappa(p) Q_1(M_f) \rangle, \tag{4.8}$$

where $m = \langle \kappa(p) M_f \rangle$ are the moments (see (4.4)) and $V = \lim_{\alpha\to 0} V_\alpha$ solves (4.2) with $f = M_f$. The above equations have to be solved for $x \in \mathbb{R}^d$ and $t > 0$, and the initial condition becomes $m(\cdot, 0) = \langle \kappa(p) M_{f_I} \rangle$. In the classical case, Levermore [60] has shown that the moment equations are symmetrizable and hyperbolic. In the present situation, this concept of hyperbolicity cannot be used since (4.8) is not a partial differential equation but a differential equation with non-local operators of the type $\lambda \mapsto \langle \mathrm{Exp}\,(\lambda \cdot \kappa(p)) \rangle$.

The system (4.8) possesses the following (formal) property: If 1 and $\frac{1}{2}|p|^2$ are included in the set of monomials and if the inelastic collision operator conserves mass and dissipates energy, i.e. $\langle Q_1(f) \rangle = 0$ and $\langle \frac{1}{2}|p|^2 Q_1(f) \rangle \le 0$ for all functions f, the total energy

$$E(t) = \int_{\mathbb{R}^{2d}} \left(\left\langle \frac{1}{2}|p|^2 M_f \right\rangle + \frac{\lambda_L^2}{2} |\nabla_x V|^2 \right) dx dp$$

is nonincreasing. To see this, we notice that for all (regular) functions f,

$$\langle \theta[V] f \rangle = 0, \quad \langle p \theta[V] f \rangle = -\langle f \rangle \nabla_x V, \quad \langle \tfrac{1}{2}|p|^2 \theta[V] f \rangle = -\langle p f \rangle \cdot \nabla_x V. \tag{4.9}$$

From the moment equations

$$\partial_t \langle M_f \rangle + \mathrm{div}_x \langle p M_f \rangle = 0, \quad \partial_t \langle \tfrac{1}{2}|p|^2 M_f \rangle + \mathrm{div}_x \langle \tfrac{1}{2}|p|^2 p M_f \rangle \le \langle p M_f \rangle \cdot \nabla_x V$$

and the Poisson equation (4.2) we obtain formally

$$\begin{aligned} \frac{dE}{dt} &\le \int_{\mathbb{R}^d} (\langle p M_f \rangle \cdot \nabla_x V + \lambda_L^2 \nabla_x V \cdot \partial_t \nabla_x V) dx \\ &= \int_{\mathbb{R}^d} (\langle p M_f \rangle \cdot \nabla_x V - V \partial_t \langle M_f \rangle) dx \\ &= \int_{\mathbb{R}^d} (\langle p M_f \rangle \cdot \nabla_x V + V \mathrm{div}_x \langle p M_f \rangle) dx = 0, \end{aligned}$$

proving the monotonicity of the total energy.

In the following section we will specify the choice of the monomials, which enables us to give a more explicit expression of the system (4.8).

Quantum hydrodynamic equations. In classical fluiddynamics, the Euler equations are derived from the Boltzmann equation by using the monomials $\kappa(p) = (1, p, |p|^2/2)$ in the moment equations. In this subsection, we derive the quantum counterpart, the so-called *quantum hydrodynamic (QHD) equations* (see [27, 51]).

Let $\kappa(p) = (1, p, |p|^2/2)$. The moments $n := m_0$, $nu := m_1$, and $ne := m_2$ are called the *particle, current, and energy densities*, respectively. We also define the *velocity* $u = nu/n$ and the *energy* $e = ne/n$. In this situation, the quantum Maxwellian can be written as $M_f = \mathrm{Exp}\,(\lambda_0 + \lambda_1 \cdot p + \lambda_2|p|^2)$ or, equivalently, as

$$M_f(x,t) = \mathrm{Exp}\,\Big(A(x,t) - \frac{|p - w(x,t)|^2}{2T(x,t)}\Big), \tag{4.10}$$

where A, w, and T are defined in terms of λ_0, λ_1, and λ_2. In the following we will give a more explicit expression for the quantum moment equations (4.8).

Using (4.9) and observing that the second and third moments can be written as

$$\langle p \otimes p M_f\rangle = P + nu \otimes u, \quad \text{where } P = \langle (p-u)\otimes(p-u)M_f\rangle,$$
$$\langle \tfrac{1}{2}p|p|^2 M_f\rangle = S + (P + neI)u, \quad \text{where } S = \langle \tfrac{1}{2}(p-u)|p-u|^2 M_f\rangle,$$

the quantum moment equations (4.8) become

$$\partial_t n + \mathrm{div}(nu) = \langle Q_1(M_f)\rangle, \tag{4.11}$$
$$\partial_t(nu) + \mathrm{div}(nu\otimes u) + \mathrm{div}\,P - n\nabla V = \langle pQ_1(M_f)\rangle, \tag{4.12}$$
$$\partial_t(ne) + \mathrm{div}\big((P+neI)u\big) + \mathrm{div}\,S - nu\cdot\nabla V = \langle \tfrac{1}{2}|p|^2 Q_1(M_f)\rangle, \tag{4.13}$$

where $u\otimes u$ denotes the matrix with components $u_j u_k$, P is the stress tensor, S the (quantum) heat flux, and I is the identity matrix in $\mathbb{R}^{d\times d}$. The electric potential is given by (4.2) with $f = M_f$ or, in the above notation, by

$$\lambda_L^2 \mathit{\Delta} V = n - C(x). \tag{4.14}$$

The above system, which is solved for $x \in \mathbb{R}^d$ and $t > 0$ with initial conditions for $n(\cdot,0)$, $nu(\cdot,0)$, and $ne(\cdot,0)$, is called the *quantum hydrodynamic equations*. The quantum correction only appears in the terms P and S. We can derive an explicit expression in the $O(\varepsilon^4)$ approximation. For this, we need to expand the quantum Maxwellian M_f in terms of ε^2. As the computations are quite involved, we only sketch the expansion and refer to [51] for details.

The quantum exponential can be expanded in terms of ε^2 yielding $\mathrm{Exp}\, f = e^f - (\varepsilon^2/8)e^f B + O(\varepsilon^4)$, where B is a polynomial in the derivatives of f up to second order. This allows for an expansion of the moments

$$(n, nu, ne) = \int_{\mathbb{R}^d} \mathrm{Exp}\,\left(A - \frac{|p-w|^2}{2T}\right)\Big(1, p, \frac{1}{2}|p|^2\Big)dp,$$

of the stress tensor

$$\begin{aligned} P = nTI + \frac{\varepsilon^2}{12}n\Big\{\Big(\frac{d}{2}+1\Big)\nabla\log T\otimes\nabla\log T - \nabla\log T\otimes\nabla\log n \\ - \nabla\log n\otimes\nabla\log T - (\nabla\otimes\nabla)\log(nT^2) + \frac{R^\top R}{T}\Big\} \quad (4.15)\\ + \frac{\varepsilon^2}{12}T\mathrm{div}\Big(n\frac{\nabla\log T}{T}\Big)I + O(\varepsilon^4), \quad (4.16)\end{aligned}$$

and of the quantum heat flux

$$\begin{aligned} S = &-\frac{\varepsilon^2}{12}n\Big\{\Big(\frac{d}{2}+1\Big)R\nabla\log\Big(\frac{n}{T}\Big)+\Big(\frac{d}{2}+2\Big)\operatorname{div}R+\frac{3}{2}\Delta u\Big\} \\ &+\frac{\varepsilon^2}{12}\left(\frac{d}{2}+1\right)n\Big\{R\nabla\log\Big(\frac{n}{T^2}\Big)+\operatorname{div}R\Big\}+O(\varepsilon^4), \end{aligned} \tag{4.17}$$

where the matrix R with components $R_{ij} = \partial u_i/\partial x_j - \partial u_j/\partial x_i$ is the anti-symmetric part of the velocity gradient and $R^\top$ is the transpose of R. In the semi-classical case $\varepsilon = 0$ the stress tensor reduces to the classical expression $P = nTI$. The term S is purely quantum and vanishes if $\varepsilon = 0$. The energy density is the sum of the thermal, kinetic, and quantum energy,

$$\begin{aligned} ne = \frac{d}{2}nT+\frac{1}{2}n|u|^2-\frac{\varepsilon^2}{24}n\Big\{&\Delta\log n-\frac{1}{T}\operatorname{tr}(R^\top R)+\frac{d}{2}|\nabla\log T|^2-\Delta\log T \\ &-\nabla\log T\cdot\nabla\log n\Big\}+O(\varepsilon^4), \end{aligned} \tag{4.18}$$

where "tr" denotes the trace of a matrix.

A simplified quantum hydrodynamic model up to order $O(\varepsilon^4)$ can be obtained under the assumptions that the inelastic collision part vanishes, $Q_1 = 0$, that the temperature is slowly varying, $\nabla\log T = O(\varepsilon^2)$, and finally, that the vorticity is small, $R = O(\varepsilon^2)$:

$$\partial_t n + \operatorname{div}(nu) = 0, \tag{4.19}$$

$$\partial_t(nu)+\operatorname{div}(nu\otimes u)+\nabla(nT)-\frac{\varepsilon^2}{12}\operatorname{div}\big(n(\nabla\otimes\nabla)\log n\big)-n\nabla V = 0, \tag{4.20}$$

$$\partial_t(ne)+\operatorname{div}\big((P+neI)u\big)-\frac{\varepsilon^2}{8}\operatorname{div}(n\Delta u)-nu\cdot\nabla V = 0, \tag{4.21}$$

with the stress tensor and energy density, respectively,

$$P = nTI-\frac{\varepsilon^2}{12}n(\nabla\otimes\nabla)\log n, \quad ne = \frac{d}{2}nT+\frac{1}{2}n|u|^2-\frac{\varepsilon^2}{24}n\Delta\log n. \tag{4.22}$$

We notice that if we choose $\kappa(p) = (1, p)$, we obtain the *isothermal quantum hydrodynamic equations* (4.19)-(4.20) with constant temperature $T = 1$.

The system (4.19)-(4.21) corresponds to Gardner's QHD model except for the dispersive velocity term $(\varepsilon^2/8)\operatorname{div}(n\Delta u)$. The differences between our QHD equations and Gardner's model can be understood as follows. In both approaches, closure is obtained by assuming that the Wigner function f is in equilibrium. However, the notion of "equilibrium" is different. A quantum system, which is characterized by its energy operator $W^{-1}(h)$, with the Weyl quantization W^{-1} and the Hamiltonian $h(p) = |p|^2/2 + V(x)$, attains its minimum of the relative (von Neumann) entropy in the mixed state with Wigner function $f_Q = \operatorname{Exp}(-h/T_0)$. This state represents the *unconstrained* quantum equilibrium. The expansion of f_Q in terms of ε^2 was first given in [74],

$$f_Q(x,p) = \exp(-h(x,p)/T_0)(1+\varepsilon^2 f_2(x,p)) + O(\varepsilon^4)$$

with an appropriate function f_2. As a definition of the quantum equilibrium *with* moment constraints, Gardner employed this expansion of f_Q and modified it mimicking the moment-shift of the Gibbs state in the classical situation:

$$\widetilde{f}_Q(x,p) = n(x)\,\exp\Big(-\frac{h(x,p-u(x))}{T(x)}\Big)\big(1+\varepsilon^2 f_2(x,p-u(x))\big) + O(\varepsilon^4).$$

In contrast to the classical case, $\widetilde{f}_Q$ is *not* the constrained minimizer for the relative von Neumann entropy. On the other hand, the equilibrium state M_f used here is a genuine minimizer of the relative entropy with respect to the given moments. It has been shown in [51] that both approaches coincide if the temperature is constant and if only the particle density is prescribed as a constraint.

Equations (4.19)-(4.22) are of hyperbolic-dispersive type, and the presence of the nonlinear third-order differential operators in (4.20) and (4.21) makes the analysis of the system quite difficult. In particular, it is not clear if the electron density stays positive if it is positive initially. Since the total mass $\int n dx$ and the total energy,

$$\begin{aligned} E(t) = \int_{\mathbb{R}^d} \Big(&\frac{d}{2}nT + \frac{1}{2}n|u|^2 + \frac{\lambda^2}{2}|\nabla V|^2 + \frac{\varepsilon^2}{6}|\nabla\sqrt{n}|^2 + \frac{\varepsilon^2 d}{48}n|\nabla \log T|^2 \\ &+ \frac{\varepsilon^2}{24T}n\,\mathrm{tr}(R^\top R)\Big)dx, \end{aligned} \tag{4.23}$$

are conserved quantities of the quantum moment equations (4.11)-(4.18) (if $Q_1 = 0$) [51], this provides some Sobolev estimates. However, this estimate seems to be not strong enough to prove the existence of weak solutions to the system. Indeed, for a special model, a nonexistence result of weak solutions to the QHD equations has been proved [35]. This result is valid for the one-dimensional isothermal stationary equations, solved in a bounded interval with Dirichlet boundary conditions for the electron density and boundary conditions for the electric potential, the electric field, and the quantum Bohm potential at the left interval point. Moreover, the term Tn_x in (4.20) has been replaced by a more general pressure function $p(n)$ satisfying a growth condition.

The nonexistence result is valid for sufficiently large current densities. On the other hand, for "small" current densities fulfilling a subsonic condition related to classical fluiddynamics, some existence results for the stationary and transient equations have been achieved [42, 43, 45, 47].

The QHD equations contain two parameters: the (scaled) Planck constant ε and the Debye length λ_L. In special regimes of the physical parameters, these constants may be small compared to one, such that the semi-classical limit $\varepsilon \to 0$ or the quasi-neutral limit $\lambda_L \to 0$ may be of interest, leading to simpler models. In fact, the QHD equations reduce in the semi-classical limit to the

Euler equations. This limit has been proved in the one-dimensional isothermal steady state for sufficiently small current densities in [41] and for arbitrary large current densities (after adding an ultra-diffusive term in (4.20)) in [36]. The quasi-neutral limit in the isentropic QHD model has been performed in [62], showing that the current density consists, for small Debye length, of a divergence-free vector field connected with the incompressible Euler equations and a highly oscillating gradient vector coming from high electric fields.

The nonisothermal QHD equations have been first solved numerically by Gardner using a finite-difference upwind method, considering the third-order term as a perturbation of the classical Euler equations [37]. However, hyperbolic schemes have the disadvantage that the numerical diffusion may influence the numerical solution considerably [56]. This can be seen in Figure 4.2 (left). The figure shows the current-voltage characteristics of a one-dimensional resonant tunneling diode, computed from the QHD equations (4.19)-(4.21) without the dispersive velocity term but including heat conductivity and relaxation-time terms of Baccarani-Wordeman type. The tunneling diode consists of three regions: the high-doped contact regions and a low-doped channel region. In the channel, a double-potential barrier is included (see [51] for the physical and numerical details).

Due to the numerical viscosity introduced by the upwind method, the solution of Gardner's model strongly depends on the mesh size. On the other hand, the solution to the new QHD equations (4.19)-(4.21) presented in [51] is much less mesh depending (see Figure 4.2 right).

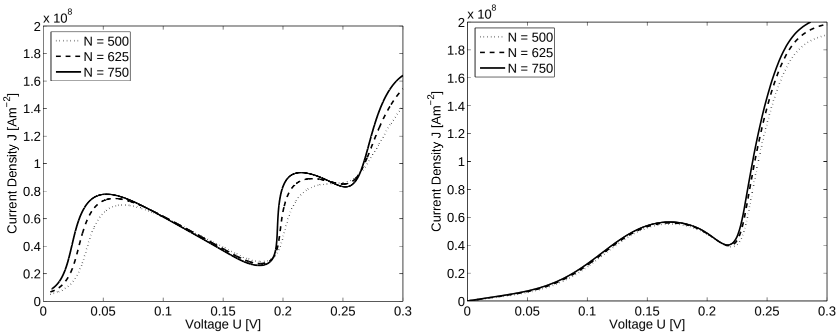

Fig. 4.2. Influence of the number of discretization points N on the current-voltage characteristics for Gardner's QHD equations (left) and for the new QHD model (right).

Notice that the main physical effect of a tunneling diode is that there exists a region in which the current density is decreasing although the voltage is increasing. This effect is called *negative differential resistance* and it is employed, for instance, to devise high-frequency oscillator devices.

The effect of the dispersive velocity term is a "smoothing" of the current-voltage curve. In order to study the influence of this term, we replace the factor $\varepsilon^2/8$ in (4.21) by $\delta^2/8$ and choose various values for δ. Clearly, only $\delta = \varepsilon$ corresponds to the physical situation. Figure 4.3 shows that the characteristics become "smoother" for larger values of δ.

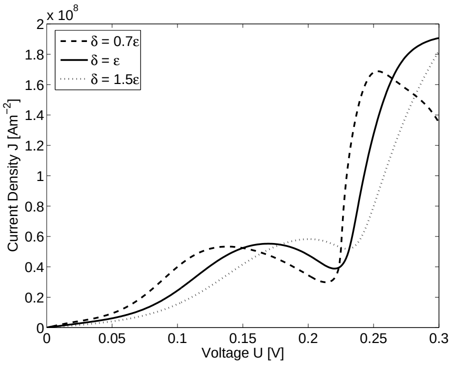

Fig. 4.3. Influence of the dispersive velocity term $(\delta^2/8)(nu_{xx})_x$ on the current-voltage curve.

Viscous quantum hydrodynamic equations. We model the inelastic collisions as electron interactions with a heat bath of oscillators in thermal equilibrium (which models the semiconductor crystal). Castella et al. [23] derived for such a situation the collision operator

$$Q_1(w) = \nu \Delta_x w + \nu_1 \Delta_p f + \nu_2 \mathrm{div}_x(\nabla_p f) + \frac{1}{\tau}\mathrm{div}_p(pf).$$

The parameters ν, ν_1, $\nu_2 \geq 0$ constitute the phase-space diffusion matrix, and $\tau > 0$ is a friction parameter, the relaxation time. If $\nu = 0$ and $\nu_2 = 0$, this gives the Caldeira-Leggett operator [20]. This model allows to incorporate inelastic scattering in the quantum hydrodynamic equations. Indeed, using the definition of the moments, we compute

$$\langle Q_1(M_f)\rangle = \nu \Delta_x n, \quad \langle p Q_1(M_f)\rangle = \nu \Delta_x(nu) - \nu_2 \nabla_x n - \frac{nu}{\tau},$$
$$\langle \tfrac{1}{2}|p|^2 Q_1(M_f)\rangle = \nu \Delta_x(ne) + d\nu_1 n - \nu_2 \mathrm{div}_x(nu) - \frac{2ne}{\tau}.$$

For simplicity, we suppose in the following that $\nu_1 = \nu_2 = 1/\tau = 0$. Assuming as in the previous section that the temperature gradients and the vorticity are of order ε^2, we obtain the *viscous quantum hydrodynamic equations*:

$$\partial_t n + \operatorname{div}(nu) = \nu \Delta n,$$
$$\partial_t(nu) + \operatorname{div}(nu \otimes u) + \nabla(nT) - \frac{\varepsilon^2}{12}\operatorname{div}\big(n(\nabla \otimes \nabla)\log n\big) - n\nabla V = \nu\Delta(nu),$$
$$\partial_t(ne) + \operatorname{div}\big((P + neI)u\big) - \frac{\varepsilon^2}{8}\operatorname{div}(n\Delta u) - nu \cdot \nabla V = \nu\Delta(ne),$$

where P and ne are defined in (4.22), and V is given by (4.14). Notice that ν is of the same order as ε^2 [40].

Due to the dissipative terms on the right-hand side of the above system, the total energy

$$E(t) = \int_{\mathbb{R}^d} \Big(\frac{d}{2}nT + \frac{1}{2}n|u|^2 + \frac{\lambda^2}{2}|\nabla V|^2 + \frac{\varepsilon^2}{6}|\nabla\sqrt{n}|^2\Big)dx$$

is no longer conserved but at least bounded:

$$\frac{dE}{dt} + \frac{\nu}{\lambda_L^2}\int_{\mathbb{R}^d} n(n - C)dx = 0.$$

However, it is not clear how to prove the existence of weak solutions or the positivity of the particle density from this equation.

A partial existence result, for sufficiently small current densities in the isothermal stationary model, is presented in [40]. The main idea is the observation that, in the one-dimensional steady state, we can integrate (4.24) yielding $nu - \nu n_x = J_0$ for some integration constant J_0 which we call the effective current density (since it satisfies $(J_0)_x = 0$). A computation now shows that

$$\Big(\frac{(nu)^2}{n}\Big)_x - \nu(nu)_{xx} = -\nu^2 n\big(n(\log n)_{xx}\big)_x + \Big(\frac{J_0^2}{n}\Big)_x + 2\nu J_0(\log n)_{xx}.$$

Hence, the coefficient of the quantum term becomes $\varepsilon^2/12+\nu^2$, and the viscosity term transforms to $2\nu J_0(\log n)_{xx}$. The smallness condition on the current density is needed in order to control the convective part $(J_0^2/n)_x$. Also in [40], the inviscid limit $\nu \to 0$ and the semi-classical limit $\varepsilon \to 0$ have been performed.

The isothermal viscous model has been numerically solved in [53, 56]. The viscosity ν has the effect to “smoothen” the current-voltage characteristics for a tunneling diode, as can be seen from Figure 4.4 (left). We refer to [53] for details of the employed parameters. The curves are computed from the *isothermal* model. Their behavior is unphysical due to the jump from a low-current to a high-current state. This effect can be explained by the constant temperature assumption. Indeed, in Figure 4.4 (right) a curve computed from the *nonisothermal* equations is presented. The characteristic shows the correct physical behavior but the viscosity leads to rather small peak-to-valley ratios (ratio of maximal to minimal current density).

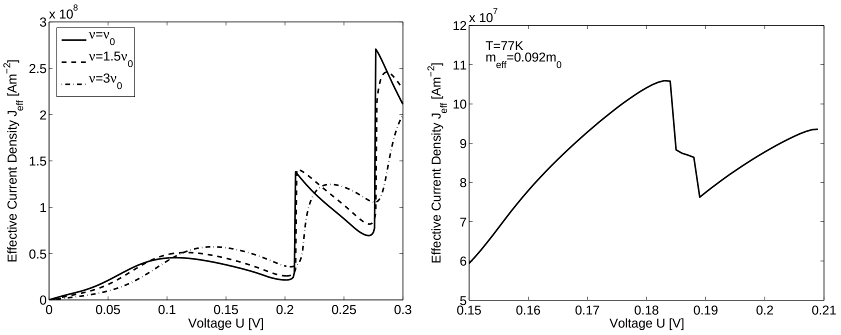

Fig. 4.4. Current voltage characteristics for a tunneling diode for the viscous QHD model. Left: isothermal case for various values of the viscosity; right: non-isothermal model.

4.3 Quantum moment diffusion models

In this section we derive quantum moment diffusion equations from a BGK-type Wigner equation using a Chapman-Enskog method. For special choices of the moments, the quantum energy-transport and the quantum drift-diffusion equations in the $O(\varepsilon^4)$ approximation are obtained.

General quantum moment diffusion equations. We consider the Wigner-Boltzmann equation (4.1) in the diffusion scaling $x' = \alpha x$, $t' = \alpha^2 t$, where $0 < \alpha \ll 1$ is as in the previous section (neglecting the primes):

$$\alpha^2 \partial_t f_\alpha + \alpha(p \cdot \nabla_x f_\alpha + \theta[V_\alpha] f_\alpha) = Q(f_\alpha), \quad (x,p,t) \in \mathbb{R}^{2d} \times (0,\infty). \tag{4.24}$$

Our aim is to perform a Chapman-Enskog expansion in the corresponding moment equations and to perform the formal limit $\alpha \to 0$. For this, we proceed similarly as in [26] using only monomials of even order, for instance $\kappa(p) = (1, \frac{1}{2}|p|^2, \ldots)$. Then the quantum Maxwellian M_f is the formal solution of the constrained minimization problem (4.3) with given moments $m_0(x,t), \ldots, m_N(x,t)$ with respect to the above set of monomials.

We assume that the collision operator can be written as

$$Q(f_\alpha) = Q_0(f_\alpha) + \alpha^2 Q_1(f_\alpha),$$

with $Q_0(f_\alpha)$ modeling the elastic scattering and $Q_1(f_\alpha)$ the inelastic scattering processes. In contrast to the previous section, we assume here that the elastic collisions are modeled by a BGK-type operator [18],

$$Q_0(f) = \frac{1}{\tau}(M_f - f),$$

where $\tau = \tau(x,t) > 0$ is the relaxation time. Then $Q_0(f)$ satisfies the properties (4.7). Concerning inelastic scattering, we suppose only that it preserves the mass, i.e. $\langle Q_1(f) \rangle = 0$ for all functions f.

Multiplying (4.24) by $\kappa(p)/\alpha$, integrating over the momentum space, and using condition (ii) in (4.7), we obtain the moment equations

$$\partial_t\langle\kappa(p)f_\alpha\rangle + \alpha^{-1}(\mathrm{div}_x\langle\kappa(p)pf_\alpha\rangle + \langle\kappa(p)\theta[V]f_\alpha\rangle) = \langle\kappa(p)Q_1(f_\alpha)\rangle.$$

In order to derive the diffusion models, we employ the Chapman-Enskog expansion $f_\alpha = M_{f_\alpha} + \alpha f_\alpha^1$, which defines f_α^1. The formal limit $\alpha \to 0$ in (4.24) gives $Q_0(f) = 0$, where $f = \lim_{\alpha\to 0} f_\alpha$ and hence $f = M_f$, by condition (i) in (4.7). Inserting the Chapman-Enkog expansion in the above moment equations, observing that the integrals $\langle\kappa(p)pM_{f_\alpha}\rangle$ and $\langle\kappa(p)\theta[V_\alpha]M_{f_\alpha}\rangle$ vanish, since $\kappa_i(p)$ is even in p, and performing the limit $\alpha \to 0$, we conclude that

$$\partial_t\langle\kappa(p)M_f\rangle + \mathrm{div}_x\langle\kappa(p)pf^1\rangle + \langle\kappa(p)\theta[V]f^1\rangle = \langle\kappa(p)Q_1(M_f)\rangle, \tag{4.25}$$

where $f^1 = \lim_{\alpha\to 0} f_\alpha^1$. It remains to determine the limit f^1. Since Q_0 is a BGK-type operator, it holds, using (4.24),

$$f_\alpha^1 = -\frac{\tau}{\alpha}Q_0(f_\alpha) = -\tau\big(\alpha\partial_t f_\alpha + p\cdot\nabla_x f_\alpha + \theta[V_\alpha]f_\alpha - \alpha Q_1(f_\alpha)\big),$$

which implies in the limit $\alpha \to 0$ that $f^1 = -\tau(p\cdot\nabla_x M_f + \theta[V]M_f)$. Inserting this expression for f^1 into (4.25) we obtain the general quantum diffusion equations

$$\begin{aligned}\partial_t m - \mathrm{div}\big(\tau\mathrm{div}\langle p\otimes p\kappa(p)M_f\rangle + \tau\langle\kappa(p)p\theta[V]M_f\rangle\big) + \langle\kappa(p)\theta[V]f^1\rangle \\ = \langle\kappa(p)Q_1(M_f)\rangle,\end{aligned} \tag{4.26}$$

where we recall that $m = \langle\kappa(p)M_f\rangle$. With the notation (4.5) we see that the expression

$$\begin{aligned}\mathrm{div}(\tau\mathrm{div}\langle p\otimes p\kappa_i(p)M_f\rangle) &= \sum_{j,k,\ell}\frac{\partial}{\partial x_j}\Big(\tau\big\langle p_jp_k\kappa_i\kappa_\ell\mathrm{Exp}\,(\lambda\cdot\kappa)\big\rangle\frac{\partial\lambda_\ell}{\partial x_k}\Big) \\ &=: \mathrm{div}(B:\nabla\lambda)\end{aligned}$$

can be interpreted as a diffusion term, and (4.26) can be formulated in a compact form as

$$A\partial_t\lambda - \mathrm{div}(B:\nabla\lambda) = g(\lambda),$$

where $A = \langle\kappa\otimes\kappa M_f\rangle$ and $g(\lambda)$ denotes the lower-order terms in λ. A more explicit expression can be derived in the cases $N = 1$ and $N = 0$ which will be discussed in the following subsections.

Quantum energy-transport equations. Let $N = 1$ and $\kappa(p) = (1, \frac{1}{2}|p|^2)$. For simplicity, we also assume that the relaxation time is constant, $\tau = 1$. Then we can simplify the quantum diffusion equations of the previous subsection. Indeed, employing the formulas (4.9) and

$$\langle\tfrac{1}{2}p|p|^2\theta[V]f\rangle = -(P + neI)\nabla V + \tfrac{\varepsilon^2}{8}n\nabla\Delta V \quad \text{for all functions } f,$$

we obtain from (4.26) the evolution equations for the particle density $m_0 = n$ and the energy density $m_2 = ne$ (see [26]):

$$\partial_t n - \operatorname{div} J_0 = 0, \quad \partial_t(ne) - \operatorname{div} J_2 - J_0 \cdot \nabla V = \langle \tfrac{1}{2}|p|^2 Q_1(f)\rangle, \tag{4.27}$$

$$J_0 = \operatorname{div} P - n\nabla V, \quad J_2 = \operatorname{div} U - (P + neI)\nabla V + \frac{\varepsilon^2}{8} n\nabla \Delta V, \tag{4.28}$$

where $P = \langle p \otimes p M_f\rangle$ is the stress tensor, $U = \langle \frac{1}{2}|p|^2 p \otimes p M_f\rangle$ is a fourth-order moment, and V is given by (4.14). The variables J_0 and J_2 are the particle and energy current densities, respectively. Noticing that the quantum Maxwellian can be written here as

$$M_f(x,t) = \operatorname{Exp}\left(A(x,t) - \frac{|p|^2}{2T(x,t)}\right),$$

one can show that the quantum fluid entropy

$$\eta(t) = \int_{\mathbb{R}^d} M_f(\operatorname{Log} M_f - 1)dxdp = \int_{\mathbb{R}^d} n(A - ne/T + 1)dx$$

is nonincreasing [26].

More explicit equations are obtained in the $O(\varepsilon^4)$ approximation. For this, we need to expand the terms P, U and the energy $ne = \int \frac{1}{2}|p|^2 \operatorname{Exp}(A - |p|^2/2T)dp$ in terms of ε^2. If $\nabla \log T = O(\varepsilon^2)$ and up to order $O(\varepsilon^4)$, some tedious computations lead to the expressions

$$P = nTI - \frac{\varepsilon^2}{12} n(\nabla \otimes \nabla)\log n, \quad ne = \frac{d}{2} nT - \frac{\varepsilon^2}{24} n\Delta \log n, \tag{4.29}$$

$$U = \frac{1}{2}(d+2)nT^2 I - \frac{\varepsilon^2}{24} nT(\Delta \log nI + (d+4)(\nabla \otimes \nabla)\log n),$$

Equations (4.27)-(4.28) with the above constitutive relations for P, U, and ne are called the *quantum energy-transport equations*. Notice that the expressions of P and U differ from those presented in [26]. We expect that this $O(\varepsilon^4)$ model possesses an entropic formulation similar to the classical energy-transport equations [24] but unfortunately, no entropic structure is currently known.

The quantum drift-diffusion equations. In this subsection we set $N = 0$ and choose $\kappa_0(p) = 1$. Then the quantum Maxwellian reads as $M_f(x,t) = \operatorname{Exp}(A(x,t) - |p|^2/2)$, and similar as in the previous subsection, we obtain

$$\partial_t n - \operatorname{div} J = 0, \quad J = \operatorname{div} P - n\nabla V,$$

where n and P are defined by

$$n = \int_{\mathbb{R}^d} \operatorname{Exp}\left(A - \frac{|p|^2}{2}\right)dp, \quad P = \int_{\mathbb{R}^d} p \otimes p \operatorname{Exp}\left(A - \frac{|p|^2}{2}\right)dp.$$

Again, the electric potential V is given selfconsistently by (4.14). Some analytical properties and numerical results for this nonlocal equation can be found in [34]. In the $O(\varepsilon^4)$ approximation, we can simplify the above model. Indeed, for $T = 1$, we obtain from (4.29) $\mathrm{div}P = \nabla n - \varepsilon^2 n\nabla(\Delta\sqrt{n}/6\sqrt{n}) + O(\varepsilon^4)$, and up to order $O(\varepsilon^4)$ the *quantum drift-diffusion equations*

$$\partial_t n + \frac{\varepsilon^2}{6}\mathrm{div}\Big(n\nabla\Big(\frac{\Delta\sqrt{n}}{\sqrt{n}}\Big)\Big) - \mathrm{div}(\nabla n - n\nabla V) = 0.$$

This fourth-order equation is of parabolic type which simplifies the analysis considerably, in particular compared to the third-order dispersive quantum hydrodynamic equations (4.19)-(4.21). Notice that the quantum term can be written as

$$\mathrm{div}\Big(n\nabla\Big(\frac{\Delta\sqrt{n}}{\sqrt{n}}\Big)\Big) = \frac{1}{2}\mathrm{div}\,\mathrm{div}\big(n(\nabla\otimes\nabla)\log n\big),$$

where $\nabla\otimes\nabla$ denotes the Hessian.

The quantum drift-diffusion equations can be also derived in the relaxation-time limit from the isothermal QHD model including relaxation terms. This limit has been made rigorous in [46], for solutions close to the equilibrium state.

The main mathematical difficulty is to prove the nonnegativity of the solutions. Since the equation is of fourth order, maximum principle arguments cannot be applied. The main idea of the existence analysis in the one-dimensional situation is the observation that the functional $\eta_0(t) = \int(n - \log n)dx$ is nonincreasing [54]. More precisely, if the equations are considered on a bounded interval such that $n = 1$ and $n_x = 0$ on the boundary,

$$\frac{d\eta_0}{dt} + \frac{\varepsilon^2}{12}\int_I(\log n)_{xx}^2 dx + \int_I(\log n)_x^2 dx + \frac{1}{\lambda_L^2}\int_I(n - C)\log n dx = 0.$$

By Poincaré's inequality, this provides an H^2 bound (if $C \in L^\infty(I)$) and hence an L^∞ bound for $w = \log n$, showing that $n = e^w$ is nonnegative (we loose positivity due to an approximation procedure). Applying a fixed-point argument, the existence of weak solutions has been proved in [54, 57]. The one-dimensional equations are by now well understood and the regularity, long-time behavior, and numerical approximation of nonnegative weak solutions have been studied [30, 50, 55, 57].

Unfortunately, the above idea does not apply in the multi-dimensional case since the functional $\int(n - \log n)dx$ seems not to be nonincreasing anymore. The new idea is to show that the entropy $\eta_1(t) = \int n(\log n - 1)dx$ is bounded,

$$\frac{d\eta_1}{dt} + \frac{\varepsilon^2}{12}\int_{\mathbb{R}^d} n|(\nabla\otimes\nabla)\log n|^2 dx + 4\int_{\mathbb{R}^d}|\nabla\sqrt{n}|^2 dx + \frac{1}{\lambda_L^2}\int_{\mathbb{R}^d}(n - C)n dx = 0,$$

where $\nabla\otimes\nabla$ denotes the Hessian. Since the entropy production integral can be estimated as

$$\int_{\mathbb{R}^d}|(\nabla\otimes\nabla)\sqrt{n}|^2 dx \le c\int_{\mathbb{R}^d} n|(\nabla\otimes\nabla)\log n|^2 dx,$$

for some constant $c > 0$ which depends on the space dimension d, this provides estimates for $\sqrt{n}$ in H^2 and shows that $n = (\sqrt{n})^2 \geq 0$. These estimates allow for a fixed-point argument (see [38, 50] for a proof in the case of vanishing second-order diffusion and vanishing electric fields).

Concerning the stationary equations, an existence analysis, even in several space dimensions, can be found in [17]. When neglecting the second-order diffusion (zero temperature case) and the electric field, we obtain the so-called *Derrida-Lebowitz-Speer-Spohn equation* [28], for which additional nonincreasing functionals have been found [49].

The current-voltage characteristics for a tunneling diode, computed from the one-dimensional quantum drift-diffusion equations, are shown in Figure 4.5 (left) with the lattice temperature $T = 300\,\mathrm{K}$. We see that the model is not capable to reproduce negative differential differential effects at room temperature. However, when using a smaller lattice temperature, negative differential resistance can be observed (Figure 4.5 right).

The quantum drift-diffusion model produces good numerical results when coupled to the Schrödinger-Poisson system employed in the channel region [31]. This can be seen from Figure 4.6 in which the coupled quantum drift-diffusion Schrödinger-Poisson model is compared with the Schrödinger-Poisson system and the coupled drift-diffusion Schrödinger-Poisson equations (see [31] for details).

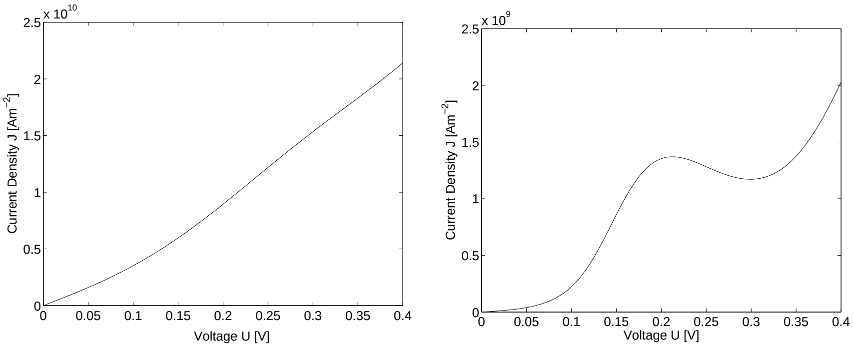

Fig. 4.5. Current voltage characteristics for a tunneling diode from the quantum drift-diffusion model for temperature $T = 300\,\mathrm{K}$ (left) and $T = 77\,\mathrm{K}$ (right).

Acknowlegdments. This work has been supported by the DFG Priority Program 1095 “Analysis, Modeling and Simulation of Multiscale Problems” under AR277/3, JU359/5. The second author has been partially supported by the DFG, grant JU359/3 (Gerhard-Hess Award). The first author thanks Maike Schulte for providing the plots of §2.

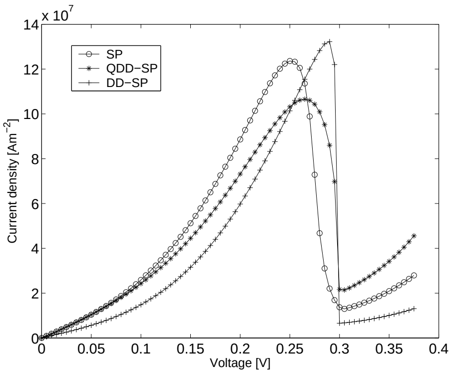

Fig. 4.6. Current voltage characteristics for a tunneling diode from the Schrödinger-Poisson system (SP), the coupled quantum drift-diffusion Schrödinger-Poisson model (QDD-SP), and the coupled drift-diffusion Schrödinger-Poisson model (DD-SP) for temperature $T = 300\,\mathrm{K}$.

References

1. M. Ancona and G. Iafrate. Quantum correction to the equation of state of an electron gas in a semiconductor. *Phys. Rev. B* 39 (1989), 9536-9540.
2. M. Ancona and H. Tiersten. Macroscopic physics of the silicon inversion layer. *Phys. Rev. B* 35 (1987), 7959-7965.
3. A. Arnold. Self-consistent relaxation-time models in quantum mechanics. *Comm. PDE* 21(3&4) (1995), 473–506.
4. A. Arnold. The relaxation-time von Neumann-Poisson equation. in: Proceedings of ICIAM 95, Hamburg (1995), Oskar Mahrenholtz, Reinhard Mennicken (eds.), *ZAMM* 76-S2 (1996), 293-296.
5. A. Arnold. Numerically absorbing boundary conditions for quantum evolution equations. *VLSI Design* 6 (1-4) (1998) 313-319.
6. A. Arnold, E. Dhamo, and C. Manzini. The Wigner-Poisson-Fokker-Planck system: global–in–time solution and dispersive effects, submitted (2005). Technical Report 10/04-N, Angewandte Mathematik, Universität Münster.
7. A. Arnold. Mathematical concepts of open quantum boundary conditions. *Transp. Theory Stat. Phys.* 30(4-6) (2001) 561-584.
8. A. Arnold, E. Dhamo, and C. Manzini. Dispersive effects in quantum kinetic equations, submitted (2005). Technical Report 07/05-N, Angewandte Mathematik, Universität Münster.
9. A. Arnold, M. Ehrhardt, I. Sofronov. Approximation, stability and fast calculation of non-local boundary conditions for the Schrödinger equation. *Commun. Mathematical Sciences* 1-3 (2003) 501-556.
10. A. Arnold, J.L. López, P.A. Markowich and J. Soler. An analysis of quantum Fokker-Planck models: A Wigner function approach. *Rev. Mat. Iberoam.* 20(3) (2004), 771–814.
11. A. Arnold, M. Schulte. Discrete transparent boundary conditions for the Schrödinger equatioon – a compact higher order scheme. in preparation 2006.

12. A. Arnold, C. Sparber. Conservative quantum dynamical semigroups for mean-field quantum diffusion models. *Comm. Math. Phys.* 251(1) (2004), 179–207.
13. A. Arnold, C. Ringhofer. Operator splitting methods applied to spectral discretizations of quantum transport equations. *SIAM J. of Num. Anal.* 32-6 (1995) 1876-1894.
14. N. Ben Abdallah and P. Degond. On a hierarchy of macroscopic models for semiconductors. *J. Math. Phys.* 37 (1996), 3308-3333.
15. N. Ben Abdallah, F. Méhats, O. Pinaud. On an open transient Schrödinger-Poisson system. *Math. Models Methods Appl. Sci.* 15-5 (2005), 667–688.
16. N. Ben Abdallah, O. Pinaud. Multiscale simulation of transport in an open quantum system: resonances and WKB interpolation. *J. Comput. Phys.* 213-1 (2006) 288–310.
17. N. Ben Abdallah and A. Unterreiter. On the stationary quantum drift-diffusion model. *Z. Angew. Math. Phys.* 49 (1998), 251-275.
18. P. Bhatnagar, E. Gross, and M. Krook. A model for collision processes in gases. I. Small amplitude processes in charged and neutral one-component systems. *Phys. Review* 94 (1954), 511-525.
19. F. Brezzi, P.A. Markowich. The three-dimensional Wigner-Poisson problem: existence, uniqueness and approximation. *Math. Methods Appl. Sci.* 14(1) (1991), 35–61.
20. A. Caldeira and A. Leggett. Path integral approach to quantum Brownian motion. *Phys. A* 121A (1983), 587-616.
21. J.A. Cañizo, J.L. López, J. Nieto. Global L^1-theory and regularity for the 3D nonlinear Wigner-Poisson-Fokker-Planck system. *J. Diff. Eq.* 198 (2004), 356–373.
22. F. Castella. The Vlasov-Poisson-Fokker-Planck System with Infinite Kinetic Energy. *Indiana Univ. Math. J.* 47(3) (1998), 939–964.
23. F. Castella, L. Erdös, F. Frommlet, and P. Markowich. Fokker-Planck equations as scaling limits of reversible quantum systems. *J. Stat. Phys.* 100 (2000), 543-601.
24. P. Degond, S. Génieys, and A. Jüngel. A system of parabolic equations in nonequilibrium thermodynamics including thermal and electrical effects. *J. Math. Pures Appl.* 76 (1997), 991-1015.
25. P. Degond, F. Méhats, and C. Ringhofer. Quantum hydrodynamic models derived from the entropy principle. *Contemp. Math.* 371 (2005), 107-131.
26. P. Degond, F. Méhats, and C. Ringhofer. Quantum energy-transport and drift-diffusion models. *J. Stat. Phys.* 118 (2005), 625-665.
27. P. Degond and C. Ringhofer. Quantum moment hydrodynamics and the entropy principle. *J. Stat. Phys.* 112 (2003), 587-628.
28. B. Derrida, J. L. Lebowitz, E. R. Speer, and H. Spohn. Fluctuations of a stationary nonequilibrium interface. *Phys. Rev. Lett.* 67 (1991), 165-168.
29. E. Dhamo, A. Arnold. An operator splitting method on the periodic Wigner-Poisson-Fokker-Planck system. in preparation, 2006.
30. J. Dolbeault, I. Gentil, and A. Jüngel. A nonlinear fourth-order parabolic equation and related logarithmic Sobolev inequalities. To appear in *Commun. Math. Sci.*, 2006.
31. A. El Ayyadi and A. Jüngel. Semiconductor simulations using a coupled quantum drift-diffusion Schrödinger-Poisson model. *SIAM J. Appl. Math.* 66 (2005), 554-572.

32. D. Ferry and J.-R. Zhou. Form of the quantum potential for use in hydrodynamic equations for semiconductor device modeling. *Phys. Rev. B* 48 (1993), 7944-7950.
33. W.R. Frensley. Wigner-function model of a resonant-tunneling semiconductor device *Phys. Rev. B* 36 (1987) 1570-1580.
34. S. Gallego and F. Méhats. Entropic discretization of a quantum drift-diffusion model. *SIAM J. Numer. Anal.* 43 (2005), 1828-1849.
35. I. Gamba and A. Jüngel. Positive solutions of singular equations of second and third order for quantum fluids. *Arch. Rat. Mech. Anal.* 156 (2001), 183-203.
36. I. Gamba and A. Jüngel. Asymptotic limits in quantum trajectory models. *Commun. Part. Diff. Eqs.* 27 (2002), 669-691.
37. C. Gardner. The quantum hydrodynamic model for semiconductor devices. *SIAM J. Appl. Math.* 54 (1994), 409-427.
38. U. Gianazza, G. Savaré, and G. Toscani. A fourth-order nonlinear PDE as gradient flow of the Fisher information in Wasserstein spaces. In preparation, 2006.
39. H.L. Gruvin, T.R. Govindan, J.P. Kreskovsky, M.A. Stroscio. Transport via the Liouville equation and moments of quantum distribution functions, *Solid State Electr.* 36 (1993), 1697–1709.
40. M. Gualdani and A. Jüngel. Analysis of the viscous quantum hydrodynamic equations for semiconductors. *Europ. J. Appl. Math.* 15 (2004), 577-595.
41. M. T. Gyi and A. Jüngel. A quantum regularization of the one-dimensional hydrodynamic model for semiconductors. *Adv. Diff. Eqs.* 5 (2000), 773-800.
42. F. Huang, H.-L. Li, A. Matsumura, and S. Odanaka. Well-posedness and stability of multi-dimensional quantum hydrodynamics in whole space. Preprint, Osaka University, Japan, 2004.
43. A. Jüngel. A steady-state quantum Euler-Poisson system for semiconductors. *Commun. Math. Phys.* 194 (1998), 463-479.
44. A. Jüngel. *Quasi-hydrodynamic Semiconductor Equations.* Birkhäuser, Basel, 2001.
45. A. Jüngel and H.-L. Li. Quantum Euler-Poisson systems: global existence and exponential decay. *Quart. Appl. Math.* 62 (2004), 569-600.
46. A. Jüngel, H.-L. Li, and A. Matsumura. The relaxation-time limit in the quantum hydrodynamic equations for semiconductors. To appear in *J. Diff. Eqs.*, 2006.
47. A. Jüngel, M. C. Mariani and D. Rial. Local existence of solutions to the transient quantum hydrodynamic equations. *Math. Models Meth. Appl. Sci.* 12 (2002), 485-495.
48. A. Jüngel and D. Matthes. A derivation of the isothermal quantum hydrodynamic equations using entropy minimization. *Z. Angew. Math. Mech.* 85 (2005), 806-814.
49. A. Jüngel and D. Matthes. An algorithmic construction of entropies in higher-order nonlinear PDEs. *Nonlinearity* 19 (2006), 633-659.
50. A. Jüngel and D. Matthes. The multi-dimensional Derrida-Lebowitz-Speer-Spohn equation. In preparation, 2006.
51. A. Jüngel, D. Matthes, and J.-P. Milišić. Derivation of new quantum hydrodynamic equations using entropy minimization. Preprint, Universität Mainz, 2005.
52. A. Jüngel and J.-P. Milišić. Macroscopic quantum models with and without collisions. To appear in *Proceedings of the Sixth International Workshop on*

Mathematical Aspects of Fluid and Plasma Dynamics, Kyoto, Japan. *Transp. Theory Stat. Phys.*, 2006.

53. A. Jüngel and J.-P. Milišić. Numerical approximation of the nonisothermal quantum hydrodynamic equations for semiconductors with viscous terms. In preparation, 2006.
54. A. Jüngel and R. Pinnau. Global non-negative solutions of a nonlinear fourth-oder parabolic equation for quantum systems. *SIAM J. Math. Anal.* 32 (2000), 760-777.
55. A. Jüngel and R. Pinnau. A positivity-preserving numerical scheme for a nonlinear fourth-order parabolic equation. *SIAM J. Num. Anal.* 39 (2001), 385-406.
56. A. Jüngel and S. Tang. Numerical approximation of the viscous quantum hydrodynamic model for semiconductors. To appear in *Appl. Numer. Math.*, 2006.
57. A. Jüngel and I. Violet. The quasineutral limit in the quantum drift-diffusion equations. Preprint, Universität Mainz, Germany, 2005.
58. N. Kluksdahl, A. M. Kriman, D. K. Ferry, and C. Ringhofer. Self–consistent study of the resonant tunneling diode. *Phys. Rev. B* 39 (1989), 7720–7735.
59. H. Kosina, M. Nedjalkov. Wigner function-based device modeling. in: *Handbook of Theoretical and Computational Nanotechnology* vol. 10 (eds: M. Rieth, W. Schommers), American Scientific Publishers, 2006
60. C. Levermore. Moment closure hierarchies for kinetic theories. *J. Stat. Phys.* 83 (1996), 1021-1065.
61. I.B. Levinson. Translational invariance in uniform fields and the equation for the density matrix in the Wigner representation. *Sov. Phys. JETP* 30 (1970) 362-367.
62. H.-L. Li and C.-K. Lin. Zero Debye length asymptotic of the quantum hydrodynamic model for semiconductors. *Commun. Math. Phys.* 256 (2005), 195-212.
63. G. Lindblad. On the generators of quantum mechanical semigroups. *Comm. Math. Phys.* 48 (1976), 119-130.
64. P.L. Lions. T. Paul. Sur les mesures de Wigner. *Rev. Math. Iberoam.*, 9(3) (1993), 553–561.
65. E. Madelung. Quantentheorie in hydrodynamischer Form. *Z. Physik* 40 (1927), 322-326.
66. P. Markowich, C. Ringhofer, and C. Schmeiser. *Semiconductor Equations.* Springer, Vienna, 1990.
67. D.A. Rodrigues, A.D. Armour. Quantum master equation descriptions of a nanomechanical resonator coupled to a single-electron transistor. *New J. Phys.* 7 (2005) 251-272.
68. B. Perthame. Time decay, propagation of low moments and dispersive effects for kinetic equations. *Comm. P.D.E.* 21(1&2) (1996), 659–686.
69. L. Ramdas Ram-Mohan. *Finite element and boundary emelent applications in quantum mechanics.* Oxford Univ. Press, 2002.
70. C. Ringhofer. A spectral method for the numerical simulation of quantum tunneling phenomena *SIAM J. Num. Anal.* 27 (1990) 32-50.
71. H. Risken. *The Fokker-Planck equation.* Springer, 1984.
72. C. Sparber, J.A. Carrillo, J. Dolbeault, P.A. Markowich. On the long time behavior of the quantum Fokker-Planck equation. *Monatsh. f. Math.* 141(3) (2004), 237–257.
73. M.A. Stroscio. Moment-equation representation of the dissipative quantum Liouville equation. *Superlattices and microstructures* 2 (1986), 83–87.

74. E. Wigner. On the quantum correction for thermodynamic equilibrium. *Phys. Rev.* 40 (1932), 749-759.
75. A. Zisowsky, A. Arnold, M. Ehrhardt, T. Koprucki. Discrete Transparent Boundary Conditions for transient kp-Schrödinger Equations with Application to Quantum-Heterostructures. *ZAMM 85* 11 (2005) 793-805.