

Kinetic and Macroscopic Equations for Semiconductors

Univ.-Prof. Dr. Ansgar Jüngel
Vienna University of Technology

Winter term 2012

*Lectures Notes for a lecture series
at the Technical University of Munich*

August 13, 2012

Contents

1	Introduction	3
2	Basic Semiconductor Physics	6
2.1	Semiconductor Crystals	7
2.2	The Schrödinger Equation	8
2.3	Electrons in a Periodic Potential	11
2.4	The Semi-Classical Picture	17
2.5	Semiconductor Statistics	21
3	Kinetic Transport Equations	28
3.1	Semi-Classical Liouville Equation	29
3.2	Semi-Classical Vlasov Equation	30
3.3	Semi-Classical Boltzmann Equation	33
3.4	Properties of the Collision Operators	38
4	Drift-Diffusion Equations	42
4.1	Scaling of the Boltzmann-Poisson system	42
4.2	Properties of the Low-Density Collision Operator	44
4.3	Derivation of the Drift-Diffusion Equations	48
4.4	Bipolar Model	50
4.5	Thermal Equilibrium State and Boundary Conditions	51

5	Hydrodynamic Equations	53
5.1	Derivation of the Hydrodynamic Equations	55
5.2	Calculation of the Collision Integrals	57
5.3	Relaxation-Time Limits	58
6	Microscopic quantum models	61
6.1	Mixed States and Density Matrix Formulation	61
6.2	Quantum Liouville Equation	64
6.3	Quantum Vlasov Equation	67
6.4	Wigner-Boltzmann Equation	69
7	Quantum Hydrodynamic Equations	71
7.1	Zero-Temperature Quantum Hydrodynamic Equations	72
7.2	Mixed-State Schrödinger Models and Quantum Hydrodynamics	75
7.3	Quantum Maxwellians	78
7.4	Wigner-Boltzmann Equations and Quantum Hydrodynamics	81

Preface

These lecture notes are based on the book by A. Jüngel “Transport Equations for Semiconductors”, Springer, 2009. In order to adapt the contents of the book to the lecture series of 30 hours, the material has been simplified and key ideas only are presented. Furthermore, we focus on some kinetic models and semi-classical equations. For more information, we refer to the above mentioned book and the semiconductor literature.

The main objective of the lecture notes is the derivation of transport equations describing the electron flow through a semiconductor device due to the application of a voltage. Depending on the device structure, the main transport phenomena may be very different, caused by diffusion, drift, scattering, or quantum-mechanical effects. The choice of the model equations depends on certain key parameters, such as the number of free electrons in the device, the mean free path of the charge carriers (i.e. the average distance between two consecutive collisions for a particle), the device dimension, and the ambient temperature.

Usually, a large number of electrons is flowing through a device such that a particle-like description using kinetic or fluid-type equations seems to be appropriate. On the other hand, electrons in a semiconductor crystal are quantum mechanical objects such that a wave-like description using the Schrödinger equation or the density-matrix formalism are necessary. For this reason, we have to devise different models which are able to describe the important physical phenomena for a particular situation or for a particular device. Moreover, since in some cases we are not interested in all the available physical information, we need simpler models which help to reduce the computation costs in the numerical simulations.

The derivations of the model equations are purely formal, although in several instances some mathematical properties are needed. It turned out to be convenient to summarize the results in form of lemmas, propositions, and theorems. However, a “proof” of a lemma, proposition, or theorem is not a proof in the strict mathematical sense, since the underlying function spaces and regularity assumptions are generally not specified. In many cases, a rigorous proof is even not available in the literature. Thus, the presentation mainly follows the rules of Mathematical Modeling.

1 Introduction

A semiconductor is a solid material whose electric conductivity is much larger than that of insulators but much smaller than that of metals, measured at room temperature. A more precise definition is that a semiconductor is a crystal with an energy gap of a few electron volt. Metals do not have an energy gap and the energy gap of insulators is larger than a few electron volt. In Section 2 we give a more precise meaning of the notion “energy band” for which some basic facts of semiconductor physics will be necessary.

As a preparation, we analyze the classical motion of one particle (electron) with mass m moving in a vacuum under the action of a force. The particle is described as a classical

particle, i.e., we associate the position vector $x \in \mathbb{R}^3$ and the velocity vector $v \in \mathbb{R}^3$ with the particle. Quantum mechanical effects are incorporated later in such a way that we obtain a semi-classical description of the electron in a semiconductor. The trajectory $(x(t), v(t))$ of the particle satisfies Newton's laws in the six-dimensional position-velocity phase space

$$\dot{x} = v, \quad m\dot{v} = F, \quad t > 0, \quad (1)$$

with initial conditions

$$x(0) = x_0, \quad v(0) = v_0, \quad (2)$$

where the dot denotes differentiation with respect to time, and F is a force. It can, for instance, be given by an electric field acting on the particle,

$$F = q\nabla V(x, t),$$

where $V(x, t)$ is the electric potential and q the charge of the particle. We assume that the force is independent of the velocity.

In semiconductors, the number of electrons M is typically very large (at least $M > 10^4$) and therefore, the numerical solution of (1)-(2) for each particle is very expensive. Since we are rather interested in the behavior of the particle *ensemble* instead of the behavior of the *individual* electrons, it seems reasonable to use a statistical description. Then we are not prescribing the initial condition (2) but the probability density $f_I(x, v)$ of the initial position and velocity of the particle. The integral

$$\int_{\Omega} f_I(x, v) dx dv$$

represents the probability to find the particle at time $t = 0$ in the subset Ω of the (x, v) -space.

Let $f(x, v, t)$ be the *probability density* or *distribution function* of the particle at time t (particle ensembles are considered in Section 4). We wish to derive an evolution equation for f . It is reasonable to assume that the distribution function is constant along the trajectory $(x(t), v(t))$:

$$f(x(t), v(t), t) = f_I(x_0, v_0), \quad t > 0,$$

since the probability to find the particle does not change along its trajectory. In fact, this condition can be derived from the so-called Liouville theorem (see [31, Section 3.1]). Differentiating this equation with respect to t gives the differential equation

$$0 = \frac{d}{dt} f(x(t), v(t), t) = \partial_t f + \dot{x} \cdot \nabla_x f + \dot{v} \cdot \nabla_v f,$$

and employing Newton's laws (1) leads to the *Liouville equation*

$$\partial_t f + v \cdot \nabla_x f + \frac{q}{m} \nabla_x V \cdot \nabla_v f = 0, \quad (x, v) \in \mathbb{R}^6, \quad t > 0. \quad (3)$$

It is supplemented with the initial condition

$$f(x, v, 0) = f_I(x, v), \quad (x, v) \in \mathbb{R}^6.$$

The Liouville equation provides a mesoscopic description of the motion of the particle.

The distribution function contains much more information than needed. Usually, only macroscopic quantities like the particle, current, and energy densities are of interest since these quantities can be measured. Therefore, we aim at deriving transport equations for these variables starting from the Liouville equation. For this, we define the particle density $n(x, t)$ and the current density $J_n(x, t)$ by

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

These integrals are also called the zeroth-order and first-order *moments*. Integrating the Liouville equation over $v \in \mathbb{R}^3$ yields

$$0 = \partial_t \int_{\mathbb{R}^3} f dv + \operatorname{div}_x \int_{\mathbb{R}^3} f v dv + \frac{q}{m} \nabla_x V \cdot \int_{\mathbb{R}^3} \nabla_v f dv = \partial_t n + \operatorname{div}_x J_n. \quad (4)$$

This equation describes the mass conservation. Indeed, integrating this equation over \mathbb{R}^3 , we find that

$$\frac{d}{dt} \int_{\mathbb{R}^3} n(x, t) dx = 0.$$

Next, multiplying (3) by v , integrating over $v \in \mathbb{R}^3$, and integrating by parts in the last term gives

$$\begin{aligned} 0 &= \partial_t \int_{\mathbb{R}^3} f v dv + \operatorname{div}_x \int_{\mathbb{R}^3} f v \otimes v dv - \frac{q}{m} \nabla_x V \cdot \int_{\mathbb{R}^3} f \nabla_v v dv \\ &= \partial_t J_n + \operatorname{div}_x \int_{\mathbb{R}^3} f v \otimes v dv - \frac{q}{m} n \nabla_x V, \end{aligned} \quad (5)$$

since $\nabla_v v$ equals the unit matrix. This equation describes the evolution of the current density, depending on the convective term $\int_{\mathbb{R}^3} f v \otimes v dv$ and the drift term $-(q/m)n\nabla_x V$. The problem is that we cannot easily express the convective term (which can be interpreted as a second-order moment) by means of the zeroth- and first-order moments n and J_n . This is called the *closure problem* since the above equations cannot be written in closed form. In these lecture notes, we show how we can eliminate this problem on a formal level. Under certain assumptions, the current density can be expressed as

$$J_n = -(\nabla_x n - n \nabla_x V).$$

Inserting this equation into (4) (and dropping the index x), we obtain the so-called *drift-diffusion equation*

$$\partial_t n - \operatorname{div}(\nabla n - n \nabla V) = 0.$$

The electric potential may be a given function or it is defined self-consistently by the Poisson equation

$$\lambda_D^2 \Delta V = n,$$

where $\lambda_D > 0$ is a constant (it contains the permittivity of the semiconductor material; see Section 2). In the latter case, the above system of equations is nonlinear since $n\nabla V$ is a “quadratic” term. Mathematically, the drift-diffusion equation for the electron density is of parabolic type and the equation for the potential is of elliptic type. We do not investigate conditions under which there exists a solution to the corresponding initial-boundary-value problems, but we remark that such a theory exists (see, e.g., [39]).

The drift-diffusion equations (together with the Poisson equation) is the most simplest semiconductor model. It is valid for semiconductors of a size of at least one micrometer, close to thermal equilibrium (small current densities, constant temperature), and for small applied voltages. In spite of its simplicity, it is very popular in industrial simulation codes. For smaller semiconductor devices, often correction terms are included in these codes.

A more complex model is given by the system (4)-(5), assuming that the second-order moment equals $\int_{\mathbb{R}^3} f v \otimes v dv = \text{div}(J_n \otimes J_n/n) + \nabla n$ (this will be made precise in Section 5):

$$\partial_t n + \text{div} J_n = 0, \quad \partial_t J_n + \text{div} \left(\frac{J_n \otimes J_n}{n} \right) + \nabla n - n \nabla V = 0.$$

These equations represent the Euler or hydrodynamic equations known in gas dynamics. There, $\text{div}(J_n \otimes J_n/n)$ is the convection, $\nabla p(n) = \nabla n$ is the derivative of the pressure $p(n) = n$, and $-n\nabla V$ is a force term.

Summarizing, we have already motivated three semiconductor models with increasing complexity:

- drift-diffusion equations for the zeroth-order moment (electron density);
- hydrodynamic equations for the first two moments (electron and current density);
- Liouville equation for the distribution function.

In these lecture notes, we will make precise the assumptions under which these models can be derived. In particular, we explain how the quantum mechanical nature of the electrons can be incorporated in the macroscopic equations.

2 Basic Semiconductor Physics

In this section, we present a short summary of the physics and main properties of semiconductors. We refer to, e.g., [1, 6, 11, 18, 27, 33, 36, 44, 46, 49] for introductory and more advanced textbooks of solid-state and semiconductor physics.

2.1 Semiconductor Crystals

In order to define a semiconductor using the notion of energy gap, we review some facts about the crystal structure of solids.

An ideal solid is made of an infinite three-dimensional array of atoms arranged in a lattice

$$L = \{n_1 a_1 + n_2 a_2 + n_3 a_3 : n_1, n_2, n_3 \in \mathbb{Z}\} \subset \mathbb{R}^3,$$

where $a_1, a_2, a_3 \in \mathbb{R}^3$ are the basis vectors of L , called *primitive vectors* of the lattice. The set L is called the *Bravais lattice*. The periodic structure of the lattice is specified in the following definitions [11, 39]:

1. The *reciprocal lattice* (or dual lattice) L^* of L is defined by

$$L^* = \{n_1 a_1^* + n_2 a_2^* + n_3 a_3^* : n_1, n_2, n_3 \in \mathbb{Z}\} \subset \mathbb{R}^3,$$

where the *primitive vectors* $a_1^*, a_2^*, a_3^* \in \mathbb{R}^3$ are the dual basis, satisfying

$$a_m \cdot a_n^* = 2\pi \delta_{mn} \quad \text{for all } m, n = 1, 2, 3. \quad (6)$$

2. A connected set $D \subset \mathbb{R}^3$ is called a *primitive cell* of L (or L^*) if the volume of D equals the volume of the parallelepiped spanned by the basis vectors of L (or L^*),

$$\text{vol}(D) = a_1 \cdot (a_2 \times a_3) \quad (\text{or } \text{vol}(D) = a_1^* \cdot (a_2^* \times a_3^*)),$$

and if the whole space \mathbb{R}^3 is covered by the union of translates of D by the primitive vectors. Here, the symbol “ \times ” denotes the vector product in \mathbb{R}^3 .

3. The special primitive cell D which consists of all points being closer to the origin than to any other point of the lattice, is called the *Wigner-Seitz cell*.
4. The Wigner-Seitz cell of the reciprocal lattice is called the (first) *Brillouin zone* (see Figure 1 for a two-dimensional example).

We give some explanations of the above definitions. What is the meaning of the reciprocal lattice? The reciprocal lattice vectors and the direct lattice vectors can be seen as conjugate variables, like time and frequency are conjugate variables in signal analysis. In fact, let $x \in L$ and $k \in L^*$ be given by

$$x = \sum_{m=1}^3 \alpha_m a_m \quad \text{and} \quad k = \sum_{n=1}^3 \beta_n a_n^*,$$

where $\alpha_m, \beta_n \in \mathbb{Z}$. Then, by (6),

$$e^{ik \cdot x} = \exp\left(i \sum_{m,n=1}^3 2\pi \delta_{mn} \alpha_m \beta_n\right) = \exp\left(2\pi i \sum_{m=1}^3 \alpha_m \beta_m\right) = 1. \quad (7)$$

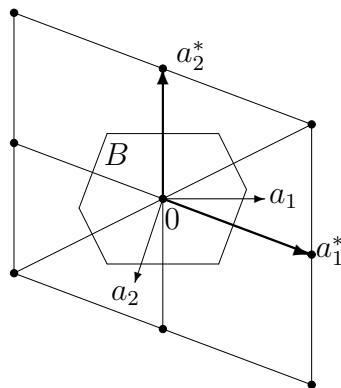


Figure 1: The primitive vectors of a two-dimensional lattice L and its reciprocal lattice L^* and the Brillouin zone B .

As the position vector x has the dimension of length, k has the dimension of inverse length and therefore, k is called a wave vector. (More precisely, k is called a *pseudo-wave vector*; see below.)

Physically, the reciprocal lattice appears in X-ray diffraction experiments with crystals. It can be shown that the intensity peaks of the reflected X-rays are obtained when the change in the wave vector Δk of the X-ray wave is an element of the reciprocal lattice [11, p. 404]. This allows one to determine the structure of the crystal lattice.

The primitive vectors a_ℓ^* of the Brillouin zone in \mathbb{R}^3 can be computed from the vectors a_m by

$$a_\ell^* = 2\pi \frac{a_m \times a_n}{a_1 \cdot (a_2 \times a_3)},$$

where (ℓ, m, n) is either $(1, 2, 3)$, $(2, 3, 1)$, or $(3, 1, 2)$. Graphically, the Brillouin zone can be constructed as follows. Draw arrows from a lattice point of L^* to its nearest neighbors and determine the mid points of the arrows. Then the planes through these points perpendicular to the arrows form the surface of the (bounded) Brillouin zone. In two space dimensions, the Brillouin zone is a hexagon or a square (see Figure 1). In three space dimensions, the zone is a polyhedron (e.g., a “capped” octahedron; see Figure 2).

2.2 The Schrödinger Equation

A semiconductor crystal consists of the nuclei, the core electrons, and the valence electrons. Their state has to be described by quantum mechanics. More precisely, the state of a quantum particle is represented by a complex-valued wave function $\phi(x, t)$, where $x \in \mathbb{R}^3$ and $t \in \mathbb{R}$. The dynamics of the wave function is given by the *Schrödinger equation*

$$i\hbar\partial_t\phi = H\phi, \quad x \in \mathbb{R}^3, \quad t > 0, \quad \phi(\cdot, 0) = \phi_I, \quad (8)$$

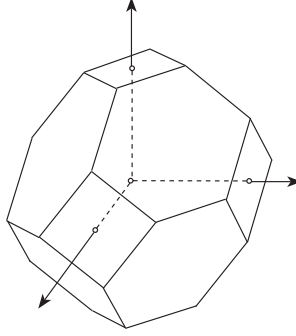


Figure 2: Brillouin zone of semiconductors like silicon, germanium, gallium arsenide etc.

where $\partial_t = \partial/\partial t$ and H is the so-called *Hamilton operator*. For instance, the Hamilton operator of a single electron with mass m moving in an electric potential $V(x)$ reads as

$$H = -\frac{\hbar^2}{2m}\Delta - qV(x), \quad x \in \mathbb{R}^3, \quad (9)$$

where $\Delta = \sum_{j=1}^3 \partial^2/\partial x_j^2$ is the Laplace operator in \mathbb{R}^3 .

Stationary states can be obtained from the ansatz $\phi(x, t) = e^{-iEt/\hbar}\psi(x)$, where E is a real number. Inserting this ansatz into (8) and dividing by $e^{-iEt/\hbar}$ gives the *stationary Schrödinger equation*

$$H\psi = E\psi \quad (10)$$

or, in the case of a single electron,

$$-\frac{\hbar^2}{2m}\Delta\psi - qV(x)\psi = E\psi, \quad x \in \mathbb{R}^3.$$

Thus, the quantum state is stationary if ψ is an eigenfunction and E is an eigenvalue of H . Physically, E describes the energy of the system if it is in the eigenstate ψ . The set of all possible energy values is represented by the spectrum of the Hamiltonian H (consisting not necessarily of eigenvalues only).

The solution ϕ of (8) with the Hamiltonian (9) can be interpreted as follows. We take the derivative

$$\begin{aligned} \partial_t|\phi|^2 &= (\partial_t\bar{\phi})\phi + \bar{\phi}(\partial_t\phi) = -\frac{i\hbar}{2m}\Delta\bar{\phi}\phi + \frac{i\hbar}{2m}\bar{\phi}\Delta\phi \\ &= -\frac{i\hbar}{2m}\operatorname{div}(\nabla\bar{\phi}\phi - \bar{\phi}\nabla\phi) = -\frac{\hbar}{m}\operatorname{div}\operatorname{Im}(\bar{\phi}\nabla\phi), \end{aligned}$$

where \bar{z} denotes the conjugate of the complex number $z \in \mathbb{C}$, $\operatorname{Im}(z)$ its imaginary part, and $\operatorname{div} u = \sum_{j=1}^3 \partial u_j/\partial x_j$ is the divergence of a vector field $u = (u_1, u_2, u_3)$. Introducing the variables

$$n = |\phi|^2, \quad J = -\frac{q\hbar}{m}\operatorname{Im}(\bar{\phi}\nabla\phi),$$

we arrive at the conservation law

$$\partial_t n - \frac{1}{q} \operatorname{div} J = 0,$$

expressing the conservation of the integral $\int_{\mathbb{R}^3} n \, dx$. According to the pioneering works of Einstein, Planck etc., we may interpret n as the *electron density* and J as the *electron current density*. The integral $\int_{\Omega} |\phi(x, t)|^2 \, dx$ is the probability to find the electron at time t in the domain Ω .

We illustrate the stationary Schrödinger equation and its solutions by two simple examples.

Example 2.1 (State of a free electron). Consider a free electron in a one-dimensional vacuum, i.e. $V(x) = 0$ for all $x \in \mathbb{R}$. We need to solve the Schrödinger equation

$$-\frac{\hbar^2}{2m} \psi'' = E\psi \quad \text{in } \mathbb{R}. \quad (11)$$

A computation shows that eigenfunctions are given by

$$\psi_k(x) = Ae^{ikx} + Be^{-ikx}, \quad x \in \mathbb{R},$$

where $k^2 = 2mE/\hbar^2$, with eigenvalues

$$E = E(k) = \frac{\hbar^2 k^2}{2m}, \quad k \in \mathbb{R}.$$

Thus, the eigenvalue problem (11) has infinitely many bounded solutions parametrized by $k \in \mathbb{R}$ and corresponding to different real-valued energies $E(k)$. The functions $e^{\pm ikx}$ are called *plane waves*. Thus, the eigenstates of a free particle are plane waves. \square

Example 2.2 (Infinite square-well potential). We consider an electron in a square-well potential. This is a one-dimensional structure of length L with a vanishing potential inside the well and an infinite potential outside. As the potential is confining the electron to the inner region, we have to solve the Schrödinger equation (10) in the interval $(0, L)$ with boundary conditions

$$\psi(0) = \psi(L) = 0$$

and potential $V(x) = 0$ for $x \in (0, L)$. The general solution of (10) is

$$\psi(x) = Ae^{(a+ik)x} + Be^{-(a+ik)x},$$

where $A, B \in \mathbb{C}$ and a and k are real numbers. Inserting this ansatz in the Schrödinger equation, we find that

$$-\frac{\hbar^2}{2m} (a + ik)^2 \psi = E\psi,$$

and thus, $-(a + ik)^2 = 2mE/\hbar^2$. The boundary conditions imply that

$$0 = \psi(0) = A + B, \quad 0 = \psi(L) = Ae^{(a+ik)L} + Be^{-(a+ik)L}.$$

The first equation shows that $B = -A$, the second one gives $e^{2(a+ik)L} = 1$, and consequently, $a = 0$ and $kL = n\pi$ for all $n \in \mathbb{Z}$. Hence, the eigenfunctions are given by

$$\psi_k(x) = A(e^{ikx} - e^{-ikx}) = C \sin(kx), \quad \text{where } k = \frac{n\pi}{L}, \quad n \in \mathbb{Z},$$

and $C = 2iA$, and the eigenvalues are

$$E(k) = \frac{\hbar^2 k^2}{2m}.$$

The integration constant C can be determined by assuming that

$$\int_0^L |\psi_k(x)|^2 dx = 1$$

holds, stating that the probability of finding the electron in the square well is equal to one. A simple computation shows that $C = \sqrt{2L}$. The system only allows for *discrete* energy states. In particular, the parameter k can take discrete values only. \square

2.3 Electrons in a Periodic Potential

The semiconductor solid can be described by ions (nuclei and core electrons) and valence electrons. These electrons are responsible for the electronic properties of the solid. The evolution of their state is quantum mechanically given by the Hamiltonian which takes into account the relevant physical phenomena, like ion vibrations, electron-ion interactions, and electron-electron scattering. We assume that the ions are fixed and in equilibrium such that we can neglect lattice vibrations and their interaction with the electrons (see [6, 44] for lattice dynamics and electron-phonon interactions).

Let the state of the ion-electron system be described by the wave function $\psi(x)$, where $x = (x_1, \dots, x_M) \in \mathbb{R}^{3M}$ is the vector of all possible positions $x_j \in \mathbb{R}^3$ of the M electrons. Then, the Hamiltonian of the quantum system (see Section 2.2) consists of the kinetic-energy part, the electron-ion interactions, and the electron-electron interactions,

$$H = -\frac{\hbar^2}{2m} \sum_{j=1}^M \Delta_j + H_{\text{ei}} + H_{\text{ee}},$$

where Δ_j is the Laplace operator acting on the x_j -variable only. In the following, we will derive explicit expressions for H_{ei} and H_{ee} :

- The lattice ions generate a periodic electrostatic potential V_{ei} ,

$$V_{\text{ei}}(x + y) = V_{\text{ei}}(x) \quad \text{for } x \in \mathbb{R}^3, \quad y \in L,$$

where L describes the lattice points (nuclei), which is the superposition of the Coulomb potentials

$$V_j(x) = \frac{Q}{4\pi\epsilon_0|x - R_j|}$$

of the crystal ions located at R_j , i.e.

$$V_{\text{ei}}(x) = \sum_{j=1}^{M_i} \frac{Q}{4\pi\epsilon_0|x - R_j|}, \quad x \in \mathbb{R}^3$$

(see Figure 3). Here, Q is the ion charge, ϵ_0 the permittivity, and M_i the number of ions. The lattice potential describes the interaction of a single electron with the ions. It is periodic with respect to the lattice. Hence, the electron-ion Hamiltonian is given by

$$H_{\text{ei}} = -q \sum_{\ell=1}^M V_{\text{ei}}(x_\ell) = - \sum_{\ell=1}^M \sum_{j=1}^{M_i} \frac{qQ}{4\pi\epsilon_0|x_\ell - R_j|}.$$

- The electron-electron interactions are modeled by

$$V_{\text{ee}}(x) = -\frac{1}{2} \sum_{j,\ell=1, j \neq \ell}^M \frac{q}{4\pi\epsilon_0|x_j - x_\ell|}, \quad x \in \mathbb{R}^{3M},$$

and the Hamiltonian is given by $H_{\text{ee}} = -qV_{\text{ee}}(x)$. The factor $\frac{1}{2}$ takes into account that the sum counts each interaction twice.

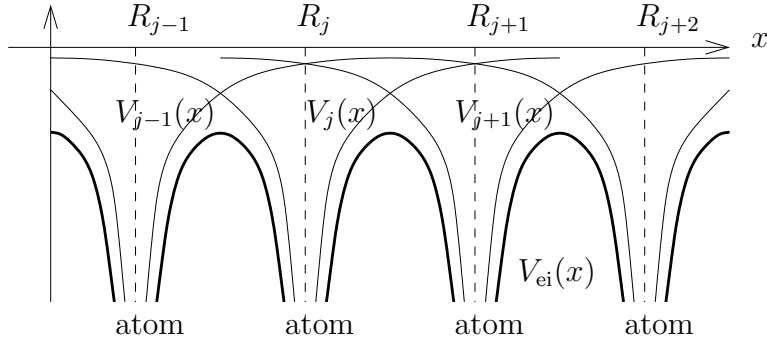


Figure 3: Potentials $V_j(x)$ of a single ion at $x = R_j$ and net potential $V_{\text{ei}}(x)$ of a one-dimensional crystal lattice.

Thus, the Hamiltonian of the system reads as

$$H = \sum_{j=1}^M \left(-\frac{\hbar^2}{2m} \Delta_j - qV_{\text{ei}}(x_j) \right) - qV_{\text{ee}}(x).$$

The solution of the eigenvalue problem $H\psi = E\psi$ is computationally very expensive, due to the presence of the potentials and the large number of electrons. In the following, we simplify the problem by making two approximations. First, we replace the electron-electron

interactions by an effective single-particle potential. This reduces the $3M$ -dimensional problem to a three-dimensional one (Hartree-Fock approximation). Second, the solution of the Schrödinger equation in the whole space \mathbb{R}^3 is reduced to the solution in a primitive cell of the lattice (Bloch decomposition).

Hartree-Fock approximation. The reduction to a single-particle potential is based on the following idea. If the electron-electron interactions can be neglected, the Schrödinger equation is the sum of single-particle Schrödinger equations. Consequently, the wave function ψ can be written as the product of the single-particle wave functions. Even in the presence of electron-electron interactions, one may try the product ansatz

$$\psi(x) = \prod_{j=1}^M \psi_j(x_j). \quad (12)$$

This approximation of the wave function is called the *Hartree approximation*. The single-particle wave functions ψ_j are determined by assuming that they minimize the energy $(\psi, H\psi)_{L^2} = \int_{\mathbb{R}^{3N}} \bar{\psi} H \psi \, dx$ under the constraint of normalized wave functions,

$$\min_{\psi} (\psi, H\psi)_{L^2} \quad \text{subject to } \|\psi_j\|_{L^2}^2 = 1 \text{ for all } j, \quad (13)$$

where $\|\psi_j\|_{L^2}^2 = \int_{\mathbb{R}^3} |\psi_j|^2 \, dx$ and $\bar{\psi}$ denotes the complex conjugate of ψ . The minimum is taken over all wave functions satisfying (12).

The above approach has a drawback. By the Pauli principle, the total wave function of an electron ensemble has to be antisymmetric (with respect to the spatial and spin variables). This is not necessarily the case if the above product ansatz is employed. To overcome this limitation, we construct a properly symmetrized wave function by a linear combination of products of the type $\psi_1(x_{j_1}) \cdots \psi_N(x_{j_N})$. Instead of going into the details, we only present the result and refer to [11, Ch. 7.2] for the computations. The result is the so-called *Hartree-Fock equation*

$$-\frac{\hbar^2}{2m} \Delta \psi_j - qV_L(x)\psi_j = E_j \psi_j, \quad x \in \mathbb{R}^3, \quad j = 1, \dots, M. \quad (14)$$

This is a single-particle equation in \mathbb{R}^3 incorporating the many-body aspect in terms of the total effective potential V_L . This potential is defined by $V_L = V_{\text{ei}} + V_{\text{eff}}$, where V_{ei} is the Coulomb potential defined above and V_{eff} is the effective single-particle potential

$$V_{\text{eff}}(x) = -q \int_{\mathbb{R}^3} \frac{n(x') - \bar{n}_{\text{ex}}(x, x')}{4\pi\epsilon_0|x - x'|} \, dx',$$

where the electron density $n(x)$ and the exchange particle density n_{ex} are given by, respectively,

$$n(x) = \sum_{j=1}^M |\psi_j(x)|^2, \quad n_{\text{ex}}(x, x') = \frac{1}{M} \sum_{j=1}^M \sum_{\ell, \parallel} \frac{\overline{\psi_j(x')\psi_\ell(x')\psi_j(x)\psi_\ell(x)}}{\overline{\psi_j(x)\psi_j(x)}}.$$

The summation is over all states ℓ with parallel spin.

Bloch decomposition. In a perfect periodic crystal, we expect that the single-electron effective potential V_L is periodic, too [6, p. 132]. Thus, one might hope that the whole-space Schrödinger problem (14) can be reduced to an eigenvalue problem on a cell of the lattice. The following result, due to Bloch [9], states that this is indeed possible.

Theorem 2.3 (Bloch). *Let V_L be a periodic potential, i.e., $V_L(x + y) = V_L(x)$ for all $x \in \mathbb{R}^3$ and $y \in L$ (the Bravais lattice). Then the eigenvalue problem for the Schrödinger operator*

$$H = -\frac{\hbar^2}{2m}\Delta - qV_L(x), \quad x \in \mathbb{R}^3,$$

can be reduced to an eigenvalue problem of the Schrödinger equation on the primitive cell D of the lattice, indexed by $k \in B$ (the Brillouin zone),

$$H\psi = E\psi \quad \text{in } D, \quad \psi(x + y) = e^{ik \cdot y}\psi(x), \quad x \in D, \quad y \in L. \quad (15)$$

For each $k \in B$, there exists a sequence $E_n(k)$, $n \geq 1$, of eigenvalues with associated eigenfunctions $\psi_{n,k}$. The eigenvalues $E_n(k)$ are real functions of k and periodic and symmetric on B . The spectrum of H is given by the union of the closed intervals $\{E_n(k) : k \in \overline{B}\}$ for $n \geq 1$ (with \overline{B} being the closure of B).

For a rigorous proof of the Bloch theorem, we refer to [42, 52], where also more properties on the energies $E_n(k)$ are stated. In the following, we give a (mathematically not rigorous) motivation of the above statement, which helps to understand the role of the vector k .

Proof. We consider the translation operator T_a , defined by $(T_a\psi)(x) = \psi(x + a)$ for $a \in L$, $x \in \mathbb{R}^3$, and functions $\psi \in L^2(\mathbb{R}^3)$. First, we claim that the eigenvalues of T_a are given by $e^{i\theta}$ for $\theta \in \mathbb{R}$. To see this, let ψ be an eigenfunction to the eigenvalue λ , i.e. $T_a\psi = \lambda\psi$. Then

$$|\lambda|^2 \|\psi\|_{L^2}^2 = \|\lambda\psi\|_{L^2}^2 = \|T_a\psi\|_{L^2}^2 = \int_{\mathbb{R}^3} |\psi(x + a)|^2 dx = \|\psi\|_{L^2}^2,$$

and thus, $|\lambda| = 1$ or $\lambda = e^{i\theta}$ for some $\theta \in \mathbb{R}$.

The Hamiltonian H commutes with all the translation operators T_a since V_L is periodic:

$$\begin{aligned} (T_a H \psi)(x) &= -\frac{\hbar^2}{2m}\Delta\psi(x + a) - qV_L(x + a)\psi(x + a) \\ &= -\frac{\hbar^2}{2m}\Delta\psi(x + a) - qV_L(x)\psi(x + a) = (HT_a\psi)(x). \end{aligned}$$

Therefore, if ψ is an eigenfunction of H , it is also an eigenfunction of T_a for any $a \in L$ and vice versa. (For this statement some mathematical properties are needed, like the self-adjointness of H and T_a ; see, e.g., [5].) Let ψ be such a simultaneous eigenvector of H and T_a for any $a \in L$. Hence, for all $j = 1, 2, 3$, there exists $\theta_j \in \mathbb{R}$ such that

$$T_{-a_j}\psi = e^{i\theta_j}\psi, \quad (16)$$

where a_1 , a_2 , and a_3 are the primitive vectors of the Bravais lattice L . We set

$$k_0 = -\frac{1}{2\pi} \sum_{\ell=1}^3 \theta_\ell a_\ell^*, \quad (17)$$

where a_1^* , a_2^* , and a_3^* are the primitive vectors of L^* . Then (7) implies that

$$k_0 \cdot a_j = -\frac{1}{2\pi} \sum_{\ell=1}^3 \theta_\ell a_\ell^* \cdot a_j = -\theta_j. \quad (18)$$

We define $\phi(x) = e^{-ik_0 \cdot x} \psi(x)$ for $x \in \mathbb{R}^3$. We claim that $\phi(x+y) = \phi(x)$ for all $x \in \mathbb{R}^3$ and $y \in L$. Since every $y \in L$ is a linear combination of the vectors a_j , it is sufficient to prove the periodicity for $y = a_j$. We obtain, using (16) and (18),

$$\begin{aligned} \phi(x) &= e^{-ik_0 \cdot x} \psi(x) = e^{-ik_0 \cdot x} (T_{-a_j} \psi)(x + a_j) = e^{-ik_0 \cdot x} e^{i\theta_j} \psi(x + a_j) \\ &= e^{-ik_0 \cdot x} e^{i\theta_j} e^{ik_0 \cdot (x+a_j)} \phi(x + a_j) = e^{i(\theta_j + k_0 \cdot a_j)} \phi(x + a_j) = \phi(x + a_j). \end{aligned}$$

It remains to show that k_0 can be restricted to the Brillouin zone. We decompose $k_0 = k + \ell$, where $k \in B$ and $\ell \in L^*$ is a point in the reciprocal lattice closest to k (see Figure 4). Then

$$\psi(x) = e^{ik_0 \cdot x} \phi(x) = e^{ik \cdot x} u(x), \quad x \in \mathbb{R}^3, \quad (19)$$

where $u(x) = e^{i\ell \cdot x} \phi(x)$ satisfies, in view of (7),

$$u(x+y) = e^{i\ell \cdot x} e^{i\ell \cdot y} \phi(x+y) = e^{i\ell \cdot x} \phi(x) = u(x)$$

for all $x \in \mathbb{R}^3$ and $y \in L$. Now, the representation (19) implies, for $x \in D$ and $y \in L$, that $\psi(x+y) = e^{ik \cdot (x+y)} u(x) = e^{ik \cdot y} \psi(x)$, which proves (15). \square

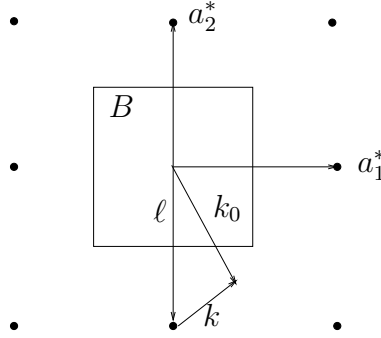


Figure 4: Illustration of $k_0 = k + \ell$ with $k \in B$ and $\ell \in L^*$.

We will often assume that the Brillouin zone can be extended to the whole space, $B = \mathbb{R}^3$, which is approximately satisfied for a sufficiently large number of atoms in the crystal and which can be justified by a scaling argument (see [31, Remark 1.6]).

The function $k \mapsto E_n(k)$ is called the *dispersion relation* and the set $\{E_n(k) : k \in B\}$ the n -th *energy band*. It shows how the energy of the n -th band depends on the (pseudo-) wave vector k . The union of ranges of E_n over $n \in \mathbb{N}$ is not necessarily the whole real line \mathbb{R} , i.e., there may exist energies E^* for which there is no number $n \in \mathbb{N}$ and no vector $k \in B$ such that $E_n(k) = E^*$. The connected components of the set of energies with this non-existence property are called *energy gaps*.

An energy gap separates two energy bands. The nearest energy band below the energy gap (if it is unique) is called the *valence band*, the nearest energy band above the energy gap is termed the *conduction band* (see Figure 5).

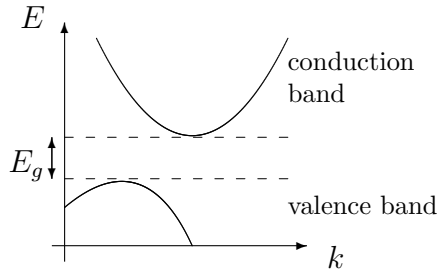


Figure 5: Schematic band structure with energy gap E_g .

Now we are able to state the definition of a semiconductor: It is a solid with an energy gap whose value is positive and smaller than a few electron volt (up to about 3 or 4 eV). In Table 1 the values of the energy gaps for some common semiconductor materials are collected.

Material	Symbol	Energy gap in eV
Indium arsenide	InAs	0.356
Germanium	Ge	0.661
Silicon	Si	1.124
Gallium arsenide	GaAs	1.424
Aluminium gallium arsenide	$\text{Al}_{0.3}\text{Ga}_{0.7}\text{As}$	1.80
Aluminium arsenide	AlAs	2.239
Gallium phosphide	GaP	2.272
Cadmium sulfur	CdS	2.514
Gallium nitride	GaN	3.44

Table 1: Energy gaps of selected semiconductors (from [46, Appendix C]; the value for $\text{Al}_{0.3}\text{Ga}_{0.7}\text{As}$ is taken from [29]).

As an example, Figure 6 shows the schematic band structures of silicon and gallium arsenide. Two different crystal directions are shown, namely the $k = (0, 0, 1)^\top$ direction

along the $+k$ axis (called the Δ line) and the $k = (1, 1, 1)^\top$ direction along the $-k$ axis (called the Λ line). The point $k = (0, 0, 0)$ is termed the Γ point. The points at the boundary of the Brillouin zone in the Λ and Δ directions are called L and X points, respectively [27, 36] (see Figure 7).

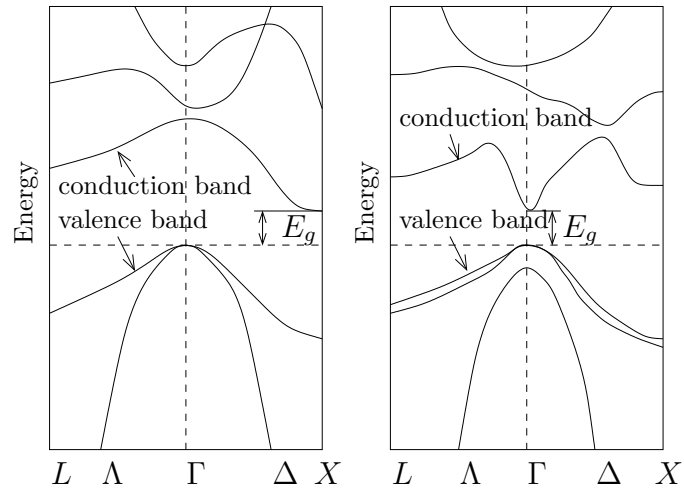


Figure 6: Schematic band structure of silicon (left) and gallium arsenide (right) (see [49, Figs. 3.7 and 3.9]).

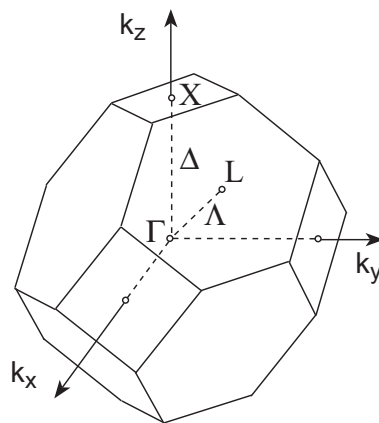


Figure 7: Brillouin zone of semiconductors like silicon, germanium, gallium arsenide etc.

2.4 The Semi-Classical Picture

In this section, we will motivate some equations which resemble the classical Newton laws but which incorporate some quantum mechanical phenomena.

Semi-classical equations of motion. We will derive heuristically the following equations:

$$\hbar\dot{x} = \nabla_k E_n(k), \quad \hbar\dot{k} = q\nabla_x V, \quad (20)$$

where x is the position of the electron at time t , k is the pseudo-wave vector introduced in Section 2.3, and the dot denotes differentiation with respect to time.

First, we motivate the left equation in (20). We assume that the electrons remain for all time in the same energy band. Then we may omit the index n in $\psi_{n,k}$. Let ψ_k be a solution of the stationary Schrödinger equation

$$-\frac{\hbar^2}{2m}\Delta\psi_k - q(V_L(x) + V(x))\psi_k = E_n(k)\psi_k \quad \text{in } D \quad (21)$$

with boundary conditions $\psi_k(x+y) = e^{ik\cdot y}\psi_k(x)$, where x and y are lattice points. Recall that the momentum is represented quantum mechanically by the operator $P\psi = -i\hbar\nabla_x\psi$, and its expectation value of a quantum system in the (normalized) state ψ_k is given by

$$\langle P \rangle_k = \int_D \bar{\psi}_k P\psi_k \, dx = \frac{\hbar}{i} \int_D \bar{\psi}_k \nabla_x \psi_k \, dx.$$

Then we define the mean velocity of this state by

$$v_n(k) = \frac{\langle P \rangle_k}{m}.$$

In the semi-classical setting, we introduce a “trajectory” of the quantum system corresponding to the mean velocity by $\dot{x} = v_n(k)$. In this interpretation, x and k are functions of time. Employing (21), we can relate the mean velocity to the energy band.

Lemma 2.4. *The semi-classical trajectory with mean velocity $v_n(k)$ is given by*

$$\dot{x} = v_n(k) = \frac{1}{\hbar} \nabla_k E_n(k), \quad t > 0.$$

Proof. By Bloch’s Theorem 2.3, ψ_k can be written as

$$\psi_k(x) = e^{ik\cdot x} u_k(x). \quad (22)$$

Differentiating (21) with respect to k and using $\nabla_k \psi_k = e^{ik\cdot x} \nabla_k u_k + ix\psi_k$ gives

$$\begin{aligned} (\nabla_k E_n)\psi_k &= -\frac{\hbar^2}{2m}\Delta_x(e^{ik\cdot x}\nabla_k u_k + ix\psi_k) \\ &\quad - (qV_L + qV + E_n)(e^{ik\cdot x}\nabla_k u_k + ix\psi_k) \\ &= \left(-\frac{\hbar^2}{2m}\Delta_x - (qV_L + qV + E_n)\right)(e^{ik\cdot x}\nabla_k u_k) - \frac{i\hbar^2}{m}\nabla_x \psi_k \\ &\quad + ix\left(-\frac{\hbar^2}{2m}\Delta_x - (qV_L + qV + E_n)\right)\psi_k. \end{aligned}$$

Observing that the last term vanishes in view of (21), multiplication of the above equation with $\bar{\psi}_k$ and integration over D yields

$$\begin{aligned} \nabla_k E_n \int_D |\psi_k|^2 dx + \frac{i\hbar^2}{m} \int_D \bar{\psi}_k \nabla_x \psi_k dx \\ = \int_D \bar{\psi}_k \left(-\frac{\hbar^2}{2m} \Delta_x - (qV_L + qV + E_n) \right) (e^{ik \cdot x} \nabla_k u_k) dx \\ = \int_D e^{ik \cdot x} \nabla_k u_k \left(-\frac{\hbar^2}{2m} \Delta_x - (qV_L + qV + E_n) \right) \bar{\psi}_k dx = 0, \end{aligned}$$

where we have used integration by parts and again (21). The boundary integral in the integration-by-parts formula vanishes since u_k is periodic on D . Thus, if ψ_k is normalized,

$$\nabla_k E_n = \frac{\hbar^2}{im} \int_D \bar{\psi}_k \nabla_x \psi_k dx = \frac{\hbar}{m} \langle P \rangle_k = \hbar v_n(k).$$

This shows the lemma. \square

The second equation in (20) is more difficult to justify (see [6, p. 220] or [36, p. 39]). If we suppose that the total energy, consisting of the band energy $E_n(k)$ and the potential energy $-qV(x)$, is constant along the trajectories $x = x(t)$, $k = k(t)$, its derivative with respect to time vanishes,

$$0 = \frac{d}{dt}(E_n(k) - qV(x)) = \nabla_k E_n(k) \cdot \dot{k} - q\nabla_x V(x) \cdot \dot{x} = v_n(k) \cdot (\hbar \dot{k} - q\nabla_x V(x)). \quad (23)$$

This identity is satisfied if $\hbar \dot{k} - q\nabla_x V = 0$, which is the second equation in (20). Clearly, this equation is not necessary for the energy to be conserved since (23) only shows that $\hbar \dot{k} - q\nabla_x V$ is perpendicular to the velocity $v_n(k)$.

Remark 2.5. The semi-classical equations (20) can be justified rigorously. The starting point is the scaled Schrödinger equation

$$ih_0 \partial_t \psi = -\frac{h_0^2}{2} \Delta \psi - \frac{h_0^2}{\varepsilon^2} V_L\left(\frac{x}{\varepsilon}\right) \psi - V(x) \psi, \quad x \in \mathbb{R}^3,$$

where $h_0 > 0$ and $\varepsilon > 0$. The combined classical and homogenization limit $h_0 \rightarrow 0$ and $\varepsilon \rightarrow 0$ is called the *semi-classical limit*. Here, the limits $h_0 \rightarrow 0$ and $\varepsilon \rightarrow 0$ are performed in such a way that the resulting semi-classical equation still contains quantum mechanical effects. Bechouche et al. [7] proved that the unscaled semi-classical equations of motion equal, in the limit $\varepsilon = h_0 \rightarrow 0$, (20). The idea of the proof is to formulate the Schrödinger equation by means of the so-called Wigner function (see Section 6.2) and to perform the limit in the Wigner equation, leading to a semi-classical Vlasov equation. \square

Effective mass tensor. The mean velocity v_n is defined by $\langle P \rangle_k = mv_n$. Employing the crystal momentum p instead of the physical momentum $\langle P \rangle_k$, we may define $p = m^* v_n$,

where m^* is another mass. In the case of a free electron motion (see Example 2.1), the mass m^* is the rest mass of the electron since $E(k) = \hbar^2|k|^2/2m$ yields $\hbar k = p = m^*v_n = m^*\nabla_k E/\hbar = m^*\hbar k/m$ and hence $m^* = m$. What is the meaning of m^* in the presence of a periodic potential? We differentiate the momentum $p = m^*v_n$ with respect to time and employ the first equation in (20),

$$\dot{p} = m^*\dot{v}_n = \frac{m^*}{\hbar} \frac{d^2 E_n}{dk^2} \dot{k} = \frac{m^*}{\hbar^2} \frac{d^2 E_n}{dk^2} \dot{p},$$

which shows that

$$(m^*)^{-1} = \frac{1}{\hbar^2} \frac{d^2 E_n}{dk^2}. \quad (24)$$

This equation is considered as a definition of the *effective mass* m^* . The right-hand side of this definition is the Hessian matrix of E_n , so the symbol $(m^*)^{-1}$ is a 3×3 matrix.

The effective mass has the advantage that under some conditions, the behavior of the electrons in a crystal can be described similarly as that of a free electron gas. In order to see this, we evaluate the Hessian of E_n near a local minimum (of the conduction band), i.e. $\nabla_k E_n(k_0) = 0$. Then $d^2 E_n(k_0)/dk^2$ is a symmetric positive definite matrix which can be diagonalized and the diagonal matrix has positive entries. We assume that the coordinates are chosen such that $d^2 E_n(k_0)/dk^2$ is already diagonal,

$$\frac{1}{\hbar^2} \frac{d^2 E_n}{dk^2}(k_0) = \begin{pmatrix} 1/m_1^* & 0 & 0 \\ 0 & 1/m_2^* & 0 \\ 0 & 0 & 1/m_3^* \end{pmatrix}.$$

Assume that the energy values are shifted in such a way that $E_n(k_0) = 0$. (This is possible by fixing a reference point for the energy.) Let us further assume that already $E_n(0) = 0$, otherwise define $\tilde{E}_n(k) = E_n(k+k_0)$. If the function $k \mapsto E_n(k)$ is smooth, Taylor's formula implies that

$$\begin{aligned} E_n(k) &= E_n(0) + \nabla_k E_n(0) \cdot k + \frac{1}{2} k^\top \left(\frac{d^2 E_n}{dk^2}(0) \right) k + \mathcal{O}(|k|^3) \\ &= \frac{\hbar^2}{2} \left(\frac{k_1^2}{m_1^*} + \frac{k_2^2}{m_2^*} + \frac{k_3^2}{m_3^*} \right) + \mathcal{O}(|k|^3) \quad \text{for } k \rightarrow 0, \end{aligned}$$

where $k = (k_1, k_2, k_3)^\top$ and $\mathcal{O}(|k|^3)$ denotes terms of order $|k|^3$. If the effective masses are equal in all directions, i.e. $m^* = m_1^* = m_2^* = m_3^*$, we can write, neglecting higher-order terms,

$$E_n(k) = \frac{\hbar^2}{2m^*} |k|^2. \quad (25)$$

This relation is valid for wave vectors k sufficiently close to a local band minimum (of the conduction band). The scalar m^* is called here the *isotropic effective mass*. Comparing this expression with the dispersion relation of a free electron gas,

$$E(k) = \frac{\hbar^2}{2m} |k|^2,$$

we infer that the energy of an electron near a band minimum (of an isotropic semiconductor) equals the energy of a free electron in a vacuum where the electron rest mass m is replaced by the effective mass m^* . Expression (25) is referred to as the *parabolic band approximation*.

Holes. When we consider the effective mass definition (24) near a maximum (of the valence band), we find that the Hessian of E_n is negative definite. This would lead to a negative effective mass. In order to obtain a positive mass, we may also change the sign for the group velocity v_n since this is consistent with the definition $p = m^*v_n$. A reversed sign in the velocity means that the particles, under the influence of an electric field, travel in the opposite direction compared to electrons. This is the case if the particles have a positive charge. Employing a positive charge leads again to a positive effective mass. The corresponding (pseudo-) particles are called *holes* (or defect electrons). Physically, a hole is a vacant orbital in a valence band. Thus, the current flow in a semiconductor crystal comes from two sources: the flow of electrons in the conduction band and the flow of holes in the valence band. It is a convention to consider the motion of the valence band vacancies rather than the electrons moving from one vacant orbital to the next (see Figure 8).

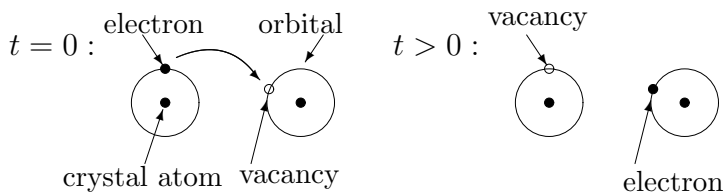


Figure 8: Motion of a valence band electron to a neighboring vacant orbital or, equivalently, of a hole in the inverse direction.

We summarize: Close to the bottom $k = 0$ of the conduction band in an isotropic semiconductor, the band energy becomes

$$E_n(k) = E_c + \frac{\hbar^2}{2m_e^*}|k|^2, \quad (26)$$

whereas near the top $k = 0$ of the valence band we have

$$E_n(k) = E_v - \frac{\hbar^2}{2m_h^*}|k|^2, \quad (27)$$

where E_c is the energy at the conduction band minimum, E_v the energy at the valence band maximum, m_e^* the effective electron mass, and m_h^* the effective hole mass. Clearly, the energy gap E_g is given by $E_g = E_c - E_v$ (see Figure 9).

2.5 Semiconductor Statistics

We will answer the question how many electrons and holes are in a semiconductor of finite size which is in thermal equilibrium (i.e. no current flow). Let $f(E)$ be the occupation

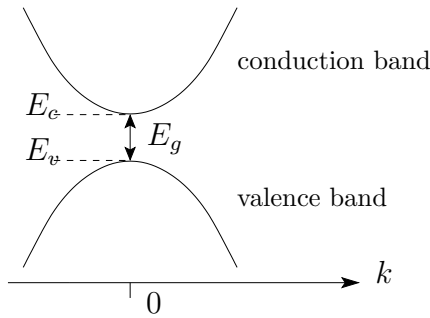


Figure 9: Schematic conduction and valence bands near the extrema at $k = 0$.

density of the quantum state of energy E . We can interpret $f(E)$ as the mean number of electrons in a quantum state of energy $E = E_n(k)$. Then the number of electrons in a given energy band n equals the sum of all $f(E_n(k))$ over all wave vectors k . In the continuum limit the sum becomes an integral:

$$N_n^* = \frac{2\text{vol}(\Omega)}{(2\pi)^d} \int_B f(E_n(k)) dk. \quad (28)$$

The factor $2\text{vol}(\Omega)/(2\pi)^d$ is called the density of states in k -space which is just a scaling factor. Here, $\text{vol}(\Omega)$ is the volume of the semiconductor, $(2\pi)^d$ is related to the volume of the Brillouin zone, and the factor 2 takes into account the two possible states of the spin of an electron (see [31, Section 1.6] for details).

Electrons are fermions, i.e. particles with half-integral spin, satisfying the following properties:

1. Electrons cannot be distinguished from each other.
2. The Pauli exclusion principle holds, i.e., each quantum state can be occupied by not more than two electrons with opposite spins.

It can be shown (by maximizing the thermodynamic entropy subject to the given total number of electrons and given total energy) that the mean number of electrons in a quantum state of energy E is given by the *Fermi-Dirac distribution function*

$$f(E) = \frac{1}{1 + e^{(E - q\mu)/k_B T}}, \quad (29)$$

where k_B is the Boltzmann constant (see [31, Lemma 1.11]). The two parameters T and μ are Lagrange multipliers coming from the constrained extremal problem. Thermodynamics shows that T can be interpreted as the *temperature* of the system and μ as the *chemical potential* [11, Chap. 5].

The properties of the Fermi-Dirac distribution can be understood as follows (also see [11, p. 298f.]). At zero temperature, this function becomes

$$f(E) = \begin{cases} 1 & \text{for } E < q\mu \\ 0 & \text{for } E > q\mu \end{cases} \quad \text{and} \quad f(q\mu) = \frac{1}{2}$$

(see Figure 10). This means that all states which have an energy smaller than the chemical potential are occupied, and all states with an energy larger than $q\mu$ are empty. Physically, this behavior comes from the Pauli principle according to which two electrons must not occupy the same quantum state. At zero temperature, the states with lowest energy are filled first. The energy of the state filled by the last particle is equal to the chemical potential $q\mu$. This number is also called the *Fermi energy* E_F . For nonzero temperature, there is a positive probability that some energy states above $q\mu$ will be occupied, i.e., some particles jump to higher energy levels due to thermal excitation.

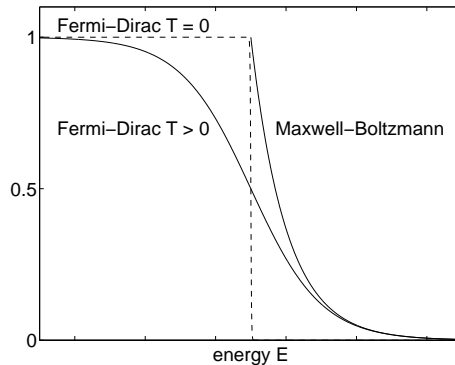


Figure 10: The Fermi-Dirac distribution at zero and nonzero temperature and the Maxwell-Boltzmann approximation.

Strictly speaking, the Fermi energy is defined as $E_F = q\mu$ only if $T = 0$. By abuse of notation, we will also employ this terminology for $T > 0$ (e.g., like in [27, Chap. 7.2]).

For energies much larger than the Fermi energy in the sense of $E - E_F \gg k_B T$, we can approximate the Fermi-Dirac distribution by the *Maxwell-Boltzmann distribution*

$$f(E) = e^{-(E-E_F)/k_B T} \quad (30)$$

since $1/(1 + e^x) \sim e^{-x}$ as $x \rightarrow \infty$ (Figure 10). Semiconductors whose electron distribution can be described by this distribution are called *nondegenerate*. Semiconductor materials in which the Fermi-Dirac distribution has to be used (for instance, in the case of high doping) are termed *degenerate*.

The electron density in a given band $E_j(k)$ is determined by the number of electrons (28), $N^* = N_j^*$, divided by the volume of the semiconductor domain:

$$n = \frac{N^*}{\text{vol}(\Omega)} = \frac{2}{(2\pi)^d} \int_B f(E_j(k)) dk, \quad \text{where } f(E) = \frac{1}{1 + e^{(E-q\mu)/k_B T}}. \quad (31)$$

We wish to formulate the integral not in the k -space but in the energy space. For this, we introduce the *Dirac delta distribution* δ as that functional which associates the value $g(0)$ with an appropriate function g , i.e. $\delta(g) = g(0)$. This is also written as $\langle \delta, g \rangle = g(0)$ for all

C^∞ functions g with compact support or as the *symbolic integral*

$$\int_{\mathbb{R}} \delta(x)g(x) dx = g(0). \quad (32)$$

We recall that this notation has to be considered with care: The symbol δ is not a function but a functional and (32) is not an integral but a symbolic representation, which is useful for the following computations.

With the Dirac distribution, the expression (31) for the electron density can be reformulated. We obtain from (32)

$$\begin{aligned} n &= \frac{2}{(2\pi)^d} \int_B \int_{\mathbb{R}} \delta(E - E_j(k))f(E) dE dk \\ &= \int_{\mathbb{R}} \left(\frac{2}{(2\pi)^d} \int_B \delta(E - E_j(k)) dk \right) f(E) dE. \end{aligned}$$

Thus, we can write

$$n = \int_{\mathbb{R}} N_j(E)f(E) dE,$$

where the integral

$$N_j(E) = \frac{2}{(2\pi)^d} \int_B \delta(E - E_j(k)) dk \quad (33)$$

is called the *density of states* of the j -th band of energy E . In the physical literature, sometimes the notation DOS instead of N_j is used. The quantity $N_j(E)\Delta E$ is approximately the number of quantum states ΔN^* between E and $E + \Delta E$. Thus, $N_j(E)$ is approximately $\Delta N^*/\Delta E$ or, in the infinitesimal sense, $N_j(E) = dN^*/dE$. Notice that the density of states in k -space is constant, but the density of states in energy space (33) generally is not.

Remark 2.6 (Rigorous formulation of (33)). The integral (33) can be formulated more rigorously by applying the *coarea formula*, which is a curvilinear generalization of Fubini's theorem [23]. The formula reads as follows. Let $B \subset \mathbb{R}^d$ be an appropriate domain, $g : B \rightarrow \mathbb{R}$ be continuous, and $E : B \rightarrow \mathbb{R}$ be continuously differentiable such that $1/|\nabla_k E_j(k)|$ is integrable. Then

$$\int_B g(k) dk = \int_{\mathbb{R}} \int_{E_j^{-1}(e)} g(k) \frac{dS_e(k)}{|\nabla_k E_j(k)|} de, \quad (34)$$

where $E_j^{-1}(e) = \{k \in B : E_j(k) = e\}$ is the level set of energy e and dS_e is a surface element. Formally, by (32), this gives

$$\begin{aligned} N_j(E) &= \frac{2}{(2\pi)^d} \int_{\mathbb{R}} \int_{\{E_j(k)=e\}} \delta(E - E_j(k)) \frac{dS_e(k)}{|\nabla_k E_j(k)|} de \\ &= \frac{2}{(2\pi)^d} \int_{\mathbb{R}} \int_{\{E_j(k)=e\}} \delta(E - e) \frac{dS_e}{|\nabla_k E_j|} de \\ &= \frac{2}{(2\pi)^d} \int_{\{E_j(k)=E\}} \frac{dS_E}{|\nabla_k E_j|}. \end{aligned} \quad (35)$$

The density of states is thus written as a surface integral over the isoenergy surface $E_j^{-1}(E)$. \square

We summarize these results in the following proposition.

Proposition 2.7 (Electron density). *The electron density n in a given band $E_j(k)$ reads as*

$$n = \int_{\mathbb{R}} N_j(E) f(E) dE,$$

where the density of states $N_j(E)$ at energy E is defined in (33) or (35) and the Fermi-Dirac distribution function $f(E)$ is given in (29).

In a similar way, we can compute the density of holes in the j -th band. Taking into account that the mean number of holes in a quantum state of energy E equals the mean number of *empty* states of energy E , $1 - f(E)$, we have

$$p = \int_{\mathbb{R}} N_j(E)(1 - f(E)) dE.$$

For the electron or hole density in the conduction or valence band, respectively, we write

$$n = \int_{\mathbb{R}} N_c(E) f(E) dE, \quad p = \int_{\mathbb{R}} N_v(E)(1 - f(E)) dE, \quad (36)$$

where $N_c(E)$ and $N_v(E)$ denote the density of states in the conduction band $E_c(k)$ and valence band $E_v(k)$, respectively.

If the energy band is parabolic, $E(k) = E_0 + \hbar^2|k|^2/2$, $k \in \mathbb{R}^3$, the electron and hole densities can be computed more explicitly.

Lemma 2.8 (Particle densities for parabolic bands). *The three-dimensional electron and hole densities in the parabolic band and Maxwell-Boltzmann approximation $q\mu - E_c$, $E_v - q\mu \ll k_B T$ are*

$$n = N_c \exp\left(\frac{q\mu - E_c}{k_B T}\right), \quad p = N_v \exp\left(\frac{E_v - q\mu}{k_B T}\right),$$

where N_c and N_v are the effective densities of states defined by

$$N_c = 2\left(\frac{m_e^* k_B T}{2\pi\hbar^2}\right)^{3/2}, \quad N_v = 2\left(\frac{m_h^* k_B T}{2\pi\hbar^2}\right)^{3/2}. \quad (37)$$

Proof. We start from (33), use spherical coordinates (ρ, θ, ϕ) and substitute $z = \hbar^2\rho^2/2m_e^*$ to obtain

$$\begin{aligned} N(E) &= \frac{2}{(2\pi)^3} \int_{\mathbb{R}^3} \delta\left(E - E_c - \frac{\hbar^2}{2m_e^*}|k|^2\right) dk \\ &= \frac{1}{4\pi^3} \int_0^{2\pi} \int_0^\pi \int_0^\infty \delta\left(E - E_c - \frac{\hbar^2}{2m_e^*}\rho^2\right) \rho^2 \sin\theta d\rho d\theta d\phi \\ &= \frac{m_e^*}{\pi^2\hbar^2} \frac{\sqrt{2m_e^*}}{\hbar} \int_0^\infty \delta(E - E_c - z) \sqrt{z} dz. \end{aligned}$$

Introducing the Heaviside function H by $H(x) = 0$ for $x < 0$ and $H(x) = 1$ for $x \geq 0$ and using (32), we obtain

$$\begin{aligned} N(E) &= \frac{m_e^*}{\pi \hbar^2} \frac{\sqrt{2m_e^*}}{\pi \hbar} \int_{\mathbb{R}} \delta(E - E_c - z) \sqrt{z} H(z) dz \\ &= \frac{m_e^*}{\pi \hbar^2} \frac{\sqrt{2m_e^*}}{\pi \hbar} \sqrt{E - E_c} H(E - E_c). \end{aligned}$$

Inserting this expression into the formula for the electron density,

$$n = \int_{\mathbb{R}} N(E) f(E) dE,$$

where $f(E) = \exp(-(E - q\mu)/k_B T)$ is given by Maxwell-Boltzmann statistics, we find that, using the substitution $x = (E - E_c)/k_B T$,

$$\begin{aligned} n &= \frac{m_e^*}{\pi \hbar^2} \frac{\sqrt{2m_e^*}}{\pi \hbar} \int_{\mathbb{R}} \sqrt{E - E_c} H(E - E_c) e^{-(E - E_c)/k_B T} dE \\ &= \frac{m_e^*}{\pi \hbar^2} \frac{\sqrt{2m_e^*}}{\pi \hbar} \int_{E_c}^{\infty} \sqrt{E - E_c} e^{-(E - E_c)/k_B T} dE \\ &= \frac{m_e^*}{\pi \hbar^2} \frac{\sqrt{2m_e^*}}{\pi \hbar} (k_B T)^{3/2} \int_0^{\infty} \sqrt{x} e^{-x - (E_c - q\mu)/k_B T} dx \\ &= \frac{m_e^*}{\pi \hbar^2} \frac{\sqrt{2m_e^*}}{\pi \hbar} (k_B T)^{3/2} \underbrace{\int_0^{\infty} \sqrt{x} e^{-x} dx}_{=\sqrt{\pi}/2} e^{-(E_c - q\mu)/k_B T} \\ &= 2 \left(\frac{m_e^* k_B T}{2\pi \hbar^2} \right)^{3/2} \exp\left(-\frac{E_c - q\mu}{k_B T}\right), \end{aligned}$$

showing the expression for the electron density. The formula for the holes is derived in a similar way. \square

Finally, we discuss some notions needed in the subsequent chapters, the intrinsic density, doping of semiconductors, and the Poisson equation.

Intrinsic density. A pure semiconductor with no impurities is called an intrinsic semiconductor. In this case, electrons in the conduction band can only come from valence band levels leaving a vacancy (hole) behind them (see Figure 8). Therefore, the number of electrons in the conduction band is equal to the number of holes in the valence band,

$$n = p = n_i.$$

The quantity n_i is called the *intrinsic density*. It can be computed in the nondegenerate parabolic band case from Lemma 2.8:

$$n_i = \sqrt{np} = \sqrt{N_c N_v} \exp\left(\frac{E_v - E_c}{2k_B T}\right) = \sqrt{N_c N_v} \exp\left(-\frac{E_g}{2k_B T}\right), \quad (38)$$

where $E_g = E_c - E_v$ is the energy gap. This allows us to determine the Fermi energy $E_F = q\mu$ of an intrinsic semiconductor:

$$\begin{aligned} E_F &= E_c + k_B T \log \frac{n}{N_c} = E_c + k_B T \log \frac{n_i}{N_c} = E_c - \frac{E_g}{2} + \frac{k_B T}{2} \log \frac{N_v}{N_c} \\ &= \frac{1}{2}(E_c + E_v) + \frac{3}{4} k_B T \log \frac{m_h^*}{m_e^*}. \end{aligned}$$

This asserts that at zero temperature, the Fermi energy lies precisely in the middle of the energy gap. Furthermore, since $\log(m_h^*/m_e^*)$ is of order one, the correction is only of order $k_B T$ for non-zero temperature. In most semiconductors at room temperature, the energy gap is much larger than $k_B T \approx 0.026$ eV. This shows that the nondegeneracy assumptions

$$\begin{aligned} E - E_F &\geq E_c - E_F = \frac{E_g}{2} - \frac{3}{4} k_B T \log \frac{m_h^*}{m_e^*} \gg k_B T, \\ E_F - E &\geq E_F - E_v = \frac{E_g}{2} - \frac{3}{4} k_B T \log \frac{m_h^*}{m_e^*} \gg k_B T \end{aligned}$$

are satisfied and that the result is consistent with our assumptions.

Doping of semiconductors. The intrinsic density is too small to result in a significant conductivity for nonzero temperature. For instance, in silicon we have $n_i \approx 6.93 \cdot 10^9 \text{ cm}^{-3}$ compared to N_c and N_v being of the order of 10^{19} cm^{-3} . Replacing some atoms in the semiconductor crystal by atoms which provide free electrons in the conduction band or free holes in the valence band allows one to increase the conductivity. Such a process is called the *doping* of a semiconductor. Impurities are called *donors* if they supply additional electrons to the conduction band, and *acceptors* if they supply additional holes to (i.e. capture electrons from) the valence band. A semiconductor which is doped with donors is termed an *n-type semiconductor*, and a semiconductor doped with acceptors is called a *p-type semiconductor*. For instance, when we dope a germanium crystal, whose atoms have each four valence electrons, with arsenic, which has five valence electrons per atom, each arsenic atom provides one additional electron. These additional electrons are only weakly bound to the arsenic atom. Indeed, the binding energy is about 0.013 eV [6, Table 28.2] which is smaller than the thermal energy $k_B T \approx 0.026$ eV at room temperature. More generally, denoting by E_d and E_a the energies of a donor electron and an acceptor hole, respectively, then $E_c - E_d$ and $E_a - E_v$ are small compared to $k_B T$ (see Figure 11). This means that the additional carriers contribute at room temperature to the electron and hole density and increase the conductivity of the semiconductor.

Poisson equation. Let $N_d(x)$, $N_a(x)$ denote the densities of the donor and acceptor impurities, respectively. Then the *doping profile* or *doping concentration* is $C(x) = N_a(x) - N_d(x)$ and the total space charge is given by

$$\rho = -qn + qp + qN_a(x) - qN_d(x) = -q(n - p - C(x)).$$

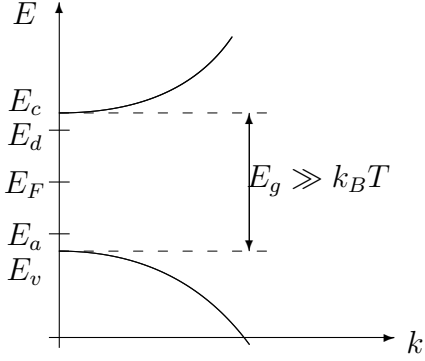


Figure 11: Illustration of the energy gap E_g and the donor and acceptor energies E_d and E_a . The Fermi energy E_F approximately lies in the middle of the energy gap for moderate temperatures.

By the Maxwell equation

$$\varepsilon_s \operatorname{div} E = \rho,$$

where ε_s is the semiconductor permittivity and $E = -\nabla V$ is the electric field with V being the electric potential, we obtain the *Poisson equation*

$$\varepsilon_s \Delta V = -\varepsilon_s \operatorname{div} E = -\rho = q(n - p - C).$$

Without the hole density (unipolar semiconductors), we find that

$$\varepsilon_s \Delta V = q(n - C). \quad (39)$$

3 Kinetic Transport Equations

We have explained in the introduction that the classical motion of M electrons in a vacuum can be modeled by the Newton equations

$$\dot{x} = v, \quad m\dot{v} = F, \quad t > 0,$$

for the position vector $x = (x_1, \dots, x_M)$, the velocity vector $v = (v_1, \dots, v_M)$, and the force vector $F = (F_1, \dots, F_M) \in \mathbb{R}^{3M}$. We assume in the following that the force is given by the electric potential V , $F_j = q\nabla_{x_j} V$, where $j = 1, \dots, M$ and q is the elementary charge. Arguing as in the introduction, the distribution function $f(x, v, t)$ satisfies the Liouville equation in the $6M$ -dimensional position-velocity phase space:

$$\partial_t f + v \cdot \nabla_x f + \frac{q}{m} \nabla_x V \cdot \nabla_v f = 0, \quad (x, v) \in \mathbb{R}^{6M}, \quad t > 0. \quad (40)$$

3.1 Semi-Classical Liouville Equation

In semiconductors, the electron ensemble cannot be described classically and the above argument is not valid. In Section 2, however, we have motivated that the motion of the electrons can be modeled semi-classically by the equations

$$\hbar\dot{x}_i = \nabla_{k_i} E_n(k_i), \quad \hbar\dot{k}_i = q\nabla_{x_i} V, \quad i = 1, \dots, M, \quad (41)$$

where E_n is the energy of the n -th band depending on the pseudo-wave vector k_i (cf. (20)). As above, we introduce the vectors $x = (x_1, \dots, x_M)$ and $k = (k_1, \dots, k_M)$. The distribution function f depends now on (x, k, t) rather than on (x, v, t) . We assume that the electrons of the ensemble stay in the same energy band so that we can drop the index n .

Taking into account (41), the Liouville equation reads as follows:

$$\begin{aligned} 0 &= \frac{d}{dt} f(x(t), k(t), t) = \partial_t f + \dot{x} \cdot \nabla_x f + \dot{k} \cdot \nabla_k f \\ &= \partial_t f + \frac{1}{\hbar} \nabla_k E \cdot \nabla_x f + \frac{q}{\hbar} \nabla_x V \cdot \nabla_k f, \end{aligned} \quad (42)$$

to be solved for $x \in \mathbb{R}^{3M}$, $k \in B^M$, and $t > 0$. Equation (42) is referred to as the *semi-classical Liouville equation*. The products are scalar products in \mathbb{R}^{6M} , i.e., they are defined as

$$\nabla_k E \cdot \nabla_x f = \sum_{i=1}^M \nabla_{k_i} E \cdot \nabla_{x_i} f, \quad \nabla_x V \cdot \nabla_k f = \sum_{i=1}^M \nabla_{x_i} V \cdot \nabla_{k_i} f,$$

and the dot on the right-hand sides denotes the usual scalar product in \mathbb{R}^3 . We have to complement the Liouville equation by initial and boundary conditions since B is a bounded set of \mathbb{R}^3 . The initial condition is given by

$$f(x, k, 0) = f_I(x, k), \quad (x, k) \in \mathbb{R}^{3M} \times B^M. \quad (43)$$

Often, periodic boundary conditions

$$f(x, k_1, \dots, k_i, \dots, k_M, t) = f(x, k_1, \dots, -k_i, \dots, k_M, t), \quad k_i \in \partial B, \quad (44)$$

for $i = 1, \dots, M$, are chosen (see, e.g., [39, formula (1.2.49)]). This formulation makes sense since B is point symmetric with respect to the origin, i.e. $k_i \in B$ if and only if $-k_i \in B$.

Remark 3.1 (Connection between the classical and semi-classical Liouville equation). We notice that in the parabolic band approximation $E(k_i) = \hbar^2 |k_i|^2 / 2m^*$ (see (25)), where m^* denotes the effective electron mass, the semi-classical Liouville equation (40) reduces to the classical Liouville equation (3) with $m = m^*$ since $v = \nabla_k E / \hbar = \hbar k / m^*$ and $\nabla_k f = (\hbar / m^*) \nabla_v f$. \square

3.2 Semi-Classical Vlasov Equation

The main disadvantage of the semi-classical Liouville initial-value problem (42)-(44) is that it has to be solved in a very high-dimensional phase space. Modeling the moderate number of $M = 10^4$ electrons, the dimension becomes $6 \cdot 10^4$ which is prohibitive for numerical simulations. In this section, we will sketch the derivation of an equation which acts in a six-dimensional phase space, by replacing the electron-ensemble electric potential by an effective single-particle potential, similar to the Hartree-Fock approximation of Section 2.3. The idea of the derivation is first to assume a certain structure of the electric force, then to integrate the Liouville equation in sub-phase spaces and finally, to carry out the formal limit $M \rightarrow \infty$, where M is the number of particles. We proceed similarly as in [39].

Let an ensemble of M electrons be given and denote by $x = (x_1, \dots, x_M)$ and $k = (k_1, \dots, k_M)$ the position and wave vector coordinates of the particles, respectively. We impose the following assumptions:

1. The motion is governed by an external electric field E_{ext} and by two-particle (long-range) interaction forces E_{int} ,

$$F_i(x, t) = -qE_{\text{ext}}(x_i, t) - \frac{q}{4\pi^3} \sum_{j=1, j \neq i}^M E_{\text{int}}(x_i, x_j), \quad i = 1, \dots, M,$$

where the interaction forces are assumed to be anti-symmetric,

$$E_{\text{int}}(x_i, x_j) = -E_{\text{int}}(x_j, x_i) \quad \text{for all } i, j. \quad (45)$$

2. The pointwise limit $E_0 = \lim_{M \rightarrow \infty} M E_{\text{int}}$ exists, i.e., the interaction force for each particle is of order $1/M$.
3. The initial density is independent of the numbering of the particles,

$$f_I(x_1, \dots, x_M, k_1, \dots, k_M) = f_I(x_{\pi(1)}, \dots, x_{\pi(M)}, k_{\pi(1)}, \dots, k_{\pi(M)}) \quad (46)$$

for all $x_i \in \mathbb{R}^3$, $k_i \in B$, $i = 1, \dots, M$, and for all permutations π of $\{1, \dots, M\}$.

4. The subensemble initial density

$$f_I^{(a)}(x_1, \dots, x_a, k_1, \dots, k_a) = \frac{1}{(4\pi^3)^{M-a}} \int_{(\mathbb{R}^3 \times B)^{M-a}} f_I dx_{a+1} \cdots dx_M dk_{a+1} \cdots dk_M$$

can be factorized,

$$f_I^{(a)} = \prod_{i=1}^a F_I(x_i, k_i), \quad (47)$$

for all $a = 1, \dots, M - 1$, where F_I is a given function.

We discuss these assumptions. We have excluded in the first condition velocity-dependent forces, which excludes magnetic fields. The first assumption, which is crucial for the derivation of the Vlasov equation, means that the force field F_i exerted on the i -th electron is given by the sum of an external electric field acting on the i -th electron and of the sum of $M - 1$ two-particle interaction forces of order $1/M$ between the i -th electron and all other electrons. The interaction force E_{int} is independent of the electron index which expresses the fact that the electrons are indistinguishable. The action-reaction law implies that the force exerted by the j -th electron on the i -th electron equals the negative force of the i -th electron on the j -th electron, i.e., E_{int} is anti-symmetric. This property and the third assumption imply that also $f(x, k, t)$ is independent of the numbering of the particles for all $t > 0$. Finally, the fourth hypothesis means that the electrons of a subensemble with a particles move independently of each other *initially*. Intuitively, this hypothesis is reasonable if a is small compared to M . A discussion of the validity of this condition, which is called the *initial chaos assumption*, can be found in [15, Chap. 2.3].

The derivation consists now of the following steps.

1. *BBGKY hierarchy*: Let $f^{(a)}$ be the distribution function of a subensemble consisting of $a < M$ electrons,

$$f^{(a)}(x_1, \dots, x_a, k_1, \dots, k_a, t) = \frac{1}{(4\pi^3)^{M-a}} \int_{(\mathbb{R}^3 \times B)^{M-a}} f(x, k, t) dx_{(a+1)} dk_{(a+1)}, \quad (48)$$

where $dx_{(a+1)} = dx_{a+1} \cdots dx_M$ and $dk_{(a+1)} = dk_{a+1} \cdots dk_M$. Now we integrate the semi-classical Liouville equation with respect to $x_{a+1}, \dots, x_M, k_{a+1}, \dots, k_M$ in order to obtain an equation for $f^{(a)}$. The result, which is just a reformulation (using the anti-symmetry of E_{int} and the third assumption), is the so-called BBGKY hierarchy (named after Bogoliubov-Born-Green-Kirkwood-Yvon):

$$\begin{aligned} 0 = & \partial_t f^{(a)} + \sum_{j=1}^a v(k_j) \cdot \nabla_{x_j} f^{(a)} - \frac{q}{\hbar} \sum_{j=1}^a E_{\text{ext}}(x_j, t) \cdot \nabla_{k_j} f^{(a)} \\ & - \frac{q}{\hbar} \sum_{j,\ell=1}^a E_{\text{int}}(x_j, x_\ell) \cdot \nabla_{k_j} f^{(a)} \\ & - (M - a) \frac{q}{4\pi^3 \hbar} \sum_{j=1}^a \text{div}_{k_j} \int_{\mathbb{R}^3 \times B} E_{\text{int}}(x_j, x_*) f_*^{(a+1)} dx_* dk_*, \end{aligned} \quad (49)$$

with initial conditions

$$f^{(a)}(x_1, \dots, x_a, k_1, \dots, k_a, 0) = f_I^{(a)}(x_1, \dots, x_a, k_1, \dots, k_a), \quad (50)$$

for $(x_1, \dots, x_a) \in \mathbb{R}^{3a}$, $(k_1, \dots, k_a) \in B^a$, where

$$f_*^{(a+1)} = f^{(a+1)}(x_1, \dots, x_a, x_*, k_1, \dots, k_a, k_*, t).$$

2. *Limit $M \rightarrow \infty$:* We assume that $f_M^{(a)}$ converges pointwise to some function $f^{(a)}$ as $M \rightarrow \infty$ (similar for its derivatives). By the second assumption, the internal field E_{int} is of order $1/M$ and vanishes in the formal limit $M \rightarrow \infty$. Moreover, $(M-a)E_{\text{int}}$ converges to E_0 . Thus, the BBGKY hierarchy becomes in the formal limit of infinitely many particles:

$$0 = \partial_t f^{(a)} + \sum_{j=1}^a v(k_j) \cdot \nabla_{x_j} f^{(a)} - \frac{q}{\hbar} \sum_{j=1}^a E_{\text{ext}}(x_j, t) \cdot \nabla_{k_j} f^{(a)} - \frac{q}{4\pi^3 \hbar} \sum_{j=1}^a \text{div}_{k_j} \int_{\mathbb{R}^3 \times B} E_0(x_j, x_*) f_*^{(a+1)} dx_* dk_*, \quad (51)$$

$$f^{(a)}(x_1, \dots, x_a, k_1, \dots, k_a, 0) = f_I^{(a)}(x_1, \dots, x_a, k_1, \dots, k_a), \quad (52)$$

where $(x_1, \dots, x_a) \in \mathbb{R}^{3a}$ and $(k_1, \dots, k_a) \in B^a$. We claim that a one-particle distribution function contains all the dynamics of this many-particle problem under the initial chaos assumption.

3. *Initial chaos assumption:* Let $f^*(x, k, t)$ solve the semiclassical Vlasov equation

$$\begin{aligned} \partial_t f^* + v(k) \cdot \nabla_x f^* - \frac{q}{\hbar} E_{\text{eff}} \cdot \nabla_k f^* &= 0, \quad x \in \mathbb{R}^3, \quad k \in B, \quad t > 0, \\ f^*(x, k, 0) &= f_I^*(x, k), \quad x \in \mathbb{R}^3, \quad k \in B, \end{aligned} \quad (53)$$

where

$$E_{\text{eff}}(x, t) = E_{\text{ext}}(x, t) + \int_{\mathbb{R}^3} n(x_*, t) E_0(x, x_*) dx_* \quad (54)$$

is the effective field and

$$n(x, t) = \int_B f^*(x, k, t) \frac{dk}{4\pi^3}$$

represents the electron density. We multiply the Vlasov equation (53), evaluated at (x_i, k_i) , by

$$Q_i = \prod_{j=1, j \neq i}^a f^*(x_j, k_j, t)$$

and sum over $i = 1, \dots, a$. Then, the time derivative in (53) becomes, for $f_i^* = f^*(x_i, k_i, t)$,

$$\sum_{i=1}^a Q_i \partial_t f_i^* = \sum_{i=1}^a \prod_{j \neq i} f_j^* \partial_t f_i^* = \partial_t \prod_{i=1}^a f_i^* = \partial_t f^{(a)}.$$

In a similar way, we compute

$$\begin{aligned} \sum_{i=1}^a Q_i v(k_i) \cdot \nabla_{x_i} f_i^* &= \sum_{i=1}^a v(k_i) \cdot \nabla_{x_i} f^{(a)}, \\ \sum_{i=1}^a Q_i E_{\text{ext}}(x_i, t) \cdot \nabla_{k_i} f_i^* &= \sum_{i=1}^a E_{\text{ext}}(x_i, t) \cdot \nabla_{k_i} f^{(a)}. \end{aligned}$$

The expression involving the limiting internal field E_0 can be reformulated as

$$\begin{aligned}
& \sum_{i=1}^a Q_i \left(\int_{\mathbb{R}^3 \times B} f^*(x_*, k_*, t) E_0(x_i, x_*) dx_* dk_* \right) \cdot \nabla_{k_i} f_i^* \\
&= \sum_{i=1}^a \operatorname{div}_{k_i} \int_{\mathbb{R}^3 \times B} \prod_{j=1}^a f^*(x_j, k_j, t) f^*(x_*, k_*, t) E_0(x_i, x_*) dx_* dk_* \\
&= \sum_{i=1}^a \operatorname{div}_{k_i} \int_{\mathbb{R}^3 \times B} f_*^{(a+1)} E_0(x_i, x_*) dx_* dk_*.
\end{aligned}$$

Putting together the above expressions, we see that the ansatz (55) solves (51)-(52).

We have shown the following result.

Theorem 3.2 (Semi-classical Vlasov equation). *Let the assumptions on page 30 hold and let f^* be a solution of the one-particle semi-classical Vlasov equation (53). Then the functions*

$$f^{(a)}(x_1, \dots, x_a, k_1, \dots, k_a, t) = \prod_{i=1}^a f^*(x_i, k_i, t) \quad (55)$$

are a solution of the limit BBGKY hierarchy (51)-(52).

Each solution of the semi-classical Vlasov equation provides a solution of the limiting semi-classical Liouville equation under the initial chaos assumption. Thus, the solution of the many-particle problem is reduced to the solution of a one-particle problem. In this sense, the Vlasov equation is derived from the Liouville equation. Figure 12 illustrates the steps of the derivation.

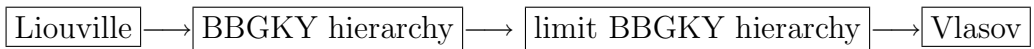


Figure 12: Illustration of the derivation of the Vlasov equation.

The Vlasov equation has the form of a Liouville equation for a single particle with the force field $-qE_{\text{eff}}$. Many-particle effects are taken into account through the effective field E_{eff} which depends on the particle density and hence, on the distribution function f^* . Therefore, (53) is a nonlinear equation with a nonlocal quadratic nonlinearity. It describes the macroscopic motion of the many-particle system with weak long-range forces. It does not provide a description of strong short-range interactions such as scattering of particles, which are considered next.

3.3 Semi-Classical Boltzmann Equation

The Vlasov equation along trajectories

$$\frac{df}{dt} = 0$$

states that the probability density f (of occupation of states) does not change in time. Scattering allows particles to jump to another trajectory. Our main assumption is that the rate of change of f due to convection and the effective field, df/dt , and the rate of change of f due to collisions, $Q(f)$, balance:

$$\frac{df}{dt} = Q(f).$$

Clearly, this equation has to be understood along trajectories,

$$\partial_t f + v(k) \cdot \nabla_x f - \frac{q}{\hbar} E_{\text{eff}} \cdot \nabla_k f = Q(f), \quad x \in \mathbb{R}^3, \quad k \in B, \quad t > 0, \quad (56)$$

where the effective field E_{eff} is given by (54).

It remains to derive an expression for $Q(f)$. We assume that scattering of particles occurs instantaneously and only changes the crystal momentum of the particles. The rate $P(x, k' \rightarrow k, t)$ at which a particle at (x, t) changes its Bloch state k' into another Bloch state k due to a scattering event is proportional to

- the occupation probability $f(x, k', t)$ and
- the probability $1 - f(x, k, t)$ that the state (x, k) is not occupied.

Here, we used a statistical version of the Pauli exclusion principle which is valid for fermions and in particular for electrons. Thus,

$$P(x, k' \rightarrow k, t) = s(x, k', k) f(x, k', t) (1 - f(x, k, t)),$$

where the proportionality factor $s(x, k', k)$ is called the *transition* or *scattering rate*. The rate of change of f due to collisions is the sum of all in-scattering rates from some k' to k minus the out-scattering rate from k to some k' ,

$$P(x, k' \rightarrow k, t) - P(x, k \rightarrow k', t),$$

for all possible Bloch states k' in the “volume element” dk' . In the limit, the sum becomes an integral and we obtain

$$\begin{aligned} (Q(f))(x, k, t) &= \int_B (P(x, k' \rightarrow k, t) - P(x, k \rightarrow k', t)) dk' \\ &= \int_B (s(x, k', k) f'(1 - f) - s(x, k, k') f(1 - f')) dk', \end{aligned} \quad (57)$$

where $f = f(x, k, t)$ and $f' = f(x, k', t)$. Equation (56), together with the effective field equation

$$E_{\text{eff}}(x, t) = E_{\text{ext}}(x, t) + \int_{\mathbb{R}^3} n(\xi, t) E_0(x, \xi) d\xi, \quad n = \int_B f \frac{dk}{4\pi^3}, \quad (58)$$

where E_{ext} and E_0 are given functions, and the collision operator (57), is called the *semi-classical Boltzmann equation*. Again we impose the initial and periodic boundary conditions

$$f(x, k, t) = f(x, -k, t), \quad x \in \mathbb{R}^3, \quad k \in \partial B, \quad t > 0, \quad (59)$$

$$f(x, k, 0) = f_I(x, k), \quad x \in \mathbb{R}^3, \quad k \in B. \quad (60)$$

When E_{ext} and E_0 are given by the Coulomb forces

$$E_0(x, y) = -\frac{q}{4\pi\varepsilon_s} \frac{x-y}{|x-y|^3}, \quad x, y \in \mathbb{R}^3, \quad x \neq y, \quad (61)$$

$$E_{\text{ext}}(x, t) = \frac{q}{4\pi\varepsilon_s} \int_{\mathbb{R}^3} C(y) \frac{x-y}{|x-y|^3} dy, \quad x, y \in \mathbb{R}^3, \quad x \neq y, \quad (62)$$

equations (56)-(58) are called the *Boltzmann-Poisson system*. This is justified by the following result.

Proposition 3.3 (Boltzmann-Poisson system). *In the case of the Coulomb forces (61) and (62), the semi-classical Boltzmann equation can be written as the Boltzmann-Poisson system*

$$\partial_t f + v(k) \cdot \nabla_x f + \frac{q}{\hbar} \nabla_x V \cdot \nabla_k f = Q(f), \quad (63)$$

$$\varepsilon_s \Delta V = q(n - C), \quad x \in \mathbb{R}^3, \quad k \in B, \quad t > 0, \quad (64)$$

with periodic boundary conditions for f on ∂B and the initial condition $f(\cdot, \cdot, 0) = f_I$.

Proof. It is well known from potential theory that the function

$$\phi(x) = -\frac{1}{4\pi} \int_{\mathbb{R}^3} \frac{g(y)}{|x-y|} dy, \quad x \in \mathbb{R}^3,$$

solves the Poisson equation $\Delta\phi = g$ in \mathbb{R}^3 under some regularity assumptions on g . Differentiation gives the formulas

$$g(x) = \Delta\phi(x) = \frac{1}{4\pi} \operatorname{div}_x \int_{\mathbb{R}^3} g(y) \frac{x-y}{|x-y|^3} dy,$$

$$0 = \operatorname{curl} \nabla\phi(x) = \frac{1}{4\pi} \operatorname{curl}_x \int_{\mathbb{R}^3} g(y) \frac{x-y}{|x-y|^3} dy.$$

This shows that $\operatorname{div} E_{\text{ext}} = qC/\varepsilon_s$, $\operatorname{curl} E_{\text{ext}} = 0$, and

$$\begin{aligned} \operatorname{div} E_{\text{eff}}(x, t) &= \operatorname{div} E_{\text{ext}}(x, t) + \operatorname{div} \int_{\mathbb{R}^3} n(x_*, t) E_0(x, x_*) dx_* \\ &= \frac{q}{\varepsilon_s} (C(x) - n(x, t)), \end{aligned} \quad (65)$$

$$\operatorname{curl} E_{\text{eff}}(x, t) = \operatorname{curl} E_{\text{ext}}(x, t) + \int_{\mathbb{R}^3} n(x_*, t) \operatorname{curl} E_0(x, x_*) dx_* = 0.$$

Since E_{eff} is vortex-free, there exists a potential V such that $E_{\text{eff}} = -\nabla V$. Thus, by (65),

$$\varepsilon_s \Delta V = -\varepsilon_s \operatorname{div} E_{\text{eff}} = q(n - C),$$

and the proposition follows. \square

Remark 3.4 (Existence of solutions). The Boltzmann equation has two nonlinearities:

- a quadratic nonlocal nonlinearity in the position variable caused by the self-consistent field E_{eff} in (58), and
- another quadratic nonlocal nonlinearity in the wave vector caused by the collision integral (57).

These nonlinearities make the mathematical analysis of the initial boundary-value problem (56)-(60) very difficult. The Boltzmann equation was first formulated by Boltzmann in 1872 for the nonequilibrium transport of dilute gases, and some properties of the solutions were shown [10]. The first result on the existence and uniqueness of solutions to the homogeneous gas-dynamics Boltzmann equation $\partial_t f = \tilde{Q}(f)$ was published by Carleman in 1933 under the assumption that f depends on the modulus of the velocity $|v|$ and t only [13]. For a very general class of collision operators, Arkeryd developed in the 1970s an L^1 theory for the homogeneous equation [2]. For the nonhomogeneous Boltzmann equation $\partial_t f + v \cdot \nabla_x f = Q(f)$, only existence results for initial data close to the equilibrium state or close to a homogeneous distribution were proved up to 1987 [15, Sec. 5.1]. The first result of global-in-time existence of so-called renormalized solutions with general initial data was then shown by Di Perna and Lions in 1989 [22] using a smoothing effect of the flow term $v \cdot \nabla_x f$, known as the velocity averaging lemma. The existence of weak solutions to the *semiconductor* Boltzmann-Poisson system was first proved by Poupaud in 1990 [40]. \square

In semiconductor crystals, scattering of electrons is due to lattice defects, phonons, and other carriers. We mention the most important collision events:

- electron-phonon scattering,
- ionized impurity scattering, and
- carrier-carrier scattering.

Carrier-carrier scattering includes electron-electron or electron-hole collisions. In the following, we only explain electron-phonon scattering since this is the most important collision mechanism.

At nonzero temperature, the atoms in the crystal lattice vibrate around their fixed equilibrium. These vibrations are quantized and the quantum of lattice vibrations is called a *phonon*. We can distinguish so-called *acoustic phonons* and *optical phonons*. Acoustic phonons arise from displacements of lattice atoms in the same direction such as sound waves. Optical phonons describe displacements in the wave vector and are able to interact

strongly with light. Denoting by $\hbar\omega_\alpha$ the energy of a phonon with frequency ω_α , the phonon occupation number N_α is computed from Bose-Einstein statistics,

$$N_\alpha = \frac{1}{e^{\hbar\omega_\alpha/k_B T} - 1},$$

where the index α refers to either “op” for optical phonons or “ac” for acoustic phonons. Notice that Bose-Einstein statistics has to be used for indistinguishable particles not obeying the Pauli exclusion principle and therefore also for phonons (see [11, p. 307ff.] for a derivation).

An electron in the Bloch state k' with conduction-band energy $E(k')$ before the collision with a phonon with quantized frequency ω_α can change to the state k after the collision if

$$E(k') - E(k) = \pm\hbar\omega_\alpha, \quad (66)$$

where the plus sign refers to phonon emission and the minus sign for phonon absorption. The transition rate $s(x, k, k')$ is nonzero only if the energy conservation condition (66) is satisfied. Therefore,

$$s_\alpha(x, k, k') = \sigma_\alpha(x, k, k') \times \left((1 + N_\alpha)\delta(E(k') - E(k) + \hbar\omega_\alpha) + N_\alpha\delta(E(k') - E(k) - \hbar\omega_\alpha) \right), \quad (67)$$

where the number $\sigma_\alpha(x, k, k')$ is assumed to be symmetric in k and k' and δ is the delta distribution. The first delta distribution contributes when an energy of $\hbar\omega_\alpha$ has been absorbed, i.e. $E(k') = E(k) - \hbar\omega_\alpha$, whereas the second term contributes when an energy of $\hbar\omega_\alpha$ has been emitted, i.e. $E(k') = E(k) + \hbar\omega_\alpha$. The factors $1 + N_\alpha$ and N_α come from the eigenvalues of the so-called creation and annihilation operators [49, Appendix B].

Generally, the phonon energy $\hbar\omega_\alpha$ can be interpreted as a function of the wave vectors k and k' . For optical (nonpolar) phonon scattering, the dependency is weak such that ω_{op} can be considered to be constant [36, Sec. 1.8]. On the other hand, the energy of acoustic phonons is rather small compared to the kinetic energy of a carrier and can be neglected near room temperature, $\hbar\omega_{\text{ac}} \approx 0$. Then (67) can be simplified for elastic acoustic phonon scattering to

$$s_{\text{ac}}(x, k, k') = \sigma_0\delta(E(k') - E(k)), \quad (68)$$

where $\sigma_0 = \sigma_{\text{ac}}(2N_{\text{ac}} + 1)$ does not depend on k nor k' .

The collision operator reads according to (57)

$$(Q_\alpha(f))(x, k, t) = \int_B (s_\alpha(x, k', k)f'(1 - f) - s_\alpha(x, k, k')f(1 - f')) dk', \quad (69)$$

where $\alpha = \text{ac, op}$. For acoustic phonon scattering in the elastic approximation, for which (68) holds, we can employ the symmetry of δ to obtain

$$\begin{aligned} \int_B (s_{\text{ac}}(x, k', k)f'f - s_{\text{ac}}(x, k, k')ff') dk' &= \int_B \sigma_0\delta(E(k') - E(k))(f'f - ff') dk' \\ &= 0, \end{aligned}$$

and the collision operator becomes

$$(Q_{\text{ac}}(f))(x, k, t) = \int_B \sigma_0 \delta(E(k') - E(k))(f' - f) dk'. \quad (70)$$

The above expression for s_α shows that the scattering rates can be highly nonsmooth. In fact, they may not be functions but distributions. As already mentioned in Section 2.5, integrals involving the delta distribution can be interpreted by employing the coarea formula (34). Indeed, let $S_\varepsilon = \{k \in B : E(k) = \varepsilon\}$ be the surface of constant energy ε , $dS_\varepsilon(k)$ the Euclidean surface element on S_ε , and $dN_\varepsilon(k) = dS_\varepsilon(k)/|\nabla_k E(k)|$ the coarea measure. Then $N(\varepsilon) = 2(2\pi)^{-3} \int_{S_\varepsilon} dN_\varepsilon$ is the density of states of energy ε (see (35)). The coarea formula can now be formulated as

$$\int_{\mathbb{R}^3} g(k) dk = \int_{\mathbb{R}} \int_{S_\varepsilon} g(k) dN_\varepsilon(k) d\varepsilon.$$

The collision integral (70), for instance, then becomes

$$(Q_{\text{ac}}(f))(x, k, t) = \int_{S_{E(k)}} \sigma_0 f(k') dN_{E(k)}(k') - f(k) \int_{S_{E(k)}} \sigma_0 dN_{E(k)}(k')$$

and does not contain delta distributions anymore.

The Boltzmann equation (56) is fundamental in deriving simpler macroscopic models for semiconductors (see below). It is the basic equation in semi-classical semiconductor modeling and usually, other models are validated by numerical comparisons with the Boltzmann equation. Nevertheless, it is important to understand its limitations (here we follow [36, Sec. 37]):

- The semiconductor Boltzmann equation is a single-particle description of a many-particle charge-carrier system. Correlations between carriers are incorporated only by the effective-field approximation.
- Quantum mechanical phenomena are only modeled in a semi-classical way. Electrons are considered as particles obeying the semi-classical Newton laws.
- Collisions are assumed to be binary and to be instantaneous in time and local in space.
- The statistical description using the probability density $f(x, k, t)$ makes only sense if the number of carriers is sufficiently large.

3.4 Properties of the Collision Operators

We analyze the low-density approximation of the collision operator (69) and its elastic approximation (70).

Low-density approximation. The low-density approximation of the collision operator (57) is derived under the assumption that the distribution function is much smaller than one such that $1 - f(x, k, t) \approx 1$.

Instead of specifying the scattering rate $s(x, k, k')$ of the collision operator, we derive a relation which is sufficient to conclude the properties. We assume that the *principle of detailed balance* [6] holds, according to which the *local* scattering probabilities vanish,

$$s(x, k', k) f'_{\text{eq}} (1 - f_{\text{eq}}) - s(x, k, k') f_{\text{eq}} (1 - f'_{\text{eq}}) = 0.$$

Here, the prime means evaluation at k' and f_{eq} is the thermal equilibrium occupation number density given by the Fermi-Dirac distribution

$$f_{\text{eq}}(x, k) = \frac{1}{1 + \exp((E(k) - E_F)/k_B T)},$$

where $E(k)$ is the band energy and E_F the Fermi energy (see Section 2.5). This shows that

$$\begin{aligned} \frac{s(x, k, k')}{s(x, k', k)} &= \frac{f'_{\text{eq}} (1 - f_{\text{eq}})}{f_{\text{eq}} (1 - f'_{\text{eq}})} = \frac{1 + e^{(E(k) - E_F)/k_B T}}{1 + e^{(E(k') - E_F)/k_B T}} \frac{e^{(E(k) - E_F)/k_B T}}{1 + e^{(E(k) - E_F)/k_B T}} \frac{1 + e^{(E(k') - E_F)/k_B T}}{e^{(E(k') - E_F)/k_B T}} \\ &= \exp \frac{E(k) - E(k')}{k_B T}. \end{aligned} \quad (71)$$

With the assumptions $1 - f_{\text{eq}} \approx 1$ and $f_{\text{eq}} \approx M(k) = \exp(-E(k)/k_B T)$ (the Maxwellian), we find that

$$\frac{s(k', k)}{M(k)} = \frac{s(k, k')}{M(k')}. \quad (72)$$

Then, using (72),

$$Q(f)(k) \approx \int_B (s(k', k) f' - s(k, k') f) dk = \int_B \frac{s(k', k)}{M(k)} (M f' - M' f) dk'.$$

This motivates the introduction of the *low-density collision operator*

$$(Q_0(f))(x, k, t) = \int_B \sigma(x, k', k) (M f' - M' f) dk', \quad (73)$$

where the *collision cross-section* $\sigma(x, k', k) = s(x, k', k)/M(k)$ is symmetric thanks to (72). For this operator, the following properties holds.

Proposition 3.5 (Low-density collision operator). *Let $\sigma(x, k, k') > 0$ be symmetric in k and k' . Then it holds:*

(1) *For all functions $f(x, k, t)$, we have*

$$\int_B (Q_0(f))(x, k, t) dk = 0 \quad \text{for } x \in \mathbb{R}^3, t > 0.$$

(2) For all nonnegative functions $f(x, k, t)$ and nondecreasing functions $\chi : \mathbb{R} \rightarrow \mathbb{R}$,

$$\int_B (Q_0(f))(x, k, t) \chi(f(x, k, t) e^{E(k)/k_B T}) dk \leq 0. \quad (74)$$

(3) The kernel $N(Q_0)$ of Q_0 is spanned by the Maxwell-Boltzmann distribution or Maxwellian

$$M(k) = e^{-E(k)/k_B T}.$$

The first property expresses the conservation of mass since integration of the Boltzmann equation with respect to (x, k) yields for the particle density $n(x, t) = \int_B f(x, k, t) dk$,

$$\begin{aligned} \partial_t \int_{\mathbb{R}^3} n(x, t) dx + \underbrace{\int_{\mathbb{R}^3} \operatorname{div}_x \int_B v(k) f dk dx}_{=0} + \frac{q}{\hbar} \int_{\mathbb{R}^3} \nabla_x V \cdot \underbrace{\int_B \nabla_k f dk}_{=0} dx \\ = \int_{\mathbb{R}^3} \underbrace{\int_B Q_0(f) dk}_{=0} dx = 0. \end{aligned}$$

Proof. The proof of the first part follows immediately from the symmetry of σ . For the second part, we compute

$$\begin{aligned} \int_{\mathbb{R}^3} Q_0(f) \chi(f/M) dk &= \int_{B^2} \sigma(Mf' - M'f) \chi(f/M) dk' dk \\ &= \int_{B^2} \sigma M M' \left(\frac{f'}{M'} - \frac{f}{M} \right) \chi\left(\frac{f}{M} \right) dk' dk. \end{aligned}$$

We add this relation to the equation in which k and k' are exchanged:

$$\begin{aligned} \int_B Q_0(f) \chi(f/M) dk \\ = -\frac{1}{2} \int_{B^2} \sigma M M' \left(\frac{f'}{M'} - \frac{f}{M} \right) \left(\chi\left(\frac{f'}{M'} \right) - \chi\left(\frac{f}{M} \right) \right) dk' dk \leq 0. \end{aligned} \quad (75)$$

Finally, the third part follows from this inequality taking $\chi(x) = x$. \square

Elastic collision operator. Some scattering mechanisms can be described or approximated by elastic collisions, like ionized impurity or acoustic phonon scattering. According to (70), the corresponding collision operator can be written as

$$(Q_{\text{el}}(f))(x, k, t) = \int_B \sigma(x, k, k') \delta(E(k') - E(k)) (f' - f) dk'.$$

We assume that the scattering rate σ is positive and symmetric,

$$\sigma(x, k, k') = \sigma(x, k', k) > 0, \quad x \in \mathbb{R}^3, \quad k, k' \in B. \quad (76)$$

Then the following properties were proved by Ben Abdallah and Degond [8].

Proposition 3.6 (Elastic collision operator). *Let the condition (76) hold. Then:*

(1) *For all (regular) functions $f(x, k, t)$,*

$$\int_B (Q_{\text{el}}(f))(x, k, t) dk = \int_B (Q_{\text{el}}(f))(x, k, t) E(k) dk = 0 \quad \text{for } x \in \mathbb{R}^3, t > 0.$$

(2) *The operator $-Q_{\text{el}}$ is symmetric and nonnegative in the sense*

$$-\int_B Q_{\text{el}}(f)f dk \geq 0 \quad \text{for all functions } f.$$

(3) *The kernel $N(Q_{\text{el}})$ of Q_{el} consists of all functions which depend only on the energy, being of the form $F(x, E(k), t)$.*

The first property expresses the conservation of mass and energy. The energy conservation only holds in the absence of external forces. Indeed, defining the energy density $ne = \int_{\mathbb{R}^3} f E(k) dk / 4\pi^3$ and integrating the Boltzmann equation (56) gives

$$\frac{d}{dt} \int_{\mathbb{R}^3} ne(x, t) dx = \int_{\mathbb{R}^3} \int_B \partial_t f E(k) \frac{dk}{4\pi^3} dx = - \int_{\mathbb{R}^3} \int_B \text{div}_x(vEf) \frac{dk}{4\pi^3} dx = 0.$$

Proof. (1) The first property follows from the symmetry of σ and δ ,

$$\begin{aligned} \int_{B^2} Q_{\text{el}}(f) E^{i-1} dk' dk &= \int_{B^2} \sigma(x, k, k') \delta(E' - E) f' E^{i-1} dk' dk \\ &\quad - \int_{B^2} \sigma(x, k, k') \delta(E - E') f' (E')^{i-1} dk dk' \\ &= \int_{B^2} \sigma(x, k, k') \delta(E' - E) f' E^{i-1} dk' dk \\ &\quad - \int_{B^2} \sigma(x, k, k') \delta(E' - E) f' E^{i-1} dk dk' = 0, \end{aligned}$$

where $E' = E(k')$ and $i = 1, 2$. We have used that $\delta(E' - E)E = \delta(E' - E)E'$.

(2) A computation similar as above gives for functions f and g :

$$\begin{aligned} \int_B Q_{\text{el}}(f)g dk &= \frac{1}{2} \int_{B^2} \sigma(x, k, k') \delta(E' - E) (f' - f)g dk' dk \\ &\quad + \frac{1}{2} \int_{B^2} \sigma(x, k', k) \delta(E - E') (f - f')g' dk dk' \\ &= -\frac{1}{2} \int_{B^2} \sigma(x, k, k') \delta(E' - E) (f' - f)(g' - g) dk' dk \\ &= \int_B Q_{\text{el}}(g)f dk. \end{aligned}$$

This shows that $-Q_{\text{el}}$ is symmetric. Moreover, it is nonnegative, since the choice $f = g$ leads to

$$-\int_B Q_{\text{el}}(f)f dk = \frac{1}{2} \int_{B^2} \sigma(x, k, k') \delta(E' - E) (f' - f)^2 dk' dk \geq 0. \quad (77)$$

(3) Let $f \in N(Q_{el})$. Then (77) implies that

$$\delta(E(k') - E(k))(f(k') - f(k))^2 = 0 \quad \text{for } k, k' \in \mathbb{R}^3.$$

Since the support of the delta distribution is concentrated at the origin we must have $f(k') = f(k)$ at all points $k, k' \in \mathbb{R}^3$ for which $E(k') = E(k)$. Thus, f is constant on each energy surface $\{k \in \mathbb{R}^3 : E(k) = \varepsilon\}$ for $\varepsilon \in \mathbb{R}$ which means that f is a function of $E(k)$ only. \square

4 Drift-Diffusion Equations

In this and the following section, we are concerned with the formal derivation of semi-classical macroscopic transport models from the semiconductor Boltzmann equation. We start in this section with the derivation of drift-diffusion equations, which are the simplest semiconductor model in the hierarchy. It was first derived by van Roosbroeck in 1950 [50]. In this section, we will employ the low-density operator (73). The derivation was made rigorous by Poupaud [41].

The starting point of the derivation is the semiconductor Boltzmann equation (56) for the distribution function $f = f(x, k, t)$,

$$\partial_t f + v(k) \cdot \nabla_x f + \frac{q}{\hbar} \nabla_x V \cdot \nabla_k f = Q(f), \quad x \in \mathbb{R}^3, k \in B, t > 0, \quad (78)$$

with the initial datum $f(\cdot, \cdot, 0) = f_I$ in $\mathbb{R}^3 \times B$, together with the Poisson equation for the electric potential V ,

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

where $v(k) = \nabla_k E/\hbar$ denotes the group velocity with the energy band $E(k)$ depending on the pseudo wave vector k , $Q(f)$ is the collision operator, $n = \int_B f dk/4\pi^3$ the electron density, $C = C(x)$ the doping profile, and B is the Brillouin zone.

4.1 Scaling of the Boltzmann-Poisson system

Before we explain the assumptions needed to derive the drift-diffusion model, we scale the Boltzmann equation in order to identify small parameters. We introduce the domain diameter L and the *mean free path* λ , which is the distance a particle travels between two consecutive scattering events. Furthermore, we introduce the reference values

- the reference length $\lambda_0 = \sqrt{L\lambda}$,
- the reference velocity $v_0 = \sqrt{k_B T_L/m^*}$,
- the reference potential $U_T = k_B T_L/q$ (thermal voltage), where T_L is the lattice temperature.

This means that the kinetic energy $m^*v_0^2/2 = k_B T/2$, the electric energy $qU_T = k_B T$, and the thermal energy $k_B T_L$ are of the same order. Thus, we consider the case of small electric fields only. Further reference values are

- the time $\tau_0 = L/v_0$, which a particle with the typical velocity v_0 needs to cross the domain,
- the typical time $\tau = \lambda/v_0$ between two consecutive collisions,
- the reference wave vector $k_0 = m^*v_0/\hbar$, corresponding to the momentum $\hbar k_0 = m^*v_0$.

Thus, the variables are scaled as follows:

$$t = \tau_0 t_s, \quad x = \lambda_0 x_s, \quad k = k_0 k_s, \quad v(k) = v_0 v_s(k_s), \quad V = U_T V_s,$$

where t_s, x_s, k_s etc. are the scaled quantities. Finally, the collision operator is assumed to be of order $1/\tau$,

$$Q(f) = \frac{1}{\tau} Q_s(f).$$

With this scaling, the Boltzmann equation (78) becomes,

$$\frac{1}{\tau_0} \partial_{t_s} f + \frac{v_0}{\lambda_0} v_s(k) \cdot \nabla_{x_s} f + \frac{U_T}{\lambda_0 k_0} \nabla_{x_s} V_s \cdot \nabla_{k_s} f = \frac{1}{\tau} Q_s(f).$$

Multiplication with τ gives

$$\underbrace{\frac{\tau}{\tau_0}}_{=\lambda/L} \partial_{t_s} f + \underbrace{\frac{v_0 \tau}{\lambda_0}}_{=\lambda/\lambda_0} v_s(k) \cdot \nabla_{x_s} f + \frac{q}{\hbar} \frac{U_T \tau}{\lambda_0 k_0} \nabla_{x_s} V_s \cdot \nabla_{k_s} f = Q_s(f).$$

Using

$$\frac{q}{\hbar} \frac{U_T \tau}{\lambda_0 k_0} = \frac{q}{\hbar} \frac{k_B T_L}{q} \frac{\lambda}{v_0} \frac{1}{\sqrt{L\lambda}} \frac{\hbar}{m^* v_0} = \frac{k_B T_L}{m^* v_0^2} \sqrt{\frac{\lambda}{L}} = \sqrt{\frac{\lambda}{L}}$$

and omitting the index “s”, we infer that

$$\alpha^2 \partial_t f + \alpha (v(k) \cdot \nabla_x f + \nabla_x V \cdot \nabla_k f) = Q(f), \quad (79)$$

where $\alpha = \lambda/\lambda_0 = \sqrt{\lambda/L}$ is the ratio of the mean free path and the reference length. Scaling the particle and doping concentrations by k_0 , i.e. $n = k_0 n_s$ and $C = k_0 C_s$, the Poisson equation becomes

$$\frac{\varepsilon_s U_T}{\lambda_0^2} \Delta_s V_s = q k_0 (n_s - C_s).$$

Dividing this equation by $q k_0$ and omitting again the index “s”, it follows that

$$\lambda_D^2 \Delta V = n - C(x), \quad (80)$$

where

$$\lambda_D^2 = \frac{\varepsilon_s U_T}{q \lambda_0^2 k_0} \quad (81)$$

is the (squared) scaled *Debye length*.

Now, we are able to specify our assumptions, following [41] (also see [39]):

1. The energy band is given by the parabolic approximation $E(k) = E_c + \hbar^2 |k|^2 / 2m^*$, where E_c is the conduction band minimum.
2. The collision operator is given by the low-density approximation (see (73))

$$(Q(f))(x, k, t) = \int_B \sigma(x, k, k') (Mf' - M'f) dk',$$

where the collision cross-section $\sigma(x, k, k')$ is positive and symmetric in k' and k , $M(k) = e^{-E(k)/k_B T_L}$ is the Maxwellian, and $f' = f(k')$, $M' = M(k')$.

3. The mean free path is very small compared to the device diameter, i.e. $\alpha \ll 1$.

The first assumption implies that the mean velocity can be written as $v(k) = \hbar k / m^*$. We can extend the Brillouin zone to the whole space and write $B = \mathbb{R}^3$ in the continuum limit. The second condition prescribes a linear collision operator which excludes nondegenerate materials. The diffusion approximation of the Boltzmann equation with degenerate Fermi-Dirac statistics was performed by Golse and Poupaud [26]. The third hypothesis means that collisions occur frequently in the material.

In the parabolic-band approximation, the scaled velocity becomes $v(k) = k$ and the scaled collision operator can be written as

$$(Q(f))(x, k, t) = \int_{\mathbb{R}^3} s(x, k, k') (Mf' - M'f) dk', \quad (82)$$

where we have set $s(x, k, k') = N e^{-E_c/k_B T_L} \sigma(x, k, k')$, the scaled Maxwellian equals $M(k) = N^{-1} e^{-|k|^2/2}$ and $N = 2(2\pi)^{-3/2}$ is such that the Maxwellian is normalized, i.e. $\int_{\mathbb{R}^3} M(k) dk / 4\pi^3 = 1$.

4.2 Properties of the Low-Density Collision Operator

We will analyze the kernel $N(Q)$ and the range $R(Q)$ of the collision operator (82), where

$$N(Q) = \{f : Q(f) = 0\}, \quad R(Q) = \{g : \text{there exists } f \text{ such that } Q(f) = g\}.$$

To this end, we introduce, for fixed $x \in \mathbb{R}^3$, the total cross-section

$$S(k) = \int_{\mathbb{R}^3} s(x, k, k') M(k') dk', \quad k \in \mathbb{R}^3,$$

and the Banach spaces X and Y , which consist of all measurable functions $f : \mathbb{R}^3 \rightarrow \mathbb{R}$ such that $\|f\|_X$ and $\|f\|_Y$ are finite, where

$$\begin{aligned}\|f\|_X^2 &= \int_{\mathbb{R}^3} f(k)^2 S(k) M(k)^{-1} dk, \\ \|f\|_Y^2 &= \int_{\mathbb{R}^3} f(k)^2 S(k)^{-1} M(k)^{-1} dk.\end{aligned}$$

By Proposition 3.5 (3), the kernel of Q is spanned by the Maxwellian $M(k)$. For the analysis of the range of Q , we employ the following version of the *Fredholm alternative*.

Lemma 4.1 (Fredholm alternative). *Let X be a Hilbert space and $Q : X \rightarrow X$ be a linear, continuous, and closed operator (i.e. $R(Q)$ is closed). Then*

$$Q(f) = g \text{ has a solution if and only if } g \in N(Q^*)^\perp.$$

Here, Q^* denotes the adjoint operator of Q and $N(Q^*)^\perp$ is the orthogonal complement of $N(Q^*)$. The Fredholm alternative is a consequence of the following equivalence:

$$Q(f) = g \text{ has a solution} \quad \Leftrightarrow \quad g \in R(Q) = \overline{R(Q)} = N(Q^*)^\perp.$$

We refer to, e.g., [54] for the functional analytical details.

The following lemma is a consequence of the Fredholm alternative.

Lemma 4.2. *Let the collision operator Q be given by (82).*

(1) *The equation $Q(f) = g$ has a solution $f \in X$ if and only if*

$$\int_{\mathbb{R}^3} g(k) dk = 0.$$

In this situation, any solution of $Q(f) = g$ can be written as $f + nM$, where $n = n(x)$ is a parameter.

(2) *The solution $f \in X$ of $Q(f) = g$ is unique if the orthogonality relation*

$$\int_{\mathbb{R}^3} f(k) S(k) dk = 0 \tag{83}$$

is satisfied.

Proof. (1) First we symmetrize the collision operator (82) by setting $f_s = \sqrt{S/M} f$ and $Q_s(f_s) = (SM)^{-1/2} Q(f)$. Then

$$\begin{aligned}Q_s(f_s) &= \frac{1}{\sqrt{SM}} \left(M \int_{\mathbb{R}^3} s(x, k, k') f' dk' - S f \right) \\ &= \int_{\mathbb{R}^3} s(x, k, k') \left(\frac{MM'}{SS'} \right)^{1/2} f'_s dk' - f_s.\end{aligned}$$

Since s is symmetric in k and k' by assumption, the operator $Q_s : L^2(\mathbb{R}^3) \rightarrow L^2(\mathbb{R}^3)$ is symmetric. It is possible to prove that Q_s is closed. By the Fredholm alternative, $Q_s(f_s) = g_s$ has a solution in $L^2(\mathbb{R}^3)$ if and only if $g_s \in N(Q_s^*)^\perp = N(Q_s)^\perp$ which means that

$$\int_{\mathbb{R}^3} g_s h \, dk = 0 \quad \text{for all } h \in N(Q_s).$$

The kernel of Q_s is spanned by $\sqrt{S/M}M = \sqrt{SM}$, such that the above relation is equivalent to

$$0 = \int_{\mathbb{R}^3} g_s \sqrt{SM} \, dk = \int_{\mathbb{R}^3} g \, dk,$$

since in the original variables we have $g = Q(f) = \sqrt{SM}Q_s(f_s) = \sqrt{SM}g_s$.

Let f_1 and f_2 be two solutions of $Q(f) = g$. Then, since Q is linear, $Q(f_1 - f_2) = 0$ and thus, $f_1 - f_2 \in N(Q)$. This shows that $f_2 = f_1 + nM$ for some $n = n(x)$.

(2) We only give a sketch of the proof and refer to [41] for details. It is possible to show that $-Q_s$ is coercive on $N(Q_s)^\perp$,

$$-\int_{\mathbb{R}^3} Q_s(f_s) f_s \, dk \geq c \|f_s\|_{L^2(\mathbb{R}^3)}^2 \quad \text{for all } f_s \in N(Q_s)^\perp,$$

where $c > 0$ is some constant. The proof is based on the fact that $\text{Id} + Q_s$ is a Hilbert-Schmidt operator. The coercivity property implies that Q_s (and also Q) is one-to-one on

$$\begin{aligned} N(Q_s)^\perp &= \left\{ f_s : 0 = \int_{\mathbb{R}^3} f_s w \, dk \text{ for all } w \in N(Q_s) = \text{span} \sqrt{SM} \right\} \\ &= \left\{ f_s : 0 = \int_{\mathbb{R}^3} f_s \sqrt{SM} \, dk = \int_{\mathbb{R}^3} f S \, dk \right\}, \end{aligned}$$

which proves the uniqueness of solutions on this set. \square

Finally, we prove some properties of the solution of the operator equations

$$Q(h_i) = k_i M(k), \quad i = 1, 2, 3. \quad (84)$$

These equations have solutions, due to Lemma 4.2, since the functions $k_i \mapsto k_i M(k)$ are odd and hence, their integrals vanish. The solutions are unique in the space of functions h_i satisfying $\int_{\mathbb{R}^3} h_i(k) S(k) \, dk = 0$. We set $h = (h_1, h_2, h_3)^\top$.

Lemma 4.3. *Assume that the collision cross-section is invariant with respect to isometric operations, i.e., for all isometric matrices $A \in \mathbb{R}^{3 \times 3}$ it holds*

$$\sigma(x, Ak, Ak') = \sigma(x, k, k') \quad \text{for all } x, k, k' \in \mathbb{R}^3. \quad (85)$$

Then there exists a scalar function $\mu_0(x) \geq 0$ such that the solutions h_i of (84) satisfy

$$\int_{\mathbb{R}^3} k \otimes h \frac{dk}{4\pi^3} = -\mu_0(x) \text{Id}, \quad (86)$$

where $k \otimes h$ is the matrix with components $k_i h_j$ and Id is the identity matrix in $\mathbb{R}^{3 \times 3}$.

In the statement of the lemma, we have omitted some technical (regularity) assumptions on the collision cross-section σ . Details can be found in [41].

Proof. Let A be the matrix of a rotation about the axis k_1 . Then $(Ak)_1 = k_1$ for all $k \in \mathbb{R}^3$. Since A is isometric, i.e. $|Ak| = |k|$, we obtain $M(Ak) = N^{-1}e^{-|Ak|^2/2} = N^{-1}e^{-|k|^2/2} = M(k)$ and $(Ak)_1 M(Ak) = k_1 M(k)$. This implies, together with assumption (85) and the transformation $w = Ak'$ with $dw = |\det A| dk' = dk'$,

$$\begin{aligned} (Q(h_1 \circ A))(k) &= \int_{\mathbb{R}^3} s(x, k, k') (M(k)h_1(Ak') - M(k')h_1(Ak)) dk' \\ &= \int_{\mathbb{R}^3} s(x, Ak, Ak') (M(Ak)h_1(Ak') - M(Ak')h_1(Ak)) dk' \\ &= \int_{\mathbb{R}^3} s(x, Ak, w) (M(Ak)h_1(w) - M(w)h_1(Ak)) dw \\ &= (Q(h_1))(Ak) = (Ak)_1 M(Ak) = k_1 M(k) = (Q(h_1))(k), \end{aligned}$$

and thus $Q(h_1 \circ A - h_1) = 0$. Another computation yields

$$\begin{aligned} \int_{\mathbb{R}^3} h_1(Ak) S(k) dk &= \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} s(x, k, k') h_1(Ak) M(k') dk' dk \\ &= \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} s(x, Ak, Ak') h_1(Ak) M(Ak') dk' dk \\ &= \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} s(x, v, w) h_1(v) M(w) dw dv = \int_{\mathbb{R}^3} h_1(v) S(v) dv \end{aligned}$$

and hence

$$\int_{\mathbb{R}^3} (h_1 \circ A - h_1) S dk = 0.$$

This is the orthogonality condition (83) which ensures the uniqueness of the solution of $Q(h_1 \circ A - h_1) = 0$. Therefore, $h_1 \circ A - h_1 = 0$. We conclude that h_1 remains invariant under a rotation about the axis k_1 . In particular, we can write $h_1(k) = H_1(k_1, |k|^2 - k_1^2)$ for some function H_1 .

Now, let A be the isometric matrix corresponding to the linear mapping $k \mapsto (-k_1, k_2, k_3)$. Since $k \mapsto k_1 M(k)$ is odd, a similar computation as above gives $Q(h_1 \circ A) = -Q(h_1)$ and

$$\int_{\mathbb{R}^3} (h_1 \circ A + h_1) S dk = 0.$$

This implies that $h_1 \circ A + h_1 = 0$. Thus, h_1 is an odd function with respect to k_1 .

In a similar way, we can show that $h_i(k) = H_i(k_i, |k|^2 - k_i^2)$ for $i = 2, 3$ and H_i are odd functions with respect to the first argument. In fact, all the functions H_i are equal since, for instance, exchanging k_1 and k_2 in

$$Q(H_1(k_1, k_2^2 + k_3^2)) = k_1 M(k_1^2 + k_2^2 + k_3^2)$$

(with a slight abuse of notation) leads to

$$Q(H_1(k_2, k_1^2 + k_3^2)) = k_2 M(k_1^2 + k_2^2 + k_3^2) = Q(H_2(k_2, k_1^2 + k_3^2))$$

or $Q(H_1 - H_2) = 0$ and thus, $H_1 = H_2$. We set $H = H_1$.

Since H is odd with respect to its first argument and $|k|^2 - k_j^2$ does not depend on k_j , we obtain

$$\int_{\mathbb{R}^3} k_i h_j(k) dk = \int_{\mathbb{R}^3} k_i H(k_j, |k|^2 - k_j^2) dk = 0 \quad \text{for all } i \neq j. \quad (87)$$

Furthermore,

$$\begin{aligned} \int_{\mathbb{R}^3} k_i h_i(k) dk &= \int_{\mathbb{R}^3} k_i H(k_i, |k|^2 - k_i^2) dk = \int_{\mathbb{R}^3} k_j H(k_j, |k|^2 - k_j^2) dk \\ &= \int_{\mathbb{R}^3} k_j h_j(k) dk \quad \text{for all } i, j. \end{aligned}$$

This means that the integral is independent of i , and we can set

$$\mu_0 = - \int_{\mathbb{R}^3} k_1 h_1(k) \frac{dk}{4\pi^3} = - \int_{\mathbb{R}^3} Q(h_1) h_1 M^{-1} \frac{dk}{4\pi^3}.$$

The parameter μ_0 depends on x since h_1 depends on x through Q . We have proved in (75) that

$$\int_{\mathbb{R}^3} Q(f) \chi(f/M) dk \leq 0 \quad \text{for all } f$$

and all nondecreasing functions χ . Choosing $\chi(x) = x$ shows that

$$\mu_0(x) = - \int_{\mathbb{R}^3} Q(h_1) h_1 M^{-1} \frac{dk}{4\pi^3} \geq 0,$$

and, in view of (87), we have shown (86). \square

4.3 Derivation of the Drift-Diffusion Equations

Now, we are in the position to derive the drift-diffusion model. Let (f_α, V_α) be a solution of the scaled Boltzmann-Poisson system

$$\alpha^2 \partial_t f_\alpha + \alpha (v(k) \cdot \nabla_x f_\alpha + \nabla_x V_\alpha \cdot \nabla_k f_\alpha) = Q(f), \quad (88)$$

$$\lambda_D^2 \Delta V_\alpha = n_\alpha - C(x), \quad (89)$$

where $n_\alpha = \int_{\mathbb{R}^3} f_\alpha dk / 4\pi^3$. We assume that f_α and V_α and their derivatives converge, as $\alpha \rightarrow 0$, pointwise to f and V , respectively, and their corresponding derivatives. The derivation consists of three steps.

1. First, we perform the (formal) limit $\alpha \rightarrow 0$ in (88). This yields

$$Q(f) = 0. \quad (90)$$

Since the kernel is spanned by the Maxwellian, $f = n(x, t)M$, where $n(x, t) = \int_{\mathbb{R}^3} f(x, k, t) dk/4\pi^3$ (notice that the Maxwellian is normalized).

2. For the second step, we introduce the *Chapman-Enskog expansion* $f_\alpha = nM + \alpha g_\alpha$. (This equation has to be considered as a definition of g_α .) Inserting the expansion in the Boltzmann equation (88) gives, after division by α ,

$$\begin{aligned} \alpha \partial_t(nM + \alpha g_\alpha) + (k \cdot \nabla_x(nM) + \nabla_x V_\alpha \cdot \nabla_k(nM)) \\ + \alpha(k \cdot \nabla_x g_\alpha + \nabla_x V_\alpha \cdot \nabla_k g_\alpha) = Q(g_\alpha), \end{aligned}$$

since $Q(nM) = nQ(M) = 0$. We perform the limit $\alpha \rightarrow 0$ to obtain

$$Q(g) = k \cdot \nabla_x(nM) + \nabla_x V \cdot \nabla_k(nM) = (\nabla_x n - n \nabla_x V) \cdot kM, \quad (91)$$

where $g = \lim_{\alpha \rightarrow 0} g_\alpha$. This operator equation is of the form (84), since $\nabla_x n - n \nabla_x V$ is a function of (x, t) only and Q is linear.

3. In the third step, we derive the evolution equations. Integrating the Boltzmann equation (88) and inserting the Chapman-Enskog expansion gives, employing the notation $\langle f \rangle = \int_{\mathbb{R}^3} f dk/4\pi^3$,

$$\partial_t \langle nM \rangle + \alpha \partial_t \langle g_\alpha \rangle + \alpha^{-1} \operatorname{div}_x \langle k(nM) \rangle + \operatorname{div}_x \langle k g_\alpha \rangle = 0.$$

Here, we have used that $\langle \nabla_x V \cdot \nabla_k f_\alpha \rangle = 0$ and $\langle Q(f_\alpha) \rangle = 0$. Since $k \mapsto kM(k)$ is an odd function, also the integral $\langle k(nM) \rangle$ vanishes. Thus, performing the limit $\alpha \rightarrow 0$,

$$\partial_t n + \operatorname{div}_x \langle k g \rangle = 0. \quad (92)$$

The flux $J_n = -\langle k g \rangle$ can be computed in terms of n and $\nabla_x V$. To this end, we employ Lemma 4.3. Let h_i be a solution of $Q(h_i) = k_i M$ ($i = 1, 2, 3$) and set $h = (h_1, h_2, h_3)^\top$. Then $g = (\nabla_x n - n \nabla_x V) \cdot h$ solves (91) and, by (86),

$$J_n = -\langle k g \rangle = -\langle k \otimes h \rangle (\nabla_x n - n \nabla_x V) = \mu_0 (\nabla_x n - n \nabla_x V).$$

The limiting Poisson equation follows directly from (89) for $V = V_\alpha$ in the formal limit $\alpha \rightarrow 0$.

Summarizing, we have proved the following result.

Theorem 4.4 (Drift-diffusion equations). *Let the assumptions at the beginning of this chapter hold, the collision cross-section is invariant with respect to isometric operations,*

and let (f_α, V_α) be a solution of the Boltzmann-Poisson system (88)-(89). Then the limit $f = \lim_{\alpha \rightarrow 0} f_\alpha$, $V = \lim_{\alpha \rightarrow 0} V_\alpha$ satisfies the drift-diffusion equations

$$\begin{aligned} \partial_t n - \operatorname{div} J_n &= 0, & J_n &= \mu_0(\nabla n - n\nabla V), \\ \lambda_D^2 \Delta V &= n - C(x), & x &\in \mathbb{R}^3, t > 0, \end{aligned} \quad (93)$$

where $\mu_0(x) \geq 0$ comes from Lemma 4.3 and $n = \int_{\mathbb{R}^3} f \, dk / 4\pi^3$ is the electron density, satisfying $n(\cdot, 0) = \int_{\mathbb{R}^3} f_I \, dk / 4\pi^3$.

The current density is the sum of the *drift current* $-\mu_0 n \nabla V$ and the *diffusion current* $\mu_0 \nabla n$, which explains the name of the model. The quantity μ_0 is called the (scaled) *electron mobility*.

The unscaled equations are obtained by scaling back to the physical variables. Employing the reference electron mobility $\mu_{n,\text{ref}} = q\tau/m^*$ and the reference current density $J_{n,\text{ref}} = qU_T k_0 \mu_{n,\text{ref}} / \lambda_0$, a calculation yields

$$\begin{aligned} \partial_t n - q^{-1} \operatorname{div} J_n &= 0, & J_n &= q\mu_n(U_T \nabla n - n\nabla V), \\ \varepsilon_s \Delta V &= q(n - C(x)), & x &\in \mathbb{R}^3, t > 0. \end{aligned}$$

These equations have to be complemented by initial conditions for the particle density,

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

The derivation of the drift-diffusion model is mainly based on the following hypotheses:

- The mean free path λ between two consecutive scattering events is much smaller than the reference length λ_0 . Typically, the mean free path is of the order 10^{-7} m.
- The electric potential is of the order of $U_T = 0.026$ V (at $T_L = 300$ K).

Thus, the drift-diffusion model is appropriate for semiconductor devices with characteristic lengths not much smaller than about $1 \mu\text{m} = 10^{-6}$ m and applied voltages much smaller than 1 V. However, in applications this model is used also for higher applied voltages (including high-field corrections). It gives reasonable results as long as the characteristic length is not much smaller than about $1 \mu\text{m}$.

4.4 Bipolar Model

In the previous section, we have derived the drift-diffusion equations for electrons. In the valence band, also the motion of holes contributes to the total current density. Since holes are quasi-particles with positive charge, under the same assumptions as in the previous section, a drift-diffusion model for the holes can be derived. Let p denote the hole density and J_p the hole current density. Then

$$\partial_t p + \operatorname{div} J_p = 0, \quad J_p = -\mu_{0,p}(\nabla p + p\nabla V).$$

Here, $\mu_{0,p}$ is the hole mobility which is considerably smaller than the electron mobility (in silicon, electron mobility: $1400 \text{ cm}^2/\text{Vs}$, hole mobility: $450 \text{ cm}^2/\text{Vs}$).

Since electron-hole pairs may be generated or recombined, we add to the right-hand side the so-called *Shockley-Read-Hall recombination-generation term*

$$R(n, p) = \frac{np - n_i^2}{\tau_p(n + n_d) + \tau_n(p + p_d)},$$

where n_i is the intrinsic density, τ_n and τ_p are the carrier life times, and the densities n_d and p_d are defined by

$$n_d = N_c \exp\left(\frac{E_t - E_c}{k_B T_L}\right), \quad p_d = N_v \exp\left(\frac{E_v - E_t}{k_B T_L}\right).$$

Here, E_t denotes the trap energy level, and N_c and N_v are the carrier effective densities of states. Notice that $n_d p_d = n_i^2$. By ‘‘trap level’’, we mean energy levels in the forbidden band region, caused by crystal impurities. They facilitate the generation of electron-hole pairs, since the jump from the valence to the conduction band can be split into two parts, each of which requires less energy than the gap energy. The Shockley-Read-Hall model is usually derived by assuming one trap level and quasi-stationarity of the dynamics of the trapped electrons (see [11, Chap. 10] or [27, Chap. 10]).

A second change concerns the Poisson equation. Including the hole density to the total space charge, it reads as

$$\lambda_D^2 \Delta V = n - p - C(x).$$

Scaling back to the physical variables, we obtain the equations

$$\partial_t n - \frac{1}{q} J_n = -R(n, p), \quad J_n = q\mu_n(U_T \nabla n - n \nabla V), \quad (94)$$

$$\partial_t p + \frac{1}{q} J_p = -R(n, p), \quad J_p = -q\mu_p(U_T \nabla p + p \nabla V), \quad (95)$$

$$\varepsilon_s \Delta V = q(n - p - C(x)), \quad x \in \mathbb{R}^3, \quad t > 0. \quad (96)$$

The unscaled recombination-generation rate remains unchanged, but the *intrinsic density* n_i becomes

$$n_i = 2 \left(\frac{\sqrt{m_e^* m_h^*} k_B T_L}{2\pi \hbar^2} \right)^{3/2} \exp\left(-\frac{E_c - E_v}{2k_B T_L}\right).$$

This is exactly the value derived in Section 2.5 (see (38)).

4.5 Thermal Equilibrium State and Boundary Conditions

When we consider the drift-diffusion equations in a bounded domain $\Omega \subset \mathbb{R}^3$, we need to impose some boundary conditions. Their definition is based on the notion of thermal equilibrium, which we explain first.

Let (n, p, V) be a solution of the unscaled drift-diffusion equations (94)-(96). The thermal equilibrium state is a steady state with no current flow, i.e.

$$\partial_t n = \partial_t p = 0 \quad \text{and} \quad J_n = J_p = 0 \quad \text{in } \Omega.$$

This implies $R(n, p) = 0$ or $np = n_i^2$ in Ω and

$$\begin{aligned} 0 &= U_T \nabla n - n \nabla V = n \nabla (U_T \ln n - V), \\ 0 &= U_T \nabla p + p \nabla V = p \nabla (U_T \ln p + V). \end{aligned}$$

It is physically reasonable to assume that the particle densities n and p are positive in Ω . (In fact, this can be proved by employing maximum principle arguments, assuming that the boundary data are positive). This yields

$$\alpha = U_T \ln n - V = \text{const.}, \quad \beta = U_T \ln p + V = \text{const.} \quad (97)$$

or

$$n = e^{\alpha/U_T} e^{V/U_T}, \quad p = e^{\beta/U_T} e^{-V/U_T} \quad \text{in } \Omega.$$

We wish to determine the constants α and β . For this, we use the equation $np = n_i^2$ and the fact that V is determined only up to an additive constant. Then the sum of the two equations in (97) yields $\alpha + \beta = U_T \ln(np) = 2U_T \ln n_i$ and, replacing V by $V + \gamma$, where $\gamma = U_T \ln n_i - \alpha$, gives

$$n = e^{(\alpha+\gamma)/U_T} e^{V/U_T} = n_i e^{V/U_T} \quad (98)$$

and

$$p = e^{(\beta-\gamma)/U_T} e^{-V/U_T} = e^{(\beta+\alpha-U_T \ln n_i)/U_T} e^{-V/U_T} = n_i e^{-V/U_T}. \quad (99)$$

The equilibrium potential satisfies the semilinear elliptic equation

$$\begin{aligned} \varepsilon_s \Delta V &= q(n - p - C) = q(n_i e^{V/U_T} - n_i e^{-V/U_T} - C) \\ &= q \left(2n_i \sinh \frac{V}{U_T} - C \right) \quad \text{in } \Omega. \end{aligned} \quad (100)$$

Now, we can define the boundary conditions. We assume that the boundary of the semiconductor domain consists of two parts: one part, called the Dirichlet boundary, on which the particle densities and the potential are prescribed,

$$n = n_D, \quad p = p_D, \quad V = V_D \quad \text{on } \Gamma_D, \quad (101)$$

and another part, the Neumann boundary, which models the insulating boundary segments on which the normal components of the current densities and the electric field vanish,

$$J_n \cdot \nu = J_p \cdot \nu = \nabla V \cdot \nu = 0 \quad \text{on } \Gamma_N.$$

In view of the expressions (94)-(95) for J_n and J_p , this is equivalent to

$$\nabla n \cdot \nu = \nabla p \cdot \nu = \nabla V \cdot \nu = 0 \quad \text{on } \Gamma_N, \quad (102)$$

where ν denotes the exterior unit normal vector to $\partial\Omega$.

It remains to determine the boundary functions n_D , p_D , and V_D . We make the following assumptions:

- The total space charge vanishes on Γ_D , $n_D - p_D - C(x) = 0$.
- The densities are in equilibrium on Γ_D , $n_D p_D = n_i^2$.
- The boundary potential is the superposition of the *built-in-potential* V_{bi} and the applied voltage U , $V_D = V_{\text{bi}} + U$.

Clearly, in thermal equilibrium we have $U = 0$. The built-in potential is the potential corresponding to the equilibrium densities given by (98) and (99):

$$n_D = n_i e^{V_{\text{bi}}/U_T}, \quad p_D = n_i e^{-V_{\text{bi}}/U_T}. \quad (103)$$

Substituting the equation $n_D - p_D - C = 0$ into $n_D p_D = n_i^2$ leads to the quadratic equation $n_D^2 - C n_D = n_i^2$ whose solution is given by

$$n_D = \frac{1}{2} \left(C + \sqrt{C^2 + 4n_i^2} \right), \quad p_D = \frac{1}{2} \left(-C + \sqrt{C^2 + 4n_i^2} \right) \quad \text{on } \Gamma_D.$$

Thus we infer from (103) that

$$V_{\text{bi}} = U_T \ln \frac{n_D}{n_i} = U_T \ln \left(\frac{C}{2n_i} + \sqrt{\frac{C^2}{4n_i^2} + 1} \right) = U_T \operatorname{arsinh} \frac{C}{2n_i}. \quad (104)$$

Therefore, the thermal equilibrium state $(n_{\text{eq}}, p_{\text{eq}}, V_{\text{eq}})$ is the (unique) solution of (100) with the boundary conditions

$$V_{\text{eq}} = V_{\text{bi}} \quad \text{on } \Gamma_D, \quad \nabla V_{\text{eq}} \cdot \nu = 0 \quad \text{on } \Gamma_N,$$

where V_{bi} is given by (104), and

$$n_{\text{eq}} = n_i e^{V_{\text{eq}}/U_T}, \quad p_{\text{eq}} = n_i e^{-V_{\text{eq}}/U_T} \quad \text{in } \Omega.$$

Furthermore, the drift-diffusion equations (94)-(96) are solved with the boundary conditions (101)-(102), where n_D and p_D are defined in (103) and $V_D = V_{\text{bi}} + U$, with V_{bi} given in (104).

5 Hydrodynamic Equations

Like in the previous chapters, the starting point is the semiconductor Boltzmann equation for the distribution function $f = f(x, k, t)$,

$$\partial_t f + v(k) \cdot \nabla_x f + \frac{q}{\hbar} \nabla_x V \cdot \nabla_k f = Q(f), \quad x \in \mathbb{R}^3, \quad k \in B, \quad t > 0,$$

where $v(k) = \nabla_k E(k)/\hbar$ is the group velocity, $E(k)$ the energy band structure depending on the (pseudo) wave vector k , $V(x, t)$ is the electric potential, computed from the Poisson

equation (89), and B is the Brillouin zone. The initial condition reads as $f(x, k, 0) = f_I(x, k)$. We assume that the collision operator is given as the sum

$$Q(f) = Q_0(f) + Q_1(f)$$

and that the mean free path λ_0 of collisions described by Q_0 is much smaller than the mean free path λ given by Q_1 .

First, we scale the Boltzmann equation and introduce some reference values:

- the reference length λ , which is the mean free path corresponding to Q_1 ,
- the reference velocity $v_0 = \sqrt{k_B T_L / m^*}$ which corresponds to a particle with kinetic energy of the order of the thermal energy $k_B T_L$,
- the reference wave vector $m^* v_0 / \hbar$,
- the reference potential $U_T = k_B T_L / q$,
- the reference times $\tau = \lambda / v_0$ and $\tau_0 = \lambda_0 / v_0$.

This defines the dimensionless variables

$$x = \lambda x_s, \quad t = \tau t_s, \quad k = \frac{m^* v_0}{\hbar} k_s, \quad v(k) = v_0 v_s(k_s),$$

and the dimensionless functions

$$V = U_T V_s, \quad Q_0(f) = \frac{1}{\tau_0} Q_{s,0}(f), \quad Q_1(f) = \frac{1}{\tau} Q_{s,1}(f).$$

Inserting this scaling into the Boltzmann equation and multiplying the resulting equation by τ_0 , we obtain,

$$\frac{\tau_0}{\tau} \partial_{t_s} f + \frac{\tau_0 v_0}{\lambda} v_s(k_s) \cdot \nabla_{x_s} f + \frac{q}{\hbar} \frac{\tau_0 U_T \hbar}{\lambda m^* v_0} \nabla_{x_s} V_s \cdot \nabla_{k_s} f = Q_{s,0}(f) + \frac{\tau_0}{\tau} Q_{s,1}(f).$$

Defining the ration $\alpha = \lambda_0 / \lambda$ between the mean free paths corresponding to the collision operators Q_0 and Q_1 , respectively, observing that

$$\frac{\tau_0 v_0}{\lambda} = \frac{\lambda_0}{\lambda} = \alpha, \quad \frac{q}{\hbar} \frac{\tau_0 U_T \hbar}{\lambda m^* v_0} = \frac{q}{\hbar} \frac{\lambda_0}{v_0} \frac{k_B T_L}{q} \frac{\hbar}{\lambda m^* v_0^2} = \frac{\lambda_0}{v_0} \frac{m^* v_0^2}{\lambda m^* v_0^2} = \frac{\lambda_0}{\lambda} = \alpha,$$

and omitting the index “s”, we conclude that

$$\alpha \partial_t f + \alpha (v(k) \cdot \nabla_x f + \nabla_x V \cdot \nabla_k f) = Q_0(f) + \alpha Q_1(f), \quad (105)$$

We assume that $\alpha \ll 1$, i.e., there are much more scattering events described by Q_0 than by Q_1 .

5.1 Derivation of the Hydrodynamic Equations

The hydrodynamic model is derived from the moment equations of (105). Let f_α be a solution of (105) and V_α be a solution of the Poisson equation (89). We introduce the following weight functions: $\kappa_0(k) = 1$, $\kappa_1(k) = v(k)$, and $\kappa_2(k) = E(k)$. The corresponding moments have a physical interpretation: $n = \langle f \rangle$ is the electron density, $J = -\langle v(k)f \rangle$ the electron current density, and $\langle E(k)f \rangle$ the energy density, relative to the distribution function f , where $\langle g \rangle = \int_B g(k) dk / 4\pi^3$. Then, the moment equations are obtained from (105) by multiplication by κ_i/α and integration over the Brillouin zone:

$$\partial_t \langle \kappa_i f_\alpha \rangle + \text{div}_x \langle v \kappa_i f_\alpha \rangle - \nabla_x V \cdot \langle \nabla_k \kappa_i f_\alpha \rangle = \alpha^{-1} \langle \kappa_i Q_0(f_\alpha) \rangle + \langle \kappa_i Q_1(f_\alpha) \rangle, \quad (106)$$

where $i = 0, 1, 2$. Unfortunately, this set of equations is not closed: The integrals $\langle v v f_\alpha \rangle = \langle v \otimes v f_\alpha \rangle$ and $\langle v E f_\alpha \rangle$ cannot be written in terms of the lower-order moments n , J , and ne . This is referred to as the *closure problem*. To solve this problem, we make some simplifying assumptions on the collision operators and perform the formal limit $\alpha \rightarrow 0$.

We impose the following assumptions:

1. The energy band is approximated by a parabolic band and $B = \mathbb{R}^3$. Then the weight functions become $\kappa_0(k) = 1$, $\kappa_1(k) = k$, and $\kappa_2(k) = \frac{1}{2}|k|^2$.
2. All moments up to second order of Q_0 vanish, i.e. $\langle \kappa_i Q_0(f) \rangle = 0$ for all functions f .
3. The kernel of Q_0 is spanned by the Maxwellians, $N(Q_0) = \{f : f(k) = M[f](k) = M(k) = \exp(\lambda_0 + \lambda_1 \cdot v(k) + \frac{1}{2}\lambda_2|k|^2)\}$, where λ_i are real numbers.
4. The collisions described by Q_1 conserve mass, i.e. $\langle Q_1(f) \rangle = 0$ for all functions $f(k)$.

The first assumption simplifies the computations below. The second condition means that the collision operator Q_0 conserves mass, momentum, and energy. For instance, a relaxation-time operator satisfies this hypothesis. The third assumption means that the equilibrium state of the system given by Q_0 is given by Maxwellians. In view of the parabolic band approximation, the Maxwellians can be written in a more common form. Instead of λ_0 , λ_1 , and λ_2 , we introduce the electron density n , the mean velocity u , and the electron temperature T by $n = \langle M \rangle$, $\lambda_2 = -1/T$, and $\lambda_1 = u/T$. Then a computation shows that

$$\begin{aligned} n &= \int_{\mathbb{R}^3} \exp(\lambda_0 + \lambda_1 \cdot k + \frac{1}{2}\lambda_2|k|^2) \frac{dk}{4\pi^3} = \int_{\mathbb{R}^3} e^{\lambda_0 - u \cdot k/T - |k|^2/2T} \frac{dk}{4\pi^3} \\ &= e^{\lambda_0 + |u|^2/2T} \int_{\mathbb{R}^3} e^{-|u-k|^2/2T} \frac{dk}{4\pi^3} = \frac{T^{3/2}}{4\pi^3} e^{\lambda_0 + |u|^2/2T} \int_{\mathbb{R}^3} e^{-|z|^2/2} dz \\ &= \frac{T^{3/2}}{4\pi^3} e^{\lambda_0 + |u|^2/2T} (2\pi)^{3/2} = \frac{2}{(2\pi)^{3/2}} T^{3/2} e^{\lambda_0 + |u|^2/2T}, \end{aligned}$$

and hence,

$$M(k) = \frac{1}{2} \left(\frac{2\pi}{T} \right)^{3/2} n e^{-|u-k|^2/2T}. \quad (107)$$

Finally, the last condition implies mass conservation for the total collision operator $Q_0 + \alpha Q_1$ which is physically reasonable.

The derivation of the hydrodynamic equations is based on two steps:

1. In the first step, the (formal) limit $\alpha \rightarrow 0$ in the Boltzmann equation (105) leads to

$$Q_0(f) = 0, \quad \text{where } f = \lim_{\alpha \rightarrow 0} f_\alpha.$$

Then, by the third assumption, $f = M$ for some n , u , and T .

2. In the second step, we perform the limit $\alpha \rightarrow 0$ in the moment equations (106), employing the first assumption on Q_0 :

$$\partial_t \langle \kappa_i M \rangle + \operatorname{div}_x \langle \kappa_i k M \rangle - \nabla_x V \cdot \langle \nabla_k \kappa_i M \rangle = \langle \kappa_i Q_1(M) \rangle, \quad i = 0, 1, 2. \quad (108)$$

We need to compute the higher-order moments.

Lemma 5.1. *Let the Maxwellian M be given by (107). Then*

$$\langle k M \rangle = nu, \quad \langle k \otimes k M \rangle = n(u \otimes u) + nT \operatorname{Id}, \quad \langle \frac{1}{2} k |k|^2 M \rangle = \frac{1}{2} nu(|u|^2 + 5T).$$

Proof. We employ the following identities:

$$\langle e^{-|z|^2/2} \rangle = 2(2\pi)^{-3/2}, \quad \langle z_i z_j e^{-|z|^2/2} \rangle = 2(2\pi)^{-3/2} \delta_{ij}.$$

Then, with the transformation $z = (k - u)/\sqrt{T}$, we obtain

$$\langle k M \rangle = \frac{1}{2} (2\pi)^{3/2} n \langle (u + \sqrt{T}z) e^{-|z|^2/2} \rangle = nu,$$

since $z \mapsto ze^{-|z|^2/2}$ is an odd function and hence, its integral vanishes. Furthermore,

$$\begin{aligned} \langle k \otimes k M \rangle &= \frac{1}{2} (2\pi)^{3/2} n \langle (u + \sqrt{T}z) \otimes (u + \sqrt{T}z) e^{-|z|^2/2} \rangle \\ &= n(u \otimes u) + \frac{1}{2} (2\pi)^{3/2} nT \langle z \otimes z e^{-|z|^2/2} \rangle = n(u \otimes u) + nT \operatorname{Id}. \end{aligned}$$

Finally, we have for $i = 1, 2, 3$:

$$\langle \frac{1}{2} k_i |k|^2 M \rangle = \frac{1}{4} (2\pi)^{3/2} n \sum_{j=1}^3 \langle (u_i + \sqrt{T}z_i)(u_j + \sqrt{T}z_j)^2 e^{-|z|^2/2} \rangle.$$

A straightforward computation shows that

$$\langle \frac{1}{2} k_i |k|^2 M \rangle = \frac{1}{2} nu_i |u|^2 + \frac{1}{2} nT \sum_{j=1}^3 (u_i + 2u_j \delta_{ij}) = \frac{1}{2} nu_i |u|^2 + \frac{5}{2} nT u_i.$$

This finishes the proof. □

Inserting the expressions of Lemma 5.1 into the moment equations (108) leads to the following result.

Theorem 5.2 (Hydrodynamic equations). *Let the above assumptions on the energy band and the collision operators hold and let (f_α, V_α) be a solution of the Boltzmann-Poisson system (105) and (89). Then the limit $f = \lim_{\alpha \rightarrow 0} f_\alpha$ equals the Maxwellian (107), where the functions n , $J_n = -nu$, and ne are solutions of the hydrodynamic equations*

$$\partial_t n - \operatorname{div} J_n = 0, \quad (109)$$

$$\partial_t J_n - \operatorname{div} \left(\frac{J_n \otimes J_n}{n} \right) - \nabla(nT) + n\nabla V = -\langle kQ_1(M) \rangle, \quad (110)$$

$$\begin{aligned} \partial_t(ne) - \operatorname{div}(J_n(e+T)) + J_n \cdot \nabla V &= \langle \frac{1}{2}|k|^2 Q_1(M) \rangle, \\ \lambda_D^2 \Delta V &= n - C(x), \end{aligned} \quad (111)$$

where $e = \frac{1}{2}|u|^2 + \frac{3}{2}T$ is the sum of the kinetic and thermal energy, and $V = \lim_{\alpha \rightarrow 0} V_\alpha$. The initial conditions are

$$n(\cdot, 0) = \int_B f_I \frac{dk}{4\pi^3}, \quad J_n(\cdot, 0) = - \int_B k f_I \frac{dk}{4\pi^3}, \quad (ne)(\cdot, 0) = \int_B \frac{1}{2}|k|^2 f_I \frac{dk}{4\pi^3}.$$

5.2 Calculation of the Collision Integrals

The production terms $\langle kQ_1(M) \rangle$ and $\langle \frac{1}{2}|k|^2 Q_1(M) \rangle$ can be specified if Q_1 is given, for instance, by the low-density operator

$$(Q_1(f))(x, k, t) = \int_{\mathbb{R}^3} \sigma(x, k, k') (M_{\text{eq}} f' - M'_{\text{eq}} f) dk', \quad (112)$$

where the collision cross-section σ is assumed to be symmetric in k and k' and $M_{\text{eq}}(k) = \frac{1}{2}(2\pi)^{3/2} e^{-|k|^2/2}$ is the Maxwellian of the thermal equilibrium state. Notice that M_{eq} is normalized, i.e. $\langle M_{\text{eq}} \rangle = 1$.

Lemma 5.3. *The low-density collision operator (112) satisfies, for all functions $f(k)$,*

$$\begin{aligned} \langle Q_1(f) \rangle &= 0, \\ \langle kQ_1(f) \rangle &= - \int_{\mathbb{R}^3} \frac{kf}{\tau_p(x, k)} \frac{dk}{4\pi^3}, \\ \langle \frac{1}{2}|k|^2 Q_1(f) \rangle &= \int_{\mathbb{R}^3} \frac{f(e_0(x, k) - \frac{1}{2}|k|^2)}{\tau_e(x, k)} \frac{dk}{4\pi^3}, \end{aligned}$$

where the momentum relaxation time τ_p , the energy relaxation time τ_e , and the averaged energy e_0 are given by, respectively,

$$\begin{aligned} \frac{1}{\tau_p(x, k)} &= \int_{\mathbb{R}^3} \sigma(x, k, k') M'_{\text{eq}} \left(1 - \frac{k'}{k}\right) dk', \\ \frac{1}{\tau_e(x, p)} &= \int_{\mathbb{R}^3} \sigma(x, k, k') M'_{\text{eq}} dk', \\ e_0(x, k) &= \left(\int_{\mathbb{R}^3} \sigma(x, k, k') M'_{\text{eq}} dk' \right)^{-1} \int_{\mathbb{R}^3} \sigma(x, k, k') \frac{1}{2}|k'|^2 M'_{\text{eq}} dk'. \end{aligned} \quad (113)$$

Furthermore, if the scattering rate σ does not depend on k and k' , then

$$\langle kQ_1(M) \rangle = \frac{J_n}{\tau_0}, \quad \langle \frac{1}{2}|k|^2Q_1(M) \rangle = -\frac{n}{\tau_0} \left(e - \frac{3}{2} \right). \quad (114)$$

where $\tau_0 = 1/\sigma$.

Proof. The first moment is given by

$$\langle kQ_1(f) \rangle = \frac{1}{4\pi^3} \int_{\mathbb{R}^6} \sigma(k, k') (M_{\text{eq}} f' - M'_{\text{eq}} f) k \, dk' \, dk,$$

and exchanging k and k' in the first sum gives

$$\begin{aligned} \langle kQ_1(f) \rangle &= \frac{1}{4\pi^3} \int_{\mathbb{R}^6} \sigma(k, k') M'_{\text{eq}} f(k' - k) \, dk' \, dk \\ &= - \int_{\mathbb{R}^3} k f \left(\int_{\mathbb{R}^3} \sigma(k, k') M'_{\text{eq}} \left(1 - \frac{k'}{k} \right) \, dk' \right) \frac{dk}{4\pi^3}, \end{aligned}$$

showing the second equation involving τ_p . The third equation follows from

$$\langle \frac{1}{2}|k|^2Q_1(f) \rangle = \frac{1}{2} \int_{\mathbb{R}^3} f \left(\int_{\mathbb{R}^3} \sigma(k, k') |k'|^2 M'_{\text{eq}} \, dk' - |k|^2 \int_{\mathbb{R}^3} \sigma(k, k') M'_{\text{eq}} \, dk' \right) \frac{dk}{4\pi^3}.$$

Furthermore, if $\sigma = \sigma(x)$, we compute

$$Q_1(f) = \sigma(x) \left(M_{\text{eq}} \int_{\mathbb{R}^3} f' \, dk' - f \int_{\mathbb{R}^3} M'_{\text{eq}} \, dk' \right) = 4\pi^3 \sigma(x) (nM_{\text{eq}} - f),$$

and hence, by the definition of J_n ,

$$\langle kQ_1(M) \rangle = \sigma(n\langle kM_{\text{eq}} \rangle - \langle kM \rangle) = \sigma J_n.$$

By the second identity in Lemma 5.1, we infer that $\langle \frac{1}{2}|k|^2M \rangle = \frac{1}{2}n|u|^2 + \frac{3}{2}nT = ne$, such that

$$\langle \frac{1}{2}|k|^2Q_1(M) \rangle = \sigma \left(n\langle \frac{1}{2}|k|^2M_{\text{eq}} \rangle - \langle \frac{1}{2}|k|^2M \rangle \right) = \sigma \left(\frac{3}{2}n - ne \right),$$

which proves the lemma. \square

5.3 Relaxation-Time Limits

By performing the so-called relaxation-time limits in the hydrodynamic model, it is possible to recover the drift-diffusion equations and to derive a new model, the energy-transport equations. We rewrite the hydrodynamic equations as follows:

$$\partial_t n - \frac{1}{q} \operatorname{div} J_n = 0, \quad (115)$$

$$\partial_t J_n - \frac{1}{q} \operatorname{div} \left(\frac{J_n \otimes J_n}{n} \right) - \frac{qk_B}{m^*} \nabla(nT) + \frac{q^2}{m^*} n \nabla V = -\frac{J_n}{\tau_p}, \quad (116)$$

$$\partial_t(ne) - \frac{1}{q} \operatorname{div} (J_n(e + k_B T)) + J_n \cdot \nabla V - \operatorname{div} (\kappa \nabla T) = -\frac{n}{\tau_e} \left(e - \frac{3}{2} k_B T_L \right), \quad (117)$$

where the energy e is given by

$$e = \frac{m^*}{2q^2} \frac{|J_n|^2}{n^2} + \frac{3}{2} k_B T,$$

and the heat conductivity is defined by $\kappa = \kappa_0 \tau_p n k_B T / m^*$, with $\kappa_0 > 0$. These equations deviate from (109)-(111) by the inclusion of the heat conduction term and by the introduction of two different relaxation mechanisms: momentum relaxation with rate τ_p and energy relaxation with rate τ_e . The reason is that we wish to consider two different time scales for momentum and energy relaxation. The coupling of the electric potential V to the electron density through the Poisson equation needs not to be considered in the subsequent considerations. Therefore, V will be treated as a given function.

First, we scale the above equations. We choose

- the reference length λ (for instance, the device diameter),
- the reference particle density C_m (for instance, the maximal value of the doping concentration),
- the reference temperature T_L (lattice temperature),
- the reference potential $U_T = k_B T_L / q$,
- the reference electron current density $J_0 = q C_m \lambda / \tau$,
- the reference time τ is given by the assumption that the thermal energy is of the same order as the geometric average of the kinetic energies needed to cross the semiconductor device in time τ and τ_p , respectively,

$$k_B T_L = \sqrt{m^* \left(\frac{\lambda}{\tau}\right)^2} \sqrt{m^* \left(\frac{\lambda}{\tau_p}\right)^2}.$$

With these reference values we can define the nondimensional variables

$$\begin{aligned} x &= \lambda x_s, & t &= \tau t_s, & n &= C_m n_s, \\ J_n &= J_0 J_{n,s}, & V &= U_T V_s, & T &= T_L T_s. \end{aligned}$$

Replacing the dimensional variables in (115)-(117) by the scaled ones, we obtain the scaled equations (omitting the index “s”)

$$\partial_t n - \operatorname{div} J_n = 0, \quad (118)$$

$$\alpha \partial_t J_n - \alpha \operatorname{div} \left(\frac{J_n \otimes J_n}{n} \right) - \nabla(nT) + n \nabla V = -J_n, \quad (119)$$

$$\partial_t(ne) - \operatorname{div} (J_n(e + T)) + J_n \cdot \nabla V - \operatorname{div} (\kappa_0 n T \nabla T) = -\frac{n}{\beta} \left(e - \frac{3}{2} \right), \quad (120)$$

with the energy

$$e = \alpha \frac{|J_n|^2}{2n^2} + \frac{3}{2}T \quad (121)$$

and the nondimensional parameters

$$\alpha = \frac{\tau_p}{\tau}, \quad \beta = \frac{\tau_e}{\tau}.$$

We consider the following formal limits:

- Limit 1: $\alpha \rightarrow 0$ and $\beta \rightarrow 0$.
- Limit 2: $\alpha \rightarrow 0$ and β fixed.
- Limit 3: $\beta \rightarrow 0$ and α fixed.

Limit 1: $\alpha \rightarrow 0$ and $\beta \rightarrow 0$. The limit $\alpha \rightarrow 0$, $\beta \rightarrow 0$ corresponds to the physical situation when the kinetic energy needed to cross the domain in time τ is much smaller than the thermal energy. Then the hydrodynamic equations (118)-(120) become in the limit $\alpha \rightarrow 0$ and $\beta \rightarrow 0$:

$$\partial_t n - \operatorname{div} J_n = 0, \quad J_n = \nabla(nT) - n\nabla V, \quad e = \frac{3}{2}.$$

Furthermore, by (121), $e = 3T/2$, and hence, the scaled temperature equals $T = 1$. The limit equations are the drift-diffusion model studied in Section 4.

Limit 2: $\alpha \rightarrow 0$ and β fixed. The limit $\alpha \rightarrow 0$ with β fixed leads to another system of equations:

$$\partial_t n - \operatorname{div} J_n = 0, \quad J_n = \nabla(nT) - n\nabla V, \quad (122)$$

$$\partial_t \left(\frac{3}{2}nT\right) - \operatorname{div} \left(\frac{5}{2}J_n T + \kappa_0 n T \nabla T\right) + J_n \cdot \nabla V = -\frac{3}{2} \frac{n}{\beta} (T - 1). \quad (123)$$

We claim that this system is of parabolic type in suitable variables. In order to see this, we introduce the so-called *entropy variables*

$$u_1 = \frac{\mu}{T}, \quad u_2 = -\frac{1}{T},$$

where the chemical potential μ links to the electron density and temperature via $n = 2(2\pi)^{-3/2} T^{3/2} \exp(\mu/T)$. The name originates from their use in nonequilibrium thermodynamics. Since

$$\frac{\mu}{T} = \log \frac{(2\pi)^{3/2}}{2} + \log \frac{n}{T^{3/2}},$$

it follows that

$$\nabla \left(\frac{\mu}{T} \right) = \frac{\nabla n}{n} - \frac{3}{2} \frac{\nabla T}{T}.$$

We conclude that

$$\begin{aligned} nT\nabla\left(\frac{\mu}{T}\right) - \frac{5}{2}nT^2\nabla\left(\frac{1}{T}\right) &= T\nabla n - \frac{3}{2}n\nabla T + \frac{5}{2}nT^2\frac{\nabla T}{T^2} = \nabla(nT), \\ \frac{5}{2}J_n T + \kappa_0 nT\nabla T &= \frac{5}{2}T\left(nT\nabla\left(\frac{\mu}{T}\right) + \frac{5}{2}nT^2\nabla\left(\frac{1}{T}\right) - n\nabla V\right) - \kappa_0 nT^3\nabla\left(\frac{1}{T}\right) \\ &= \frac{5}{2}nT^2\nabla\left(\frac{\mu}{T}\right) - \left(\frac{25}{4} + \kappa_0\right)nT^3\nabla\left(\frac{1}{T}\right). \end{aligned}$$

In the entropic variables, system (122)-(123) can be written as

$$\frac{\partial}{\partial t} \begin{pmatrix} n \\ \frac{3}{2}nT \end{pmatrix} - \operatorname{div} \begin{pmatrix} D(n, T)\nabla \begin{pmatrix} \mu/T \\ -1/T \end{pmatrix} \\ n\nabla V \begin{pmatrix} 1 \\ \frac{5}{2}T \end{pmatrix} \end{pmatrix} = \begin{pmatrix} 0 \\ -J_n \cdot \nabla V - \frac{3}{2}n(T-1)/\beta \end{pmatrix},$$

where the diffusion matrix D is given by

$$D(n, T) = nT \begin{pmatrix} 1 & \frac{5}{2}T \\ \frac{5}{2}T & (\frac{25}{4} + \kappa_0)T^2 \end{pmatrix}.$$

This matrix is symmetric and positive definite for $n > 0$ and $T > 0$ if and only if κ_0 is positive. The heat conduction term is necessary to obtain well-posedness of the energy-transport system (at least locally in time).

Limit 3: $\beta \rightarrow 0$ **with** α **fixed.** The limit $\beta \rightarrow 0$ with α fixed gives the equation $e = \frac{3}{2}$ which only means that the sum of the kinetic and thermal energy is constant in space and time. More interestingly is the limit $\beta \rightarrow 0$ in the energy-transport model (122)-(123). This yields $T = 1$ and the drift-diffusion equations

$$\partial_t n - \operatorname{div} J_n = 0, \quad J_n = \nabla n - n\nabla V.$$

The derivation of hydrodynamic models and the three relaxation-time limits are summarized in Figure 13.

6 Microscopic quantum models

We consider three alternative formulations of the quantum mechanical motion of an ensemble of electrons: the Schrödinger formulation, the density-matrix formulation, and the kinetic Wigner formulation.

6.1 Mixed States and Density Matrix Formulation

In Section 2.2 we have considered the single-state Schrödinger equation. We say that the quantum system is in a *pure state*. In applications, we have to deal often with *mixed states* which are described by a sequence of wave functions (ψ_j) , $j \in \mathbb{N}$, satisfying

$$i\partial_t \psi_j = H\psi_j, \quad t > 0, \quad \psi_j(\cdot, 0) = \psi_j^0 \quad \text{in } \mathbb{R}^3, \quad (124)$$

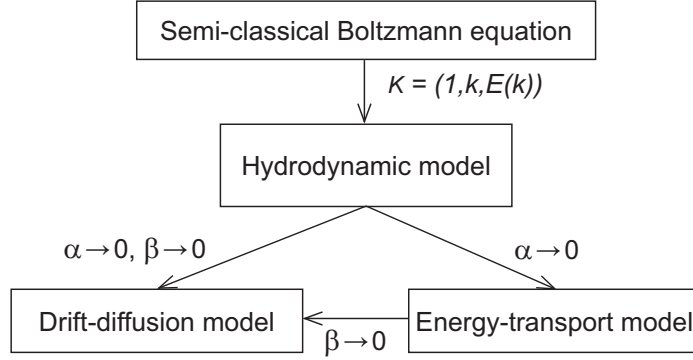


Figure 13: Derivation of hydrodynamic models and relaxation-time limits in the hydrodynamic and energy-transport equations.

where H is the quantum mechanical Hamiltonian, for instance, $H = -(\hbar^2/2m)\Delta - qV(x, t)$. Each wave function ψ_j has an occupation probability $\lambda_j \geq 0$ satisfying $\sum_{j \in \mathbb{N}} \lambda_j = 1$. A mixed quantum state describes a statistical mixture. Such a description is necessary if, for instance, only partial information about a quantum state is available. For details, we refer to the physical literature; see, e.g., [45].

An alternative formulation of mixed quantum states is given by the *density matrix*. Given the sequence (ψ_j, λ_j) , we define the *density matrix (function)*

$$\rho(x, y) = \sum_{j=1}^{\infty} \lambda_j \psi_j(x, t) \overline{\psi_j(y, t)}$$

and the *density matrix operator*

$$(\widehat{\rho}\psi)(x) = \int_{\mathbb{R}^3} \rho(x, y) \psi(y) dy, \quad \psi \in L^2(\mathbb{R}^3).$$

Mathematically, the density matrix operator is a positive, self-adjoint, and compact operator on $L^2(\mathbb{R}^3)$. The “diagonal” of the density matrix can be interpreted as the *particle density*

$$n(x, t) = 2\rho(x, x, t) = 2 \sum_{j=1}^{\infty} \lambda_j |\psi_j(x, t)|^2, \quad x \in \mathbb{R}^3, t \in \mathbb{R}. \quad (125)$$

The factor 2 takes into account the two possible states of the spin of the particles. Furthermore, the *particle current density* is defined by (using $i(a\bar{b} - \bar{a}b) = -2\text{Im}(a\bar{b})$ for complex

numbers a and b)

$$J(x, t) = \frac{i\hbar q}{m} (\nabla_r - \nabla_s) \rho(r, s, t)|_{r=s=x} \quad (126)$$

$$\begin{aligned} &= \frac{i\hbar q}{m} \sum_{j=1}^{\infty} \lambda_j (\nabla_x \psi_j(x, t) \overline{\psi_j(x, t)} - \psi_j(x, t) \overline{\nabla_x \psi_j(x, t)}) \\ &= -2 \frac{\hbar q}{m} \sum_{j=1}^{\infty} \lambda_j \text{Im}(\nabla_x \psi_j(x, t) \overline{\psi_j(x, t)}). \end{aligned} \quad (127)$$

Proposition 6.1. *The density matrix satisfies the Liouville-von Neumann equation in the “matrix” formulation*

$$i\hbar \partial_t \rho(x, y, t) = (H_x - H_y) \rho(x, y, t), \quad t > 0, \quad \rho(x, y, 0) = \rho_I(x, y), \quad x, y \in \mathbb{R}^3, \quad (128)$$

where H_x, H_y denote the Hamiltonians only acting on the variable x, y , respectively (for instance, $H_x = -(\hbar^2/2m)\Delta_x - qV(x, t)$). The initial density matrix is given by

$$\rho_I(x, y) = \sum_{j=1}^{\infty} \lambda_j \psi_j^0(x) \overline{\psi_j^0(y)}, \quad x, y \in \mathbb{R}^3.$$

Proof. We just have to compute the time derivative of $\rho(x, y, t)$ and to insert the Schrödinger equations (124):

$$\begin{aligned} i\hbar \partial_t \rho(x, y, t) &= i\hbar \sum_{j=1}^{\infty} \lambda_j (\partial_t \psi_j(x, t) \overline{\psi_j(y, t)} + \psi_j(x, t) \overline{\partial_t \psi_j(y, t)}) \\ &= \sum_{j=1}^{\infty} \lambda_j (H \psi_j(x, t) \overline{\psi_j(y, t)} - \psi_j(x, t) \overline{H \psi_j(y, t)}) \\ &= H_x \sum_{j=1}^{\infty} \lambda_j \psi_j(x, t) \overline{\psi_j(y, t)} - H_y \sum_{j=1}^{\infty} \lambda_j \psi_j(x, t) \overline{\psi_j(y, t)} \\ &= (H_x - H_y) \rho(x, y, t). \end{aligned}$$

Above, we have used that $H = \overline{H}$. □

Instead of assuming the existence of a sequence (ψ_j, λ_j) of mixed states, one may also start from the density matrix operator. More precisely, one may assume that the quantum mechanical system is described by a density matrix operator $\hat{\rho}$, which is a positive, self-adjoint, and compact operator, normalized to one, i.e. $\text{tr}(\hat{\rho}) = 1$. Here, the trace of an operator is defined by $\text{tr}(\hat{\rho}) = \sum_{j=1}^{\infty} ((\hat{\rho}^* \hat{\rho})^{1/2} u_j, u_j)_{L^2}$, where $\hat{\rho}^*$ denotes the adjoint operator and (u_j) is a complete orthonormal set of $L^2(\mathbb{R}^3)$. Then, a pure state can be defined by the property $\text{tr}(\hat{\rho}^2) = \text{tr}(\hat{\rho})$. If $\text{tr}(\hat{\rho}^2) < \text{tr}(\hat{\rho})$, the quantum system is in a mixed state [45, Section 3.4.2].

The self-adjointness and compactness of $\widehat{\rho}$ provide the existence of a complete orthonormal set (ψ_j) of eigenfunctions with eigenvalues (λ_j) . The positivity of $\widehat{\rho}$ implies that the eigenvalues are nonnegative. The density matrix operator has the unique integral representation

$$(\widehat{\rho}\psi)(x) = \int_{\mathbb{R}^3} \rho(x, y)\psi(y)dy, \quad \psi \in L^2(\mathbb{R}^3),$$

for some density matrix $\rho(x, y, t)$. The self-adjointness of $\widehat{\rho}$ implies the symmetry $\rho(x, y, t) = \rho(y, x, t)$. Furthermore, *postulating* that the density matrix operator is a solution of the Liouville-von Neumann equation in operator formulation,

$$i\hbar\partial_t\widehat{\rho} = [H, \widehat{\rho}] := H\widehat{\rho} - \widehat{\rho}H, \quad t > 0, \quad \widehat{\rho}(0) = \widehat{\rho}_I,$$

it can be shown that the density matrix satisfies the evolution equation (128) and the wave functions ψ_j solve the Schrödinger equation (124) [31, Section 10.1].

6.2 Quantum Liouville Equation

The quantum Liouville equation is the quantum analogue of the Liouville equation presented in Section 3.1. It will be derived from the electron-ensemble Liouville-von Neumann equation for the density matrix ρ ,

$$i\hbar\partial_t\rho(r, s, t) = (H_r - H_s)\rho(r, s, t), \quad \rho(r, s, 0) = \rho_I(r, s), \quad r, s \in \mathbb{R}^{3M}, \quad (129)$$

for an ensemble consisting of M electrons with mass m in a vacuum (see Section 6.1 for the introduction of this equation). We define the *Fourier transform* of a function $f : \mathbb{R}^{3M} \rightarrow \mathbb{C}$ as

$$(\mathcal{F}(f))(p) = \int_{\mathbb{R}^{3M}} f(y)e^{-iy\cdot p/\hbar} dy,$$

and its inverse,

$$(\mathcal{F}^{-1}(g))(y) = \frac{1}{(2\pi\hbar)^{3M}} \int_{\mathbb{R}^{3M}} g(p)e^{iy\cdot p/\hbar} dp,$$

for functions $g : \mathbb{R}^{3M} \rightarrow \mathbb{C}$.

For the kinetic formulation of the Liouville-von Neumann equation, we need the so-called *Wigner function* introduced by Wigner in 1932 [51]:

$$w(x, p, t) = \int_{\mathbb{R}^{3M}} \rho\left(x + \frac{y}{2}, x - \frac{y}{2}, t\right) e^{-iy\cdot p/\hbar} dy. \quad (130)$$

Setting

$$u(x, y, t) = \rho\left(x + \frac{y}{2}, x - \frac{y}{2}, t\right), \quad (131)$$

the Wigner function can be written as the Fourier transform of u , $w = \mathcal{F}(u)$. Furthermore, $u = \mathcal{F}^{-1}(w)$. or, more explicitly,

$$u(x, y, t) = \frac{1}{(2\pi\hbar)^{3M}} \int_{\mathbb{R}^{3M}} w(x, p, t) e^{iy\cdot p/\hbar} dp.$$

Since y has the dimension of a length, p/\hbar in the Fourier transform has the dimension of an inverse length and thus, p has the dimension of a momentum. We interpret p as the crystal momentum $\hbar k$. We notice that the transformation $\rho \mapsto w$ is called the *Wigner-Weyl transform*.

The evolution equation for the Wigner function is obtained by transforming the Liouville-von Neumann equation to the (x, y) variables and applying Fourier transformation. The result is expressed in the following proposition.

Proposition 6.2 (Many-particle quantum Liouville equation). *Let ρ be a solution of the Liouville-von Neumann equation (129). Then the Wigner function (130) is formally a solution of*

$$\partial_t w + \frac{p}{m} \cdot \nabla_x w + q\theta[V]w = 0, \quad t > 0, \quad w(x, p, 0) = w_I(x, p) \quad (132)$$

for $x, p \in \mathbb{R}^{3M}$, where the initial datum is given by

$$w_I(x, p) = \int_{\mathbb{R}^{3M}} \rho_I\left(x + \frac{y}{2}, x - \frac{y}{2}\right) e^{-iy \cdot p/\hbar} dy,$$

and $\theta[V]$ is a pseudo-differential operator, defined by

$$(\theta[V]w)(x, p, t) = \frac{1}{(2\pi\hbar)^{3M}} \int_{\mathbb{R}^{3M} \times \mathbb{R}^{3M}} (\delta V)(x, y, t) w(x, p', t) e^{iy \cdot (p-p')/\hbar} dp' dy, \quad (133)$$

where

$$\delta V(x, y, t) = \frac{i}{\hbar} \left(V\left(x + \frac{y}{2}, t\right) - V\left(x - \frac{y}{2}, t\right) \right).$$

Equation (132) is called the *many-particle Wigner equation* or *many-particle quantum Liouville equation*. The local term $(p/m) \cdot \nabla_x w$ is the quantum analogue of the classical transport term of the Liouville equation (see (3)). The nonlocal term $q\theta[V]w$ models the influence of the electric potential. The nonlocality has the effect that the electron ensemble “feels” an upcoming potential barrier.

Before we prove the proposition, we discuss the pseudo-differential operator. It can be written, by slight abuse of notation, as

$$\begin{aligned} (\theta[V]w)(x, p, t) &= \int_{\mathbb{R}^{3M}} (\delta V)(x, y, t) u(x, -y, t) e^{iy \cdot p/\hbar} dy \\ &= (2\pi\hbar)^{3M} \mathcal{F}^{-1}((\delta V)(x, y, t) u(x, -y, t)). \end{aligned}$$

Therefore, it acts in the Fourier space essentially as a multiplication operator. The multiplier δV is called the *symbol* of the operator. The symbol δV is a discrete directional derivative, since in the formal limit “ $\hbar \rightarrow 0$ ”, we find

$$\delta V(x, \hbar y, t) \rightarrow i \nabla_x V(x, t) \cdot y.$$

We refer to [47] for a mathematical theory of pseudo-differential operators. In particular, the Wigner equation (132) is a linear pseudo-differential equation.

Proof of Proposition 6.2. First, we derive the evolution equation for u , defined in (131), and then take the inverse Fourier transform. We compute, for $r = x + y/2$ and $s = x - y/2$,

$$\begin{aligned}\operatorname{div}_y(\nabla_x u)(x, y, t) &= \operatorname{div}_y(\nabla_r \rho + \nabla_s \rho)\left(x + \frac{y}{2}, x - \frac{y}{2}, t\right) \\ &= \frac{1}{2}(\Delta_r \rho - \Delta_s \rho)\left(x + \frac{y}{2}, x - \frac{y}{2}, t\right).\end{aligned}$$

Then the transformed Liouville-von Neumann equation for u becomes,

$$\begin{aligned}\partial_t u(x, y, t) &= \partial_t \rho(r, s, t) = -\frac{i}{\hbar}\left(-\frac{\hbar^2}{2m}(\Delta_r - \Delta_s) - qV(r, t) + qV(s, t)\right)\rho(r, s, t) \\ &= \frac{i\hbar}{m}\operatorname{div}_y(\nabla_x u)(x, y, t) + q\delta V(x, y, t)u(x, y, t)\end{aligned}$$

or

$$\partial_t u - \frac{i\hbar}{m}\operatorname{div}_y(\nabla_x u) - q(\delta V)u = 0, \quad x, y \in \mathbb{R}^{3M}, \quad t > 0.$$

The Fourier transform gives

$$\partial_t \mathcal{F}(u) - \frac{i\hbar}{m}\mathcal{F}(\operatorname{div}_y \nabla_x u) - q\mathcal{F}((\delta V)u) = 0. \quad (134)$$

The second term on the left-hand side can be written, by integrating by parts, as

$$\begin{aligned}\mathcal{F}(\operatorname{div}_y \nabla_x u)(x, p, t) &= \int_{\mathbb{R}^{3M}} \operatorname{div}_y(\nabla_x u)(x, y, t) e^{-iy \cdot p/\hbar} dy \\ &= \frac{i}{\hbar} \int_{\mathbb{R}^{3M}} p \cdot \nabla_x u(x, y, t) e^{-iy \cdot p/\hbar} dy = \frac{i}{\hbar} p \cdot \nabla_x \mathcal{F}(u)(x, p, t) \\ &= \frac{i}{\hbar} p \cdot \nabla_x w(x, p, t).\end{aligned}$$

The third-term on the left-hand side of (134) becomes, by (133),

$$\begin{aligned}\mathcal{F}((\delta V)u)(x, p, t) &= \int_{\mathbb{R}^{3M}} (\delta V)(x, y, t) u(x, y, t) e^{-iy \cdot p/\hbar} dy \\ &= (2\pi\hbar)^{-3M} \int_{\mathbb{R}^{3M}} (\delta V)(x, y, t) w(x, p', t) e^{iy \cdot (p' - p)/\hbar} dp' dy \\ &= (2\pi\hbar)^{-3M} \int_{\mathbb{R}^{3M}} (\delta V)(x, -y, t) w(x, p', t) e^{iy \cdot (p - p')/\hbar} dp' dy \\ &= -(\theta[V]w)(x, p, t).\end{aligned}$$

Therefore, (134) equals the Wigner equation (132). \square

Lemma 6.3. *The ensemble particle density n and the ensemble current density J , defined in (125) and (127), respectively, can be expressed in terms of the Wigner function as*

$$n(x, t) = \frac{2}{(2\pi\hbar)^{3M}} \int_{\mathbb{R}^{3M}} w(x, p, t) dp, \quad J(x, t) = -\frac{2}{(2\pi\hbar)^{3M}} \frac{q}{m} \int_{\mathbb{R}^{3M}} w(x, p, t) p dp.$$

The above integrals are called the zeroth and first moments of the Wigner function, respectively, in analogy to the classical situation (see Section 1).

Proof. The first identity follows from

$$n(x, t) = 2\rho(x, x, t) = 2u(x, 0, t) = 2(2\pi\hbar)^{-3M} \int_{\mathbb{R}^{3M}} w(x, p, t) dp.$$

For the proof of the second identity, we compute

$$\begin{aligned} J(x, t) &= \frac{i\hbar q}{m} (\nabla_r - \nabla_s) \rho(x, x, t) = \frac{2i\hbar q}{m} \nabla_y u(x, 0, t) \\ &= \frac{2i\hbar q}{m} \frac{1}{(2\pi\hbar)^{3M}} \int_{\mathbb{R}^{3M}} w(x, p, t) \nabla_y e^{iy \cdot p/\hbar} \Big|_{y=0} dp \\ &= -\frac{q}{m} \frac{2}{(2\pi\hbar)^{3M}} \int_{\mathbb{R}^{3M}} w(x, p, t) p dp, \end{aligned}$$

finishing the proof. \square

6.3 Quantum Vlasov Equation

The quantum Liouville equation has the same disadvantage as its classical analogue, namely that the equation needs to be solved in a very high-dimensional electron-ensemble phase space which makes its numerical solution almost unfeasible. In this section we derive the quantum analogue of the classical Vlasov equation, the quantum Vlasov equation, which acts on the six-dimensional phase space. We proceed similarly as in [39, Sec. 1.5].

Consider an ensemble of M electrons with mass m moving in a vacuum under the action of a (real-valued) potential $V(x, t)$. The motion of the particle ensemble is described by the density matrix as a solution of the Liouville-von Neumann equation (129). We impose the following assumptions:

1. The potential can be decomposed into a sum of external potentials acting on one particle and of two-particle interaction potentials,

$$V(x_1, \dots, x_M, t) = \sum_{j=1}^M V_{\text{ext}}(x_j, t) + \frac{1}{2} \sum_{j, \ell=1}^M V_{\text{int}}(x_j, x_\ell), \quad (135)$$

where the interaction potential V_{int} is symmetric, i.e. $V_{\text{int}}(x_j, x_\ell) = V_{\text{int}}(x_\ell, x_j)$ for all $j, \ell = 1, \dots, M$.

2. The limit $V_0 = \lim_{M \rightarrow \infty} M V_{\text{int}}$ exists, i.e., the interaction potential is of order $1/M$.
3. The electrons of the ensemble are initially indistinguishable in the sense of

$$\rho(r_1, \dots, r_M, s_1, \dots, s_M, 0) = \rho(r_{\pi(1)}, \dots, r_{\pi(M)}, s_{\pi(1)}, \dots, s_{\pi(M)}, 0) \quad (136)$$

for all permutations π of $\{1, \dots, M\}$ and all $r_j, s_j \in \mathbb{R}^3$.

4. The initial subensemble density matrices

$$\rho_I^{(a)}(r^{(a)}, s^{(a)}) = \int_{\mathbb{R}^{3(M-a)}} \rho_I(r^{(a)}, u_{a+1}, \dots, u_M, s^{(a)}, u_{a+1}, \dots, u_M) du_{a+1} \cdots du_M,$$

where $r^{(a)} = (r_1, \dots, r_a)$ and $s^{(a)} = (s_1, \dots, s_a)$, can be factorized for all $1 \leq a \leq M-1$:

$$\rho_I^{(a)}(r^{(a)}, s^{(a)}) = \prod_{j=1}^a R_I(r_j, s_j),$$

where R_I is a given function.

We discuss these hypotheses. The factor $\frac{1}{2}$ in (135) is necessary since each electron-electron pair in the sum of two-particle interactions is counted twice. The symmetry of the interaction potentials implies that

$$V(x_1, \dots, x_M, t) = V(x_{\pi(1)}, \dots, x_{\pi(M)}, t) \quad \text{for all } t \geq 0$$

and for all permutations π . It can be shown that this property and (136) have the consequence that

$$\rho(r_1, \dots, r_M, s_1, \dots, s_M, t) = \rho(r_{\pi(1)}, \dots, r_{\pi(M)}, s_{\pi(1)}, \dots, s_{\pi(M)}, t) \quad (137)$$

holds for all $t > 0$. Physically, this means that the electrons are indistinguishable for all time.

We claim that a one-particle density matrix contains all the dynamics of the many-particle problem. Proceeding exactly as in the classical case, we arrive at the following result.

Theorem 6.4 (Quantum Vlasov equation). *Let the hypotheses on page 67 hold and let W be a solution of the quantum Vlasov equation*

$$\begin{aligned} \partial_t W + \frac{p}{m} \cdot \nabla_x W + q\theta[V_{\text{eff}}]W &= 0, \quad x, p \in \mathbb{R}^3, \quad t > 0, \\ W(x, p, 0) &= W_I(x, p), \quad x, p \in \mathbb{R}^3, \end{aligned} \quad (138)$$

where the pseudo-differential operator $\theta[V_{\text{eff}}]$ is defined as in (133) with $M = 1$, the effective potential V_{eff} is given by

$$V_{\text{eff}}(x, t) = V_{\text{ext}}(x, t) + \int_{\mathbb{R}^3} n(z, t) V_0(x, z) dz, \quad (139)$$

the electron density is

$$n(x, t) = \frac{2}{(2\pi\hbar)^3} \int_{\mathbb{R}^3} W(x, p, t) dp, \quad (140)$$

and the initial datum equals

$$W_I(x, p) = \int_{\mathbb{R}^3} R_I\left(x + \frac{y}{2}, x - \frac{y}{2}\right) e^{-iy \cdot p/\hbar} dy, \quad x, p \in \mathbb{R}^3.$$

We define the single-state density matrix R as the inverse Fourier transform of the Wigner function,

$$W(x, p, t) = \int_{\mathbb{R}^3} R\left(x + \frac{y}{2}, x - \frac{y}{2}, t\right) e^{-iy \cdot p/\hbar} dy, \quad x, p \in \mathbb{R}^3, \quad t > 0.$$

Then the density matrix

$$\rho^{(a)}(r^{(a)}, s^{(a)}, t) = \prod_{j=1}^a R(r_j, s_j, t) \quad (141)$$

is a solution of the limit BBGKY Liouville-von Neumann equation

$$\begin{aligned} i\hbar \partial_t \rho^{(a)} = & -\frac{\hbar^2}{2m} \sum_{j=1}^a (\Delta_{r_j} - \Delta_{s_j}) \rho^{(a)} - q \sum_{j=1}^a (V_{\text{ext}}(r_j, t) - V_{\text{ext}}(s_j, t)) \rho^{(a)} \\ & - q \sum_{j=1}^a \int_{\mathbb{R}^3} (V_0(r_j, u_*) - V_0(s_j, u_*)) \rho_*^{(a+1)} du_*. \end{aligned}$$

with initial datum $\rho^{(a)}(\cdot, \cdot, 0) = \rho_I^{(a)}$ in $\mathbb{R}^{3a} \times \mathbb{R}^{3a}$.

The expression (141) is also called a *Hartree ansatz*. As the effective potential depends on the function W through (140), the quantum Vlasov equation is a *nonlinear* pseudo-differential equation.

In contrast to the classical Vlasov equation, the quantum Vlasov equation does not preserve the nonnegativity of the solution. However, if the initial single-particle density matrix $R(r, s, 0)$ is positive semi-definite, the electron density n , defined in (140), remains nonnegative for all times.

Similar to the quantum Liouville equation, the solution of the quantum Vlasov equation converges (at least formally) as “ $\hbar \rightarrow 0$ ” to a solution of the classical Vlasov equation

$$\partial_t W + \frac{p}{m} \cdot \nabla_x W + q \nabla_x V_{\text{eff}} \cdot \nabla_p W = 0.$$

6.4 Wigner-Boltzmann Equation

In the previous sections, we have considered only ballistic and hence reversible quantum transport of electrons. However, if the characteristic device length is much larger than the mean free path of the electrons, scattering phenomena between electrons and phonons or among the electrons have to be taken into account. Inspired from classical kinetic theory,

collisions may be modeled by an appropriate collision operator, which is added to the right-hand side of the quantum Liouville or Vlasov equation. This gives the *Wigner-Boltzmann equation*

$$\partial_t w + v(p) \cdot \nabla_x w + q\theta[V_{\text{eff}}]w = Q(w), \quad x, p \in \mathbb{R}^3, \quad t > 0, \quad (142)$$

which we write here for the effective single-state potential V_{eff} derived in Section 6.3. The velocity may depend on the pseudo-wave vector, $v(p) = v(\hbar k)$. In the parabolic band case, $v(p) = \hbar k/m$. This model is an example of an open quantum system since the electron ensemble interacts with some environment, such as an external phonon bath, through the collision operator $Q(w)$.

In the following, we present some spatially local collision operators which are employed in numerical simulations of the Wigner equation.

Wigner-Fokker-Planck model. The first model is the *quantum Fokker-Planck collision operator*

$$Q(w) = D_{pp}\Delta_p w + 2\gamma\text{div}_p(pw) + D_{qq}\Delta_x w + 2D_{pq}\text{div}_x(\nabla_p w), \quad (143)$$

where $\gamma > 0$ is a friction parameter and the nonnegative coefficients D_{pp} , D_{pq} , and D_{qq} constitute the phase-space diffusion matrix of the system. The first term models classical diffusion and the last two terms quantum diffusion. The corresponding *Wigner-Fokker-Planck equation* governs the dynamical evolution of an electron ensemble interacting dissipatively with an idealized heat bath consisting of an ensemble of harmonic oscillators and modeling the semiconductor lattice.

Without quantum diffusion, the collision operator

$$Q(w) = D_{pp}\Delta_p w + 2\gamma\text{div}_p(pw) \quad (144)$$

was derived by Caldeira and Leggett [12] and Diósi [21]. The Wigner equation with the Caldeira-Leggett operator is also known under the name of *quantum Brownian motion* or *quantum Langevin equation* and it received a large interest in the context of interaction between light and matter (see, for instance, [16]).

The Caldeira-Leggett scattering term does not satisfy the so-called *Lindblad condition*

$$D_{pp}D_{qq} - D_{pq}^2 \geq \frac{\gamma^2}{4},$$

which is a generic condition for quantum systems to preserve complete positivity of the density matrix along the evolution. Such a property has to be satisfied for a true quantum evolution. Thus the Wigner-Caldeira-Leggett equation is quantum mechanically not correct. The reason for this shortcoming comes from the inconsistency that the equation contains the temperature T , through its coefficients, but the $1/T \rightarrow 0$ limit was performed in [12] along the derivation of the model. In [14], the approach was improved by deriving the Fokker-Planck operator (143) with finite temperature.

Wigner-BGK model. The second model is the relaxation-time approximation or *Bhatnagar-Gross-Krook (BGK) model* [34, 43]

$$Q(w) = \frac{1}{\tau} \left(\frac{n}{n_0} w_0 - w \right),$$

where the particle density and the equilibrium density are given by, respectively,

$$n(x, t) = \frac{2}{(2\pi\hbar)^3} \int_{\mathbb{R}^3} w(x, p, t) dp, \quad n_0(x, t) = \frac{2}{(2\pi\hbar)^3} \int_{\mathbb{R}^3} w_0(x, p, t) dp,$$

and w_0 is the Wigner function of the quantum mechanical thermal equilibrium, defined, for instance in the mixed state, by the thermal equilibrium density matrix

$$\rho_{\text{eq}}(r, s) = \sum_j f(E_j) \psi_j(r) \overline{\psi_j(s)}$$

(by means of the Wigner-Weyl transformation), where (ψ_j, E_j) are the eigenfunction-eigenvalue pairs of the quantum Hamiltonian, and $f(E_j)$ is the Fermi-Dirac or Maxwell-Boltzmann distribution. The above collision operator expresses the tendency of the system to relax, in absence of external forces, to the quantum thermal equilibrium since the solution of the Wigner-BGK model with vanishing transport and electric field,

$$\partial_t w = \frac{1}{\tau} \left(\frac{n}{n_0} w_0 - w \right),$$

tends to the equilibrium Wigner function nw_0/n_0 . We remark that the relaxation term can be represented in Lindblatt form, such that positivity preservation is guaranteed for this model [3].

The kinetic quantum and kinetic semiclassical models are summarized in Figure 14.

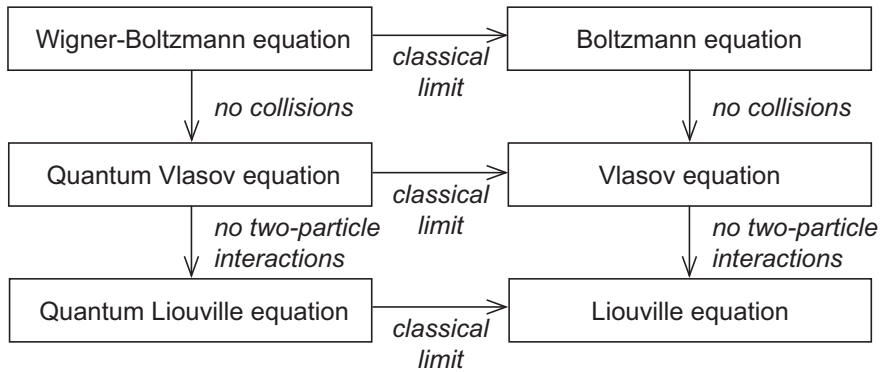


Figure 14: Semi-classical and quantum kinetic models and their relations.

7 Quantum Hydrodynamic Equations

In this section, we show that, in analogy to the semi-classical situation, quantum hydrodynamic models can be derived by employing a hydrodynamic scaling. We present two derivations: one from the (mixed-state) Schrödinger equations and one from a Wigner-Boltzmann equation.

7.1 Zero-Temperature Quantum Hydrodynamic Equations

It is well known since Madelung [37] that there exists a fluid-dynamical description of the Schrödinger equation, also called the *Madelung hydrodynamic formulation* or *quantum fluid dynamics*. In this section we consider a single electron moving in a vacuum. Electron ensembles are studied in the following sections.

The quantum evolution of the particle with mass m is described by the single-state Schrödinger equation

$$i\hbar\partial_t\psi = -\frac{\hbar^2}{2m}\Delta\psi - qV(x,t)\psi, \quad t > 0, \quad \psi(\cdot, 0) = \psi_I \quad \text{in } \mathbb{R}^3,$$

where ψ is the wave function and V the electric potential. The potential may be a given function or the solution of the Poisson equation. In the following, we assume that V is a given function. However, the following arguments do not change if V solves the Poisson equation. First we scale the equation by introducing reference values for the time τ , length λ , and potential U . We assume that the kinetic energy is of the same order as the electric energy,

$$m\left(\frac{\lambda}{\tau}\right)^2 = qU.$$

Then the scaled Schrödinger equation becomes

$$\frac{i\hbar}{q}\partial_{t_s}\psi = -\frac{\hbar^2}{2m\lambda^2}\Delta_s\psi - qUV_s(x_s, t_s)\psi,$$

and after division by $qU = m\lambda^2/\tau^2$,

$$i\frac{\hbar\tau}{m\lambda^2}\partial_{t_s}\psi = -\frac{\hbar^2\tau^2}{2m^2\lambda^2}\Delta_s\psi - V_s(x_s, t_s)\psi.$$

Introducing the scaled Planck constant as the ratio between wave energy and kinetic energy,

$$\varepsilon = \frac{\hbar/\tau}{m(\lambda/\tau)^2} = \frac{\hbar\tau}{m\lambda^2},$$

we infer that

$$i\varepsilon\partial_t\psi = -\frac{\varepsilon^2}{2}\Delta\psi - V(x,t)\psi, \quad t > 0, \quad \psi(\cdot, 0) = \psi_I \quad \text{in } \mathbb{R}^3. \quad (145)$$

In order to derive a fluid-dynamical formulation, we need to assume that the initial wave function is given in the WKB state (named after Wentzel-Kramers-Brillouin):

$$\psi_I = \sqrt{n_I}\exp(iS_I/\varepsilon), \quad (146)$$

where $n_I(x) \geq 0$ and $S_I(x) \in \mathbb{R}$ are some functions. Then, inserting the ansatz $\psi = \sqrt{n}\exp(iS/\varepsilon)$ in the Schrödinger equation leads to the following result.

Theorem 7.1 (Zero-temperature quantum hydrodynamic equations). *Let ψ be a solution of the initial-value problem (145) with initial datum (146). Then $n = |\psi|^2$, $J_n = -\varepsilon \operatorname{Im}(\bar{\psi} \nabla \psi)$ are a solution of the zero-temperature quantum hydrodynamic or Madelung equations*

$$\begin{aligned} \partial_t n - \operatorname{div} J_n &= 0, \quad \partial_t J_n - \operatorname{div} \left(\frac{J_n \otimes J_n}{n} \right) + n \nabla V + \frac{\varepsilon^2}{2} n \nabla \left(\frac{\Delta \sqrt{n}}{\sqrt{n}} \right) = 0, \\ n(\cdot, 0) &= n_I, \quad J_n(\cdot, 0) = J_I \quad \text{in } \mathbb{R}^3, \end{aligned} \quad (147)$$

where the initial data is given by $n_I = |\psi_I|^2$ and $J_I = -n_I \nabla S_I$, as long as $n > 0$ in \mathbb{R}^3 . On the other hand, let (n, S) be a (smooth) solution of

$$\partial_t n + \operatorname{div}(n \nabla S) = 0, \quad \partial_t S + \frac{1}{2} |\nabla S|^2 - V - \frac{\varepsilon^2}{2} \frac{\Delta \sqrt{n}}{\sqrt{n}} = 0, \quad t > 0, \quad (148)$$

$$n(\cdot, 0) = n_I, \quad S(\cdot, 0) = S_I \quad \text{in } \mathbb{R}^3, \quad (149)$$

such that $n > 0$ in \mathbb{R}^3 , $t > 0$. Then $\psi = \sqrt{n} \exp(iS/\varepsilon)$ solves the Schrödinger equation (145) with initial datum (146).

Proof. Let ψ be a solution of the initial-value problem (145) with initial datum (146). As long as $|\psi| > 0$, we can decompose $\psi = \sqrt{n} \exp(iS/\varepsilon)$, where $n = |\psi|^2$ and S is some phase function. Then

$$J_n = -\varepsilon \operatorname{Im}(\bar{\psi} \nabla \psi) = -\varepsilon \operatorname{Im} \left(\sqrt{n} \nabla \sqrt{n} + \frac{i}{\varepsilon} n \nabla S \right) = -n \nabla S.$$

Thus, n and J_n satisfy the initial conditions. Inserting the decomposition $\psi = \sqrt{n} \exp(iS/\varepsilon)$ into the Schrödinger equation (145) gives, after division by the factor $\exp(iS/\varepsilon)$,

$$\frac{i\varepsilon}{2} \frac{\partial_t n}{\sqrt{n}} - \sqrt{n} \partial_t S = -\frac{\varepsilon^2}{2} \left(\Delta \sqrt{n} + \frac{2i}{\varepsilon} \nabla \sqrt{n} \cdot \nabla S + \frac{i}{\varepsilon} \sqrt{n} \Delta S - \frac{\sqrt{n}}{\varepsilon^2} |\nabla S|^2 \right) - \sqrt{n} V. \quad (150)$$

The imaginary part of this equation equals

$$\partial_t n = -2\sqrt{n} \nabla \sqrt{n} \cdot \nabla S - n \Delta S = -\operatorname{div}(n \nabla S),$$

which is the first equation of (147). Dividing the real part of (150) by \sqrt{n} , then differentiating the resulting equation with respect to x and multiplying it by n , we infer, using the first equation in (147), that

$$\begin{aligned} n \nabla V + \frac{\varepsilon^2}{2} n \nabla \left(\frac{\Delta \sqrt{n}}{\sqrt{n}} \right) &= n \partial_t (\nabla S) + \frac{1}{2} n \nabla |\nabla S|^2 \\ &= \partial_t (n \nabla S) - (\operatorname{div} J_n) \nabla S + \frac{1}{2} n \nabla |\nabla S|^2 \\ &= -\partial_t J_n + \operatorname{div} \left(\frac{J_n \otimes J_n}{n} \right). \end{aligned} \quad (151)$$

For the last equality, we have employed the identity

$$\frac{1}{2}n\nabla|\nabla S|^2 = n((\nabla \otimes \nabla)S)\nabla S = \operatorname{div}(n\nabla S \otimes \nabla S) - \operatorname{div}(n\nabla S)\nabla S,$$

where $(\nabla \otimes \nabla)S$ denotes the Hessian of S . Equation (151) is the second equation in (147).

Let (n, S) be a solution of (148)-(149) with $n > 0$ and set $\psi = \sqrt{n} \exp(iS/\varepsilon)$. Then, differentiating ψ gives

$$\begin{aligned} i\varepsilon\partial_t\psi + \frac{\varepsilon^2}{2}\Delta\psi &= e^{iS/\varepsilon} \left(i\varepsilon\frac{\partial_t n}{2\sqrt{n}} - \sqrt{n}\partial_t S + \frac{\varepsilon^2}{2}\Delta\sqrt{n} + i\varepsilon\nabla\sqrt{n} \cdot \nabla S \right. \\ &\quad \left. + \frac{i\varepsilon}{2}\sqrt{n}\Delta S - \frac{\sqrt{n}}{2}|\nabla S|^2 \right) \\ &= e^{iS/\varepsilon} \left(-\frac{i\varepsilon}{2}\frac{\operatorname{div}(n\nabla S)}{\sqrt{n}} + i\varepsilon\nabla\sqrt{n} \cdot \nabla S + \frac{i\varepsilon}{2}\sqrt{n}\Delta S - \sqrt{n}V \right) \\ &= -\sqrt{n}e^{iS/\varepsilon}V = -V\psi. \end{aligned}$$

Thus, ψ solves the Schrödinger equation. \square

The system (147) is the quantum analogue of the classical pressureless Euler equations of gas dynamics, which are obtained in the classical limit $\varepsilon \rightarrow 0$. We notice that the above derivation requires an irrotational initial velocity J_n/n since $\operatorname{curl}(J_n/n) = -\operatorname{curl}(\nabla S) = 0$. The quantum term can be interpreted as a quantum self-potential with the so-called quantum or *Bohm potential* $\phi_B = \Delta\sqrt{n}/\sqrt{n}$ or as a quantum stress term:

$$\frac{\varepsilon^2}{2}n\nabla\left(\frac{\Delta\sqrt{n}}{\sqrt{n}}\right) = \frac{\varepsilon^2}{4}\operatorname{div}(n(\nabla \otimes \nabla)\log n),$$

where $P = (\varepsilon^2/4)n(\nabla \otimes \nabla)\log n$ is a nondiagonal stress tensor. The quantum hydrodynamic equations are employed in Bohmian mechanics and for the description of quantum trajectories [53].

There is a problem with the formulation (148) if vacuum occurs, i.e. if $n = 0$ locally. In this situation, the phase S is not defined which manifests in the fact that the Bohm potential may become singular at vacuum points. It is shown by Gasser and Markowich [24] that the formulation (147) has generally better mathematical properties than (148). In fact, it can be shown that $n\nabla\phi_B$ is an element of a Sobolev space with negative index and not just a distribution.

Another problem is the reconstruction of the initial datum ψ_I in terms of the variables n_I and J_I . In the above theorem it is explicitly required that ψ_I is given in terms of n_I and S_I . This problem is connected to a more general important problem in physics, the so-called *Pauli problem* [48], regarding the possibility to reconstruct a pure quantum state by knowing a finite set of measurements of the state, in our case: the particle and current densities. Here, the possible existence of vacuum points generally makes this reconstruction impossible (see [48] and references therein).

7.2 Mixed-State Schrödinger Models and Quantum Hydrodynamics

The quantum hydrodynamic model of the previous section is derived for a single particle and therefore, it does not contain a temperature term. In order to include temperature, we consider now an electron ensemble represented by a mixed state (see Section 6.1). A mixed quantum state consists of a sequence of occupation probabilities $\lambda_j \geq 0$ ($j \in \mathbb{N}$) for the j -th state ψ_j described by the scaled Schrödinger equation [25]

$$i\varepsilon \partial_t \psi_j = -\frac{\varepsilon^2}{2} \Delta \psi_j - V(x, t) \psi_j, \quad t > 0, \quad \psi_j(\cdot, 0) = \psi_j^0 \quad \text{in } \mathbb{R}^3, \quad (152)$$

where the electric potential is assumed to be given. The occupation numbers satisfy $\sum_{j=1}^{\infty} \lambda_j = 1$, which means that the probability of finding the electron ensemble in any of the quantum states is one.

We define the single-state particle and current densities of the j -th state as in the previous section as

$$n_j = |\psi_j|^2, \quad J_j = -\varepsilon \operatorname{Im}(\bar{\psi}_j \nabla \psi_j), \quad j \in \mathbb{N}.$$

We claim that, following [25], the total electron density n and current density J of the mixed state,

$$n = \sum_{j=1}^{\infty} \lambda_j |\psi_j|^2, \quad J = \sum_{j=1}^{\infty} \lambda_j J_j, \quad (153)$$

are a solution of the quantum hydrodynamic equations with a temperature tensor.

Theorem 7.2 (Quantum hydrodynamic equations). *Let ψ_j be single-state solutions of the Schrödinger equation (152) with occupation numbers λ_j of the j -th quantum state. Then (n, J) , defined in (153), is a solution of the quantum hydrodynamic equations*

$$\partial_t n - \operatorname{div} J = 0, \quad (154)$$

$$\partial_t J - \operatorname{div} \left(\frac{J \otimes J}{n} + n\theta \right) + n \nabla V + \frac{\varepsilon^2}{2} n \nabla \left(\frac{\Delta \sqrt{n}}{\sqrt{n}} \right) = 0, \quad (155)$$

where $x \in \mathbb{R}^3$ and $t > 0$, with initial conditions

$$n(\cdot, 0) = \sum_{j=1}^{\infty} \lambda_j |\psi_j^0|^2, \quad J(\cdot, 0) = -\varepsilon \sum_{j=1}^{\infty} \lambda_j \operatorname{Im}(\bar{\psi}_j^0 \nabla \psi_j^0) \quad \text{in } \mathbb{R}^3.$$

The temperature tensor θ is defined by $\theta = \theta_{\text{cu}} + \theta_{\text{os}}$, where the “current temperature” and “osmotic temperature” are given by, respectively,

$$\theta_{\text{cu}} = \sum_{j=1}^{\infty} \lambda_j \frac{n_j}{n} (u_{\text{cu},j} - u_{\text{cu}}) \otimes (u_{\text{cu},j} - u_{\text{cu}}),$$

$$\theta_{\text{os}} = \sum_{j=1}^{\infty} \lambda_j \frac{n_j}{n} (u_{\text{os},j} - u_{\text{os}}) \otimes (u_{\text{os},j} - u_{\text{os}}),$$

and the variables

$$u_{\text{cu},j} = -\frac{J_j}{n_j}, \quad u_{\text{cu}} = -\frac{J}{n}, \quad u_{\text{os},j} = \frac{\varepsilon}{2} \nabla \log n_j, \quad u_{\text{os}} = \frac{\varepsilon}{2} \nabla \log n$$

are called the “current velocities” and “osmotic velocities”, respectively.

The notion “osmotic” comes from the fact that the quantum term can be written as the divergence of the quantum stress tensor $P = (\varepsilon^2/4)n(\nabla \otimes \nabla) \log n$ [25].

Proof. The pair (n_j, J_j) solves the single-state quantum hydrodynamic equations (147) with initial conditions

$$n_j(\cdot, 0) = |\psi_j^0|^2, \quad J_j(\cdot, 0) = -\varepsilon \text{Im}(\bar{\psi}_j^0 \nabla \psi_j^0).$$

Multiplication of (147) by λ_j and summation over j yields

$$\begin{aligned} \partial_t n - \text{div} J &= 0, \\ \partial_t J - \sum_{j=1}^{\infty} \lambda_j \text{div} \left(\frac{J_j \otimes J_j}{n_j} \right) + n \nabla V + \frac{\varepsilon^2}{2} \sum_{j=1}^{\infty} \lambda_j n_j \nabla \left(\frac{\Delta \sqrt{n_j}}{\sqrt{n_j}} \right) &= 0. \end{aligned} \quad (156)$$

We rewrite the second and fourth term of the second equation. With the definitions of the “current temperature” and “current velocity”, we obtain

$$\begin{aligned} \sum_{j=1}^{\infty} \lambda_j \text{div} \left(\frac{J_j \otimes J_j}{n_j} \right) &= \sum_{j=1}^{\infty} \lambda_j \text{div} (n_j u_{\text{cu},j} \otimes u_{\text{cu},j}) \\ &= \sum_{j=1}^{\infty} \lambda_j \text{div} (n_j (u_{\text{cu},j} - u_{\text{cu}}) \otimes (u_{\text{cu},j} - u_{\text{cu}}) + 2n_j u_{\text{cu},j} \otimes u_{\text{cu}}) - \text{div} (n u_{\text{cu}} \otimes u_{\text{cu}}) \\ &= \text{div} (n \theta_{\text{cu}}) + 2 \sum_{j=1}^{\infty} \text{div} \left(\lambda_j J_j \otimes \frac{J}{n} \right) - \text{div} \left(\frac{J \otimes J}{n} \right) = \text{div} (n \theta_{\text{cu}}) + \text{div} \left(\frac{J \otimes J}{n} \right). \end{aligned}$$

Furthermore, employing the definitions of the “osmotic temperature” and “osmotic velocity”, we compute

$$\begin{aligned} \frac{\varepsilon^2}{2} \sum_{j=1}^{\infty} \lambda_j n_j \nabla \left(\frac{\Delta \sqrt{n_j}}{\sqrt{n_j}} \right) &= \frac{\varepsilon^2}{4} \sum_{j=1}^{\infty} \lambda_j \text{div} \left((\nabla \otimes \nabla) n_j - \frac{\nabla n_j \otimes \nabla n_j}{n_j} \right) \\ &= \frac{\varepsilon^2}{4} \sum_{j=1}^{\infty} \lambda_j \text{div} \left((\nabla \otimes \nabla) n_j + \frac{n_j}{n} \frac{\nabla n \otimes \nabla n}{n} - 2 \frac{\nabla n \otimes \nabla n_j}{n} \right. \\ &\quad \left. - n_j \left(\frac{\nabla n_j}{n_j} - \frac{\nabla n}{n} \right) \otimes \left(\frac{\nabla n_j}{n_j} - \frac{\nabla n}{n} \right) \right) \\ &= \frac{\varepsilon^2}{4} \text{div} \left((\nabla \otimes \nabla) n - \frac{\nabla n \otimes \nabla n}{n} \right) - \text{div} (n \theta_{\text{os}}) \\ &= \frac{\varepsilon^2}{2} n \nabla \left(\frac{\Delta \sqrt{n}}{\sqrt{n}} \right) - \text{div} (n \theta_{\text{os}}). \end{aligned}$$

Inserting these expressions into (156) gives (155). \square

The temperature tensor cannot be expressed in terms of the total particle and current densities without further assumptions, and as in the derivation of the semi-classical hydrodynamic equations, we need a closure condition to obtain a closed set of equations. In the literature, the following closures were employed.

Assume that the temperature tensor is diagonal with equal entries on the diagonal, $\theta = T \text{Id}$, where T is a scalar temperature and Id the identity matrix. Then we can close the equations (154)-(155) by taking T to be constant and refer to this case as the *isothermal quantum hydrodynamic model*. If T is given by $T(n) = T_0 n^\alpha$ for some $\alpha > 0$, we refer to (154)-(155) as the *isentropic quantum hydrodynamic model*.

Boundary conditions. When the quantum hydrodynamic equations are considered in a bounded domain, some boundary conditions are needed. In the literature, the following boundary conditions for irrotational flows were suggested [30]. We consider the steady state isothermal equations

$$\text{div } J = 0, \quad -\text{div} \left(\frac{J \otimes J}{n} \right) - \nabla n + n \nabla V + \frac{\varepsilon^2}{6} n \nabla \left(\frac{\Delta \sqrt{n}}{\sqrt{n}} \right) = 0 \quad \text{in } \Omega$$

and we assume that the velocity J/n is irrotational and that there exists a velocity potential S such that $J = -n \nabla S$. Since $\text{div} (J \otimes J/n) = \frac{1}{2} n \nabla |\nabla S|^2$, we can write the momentum equation as

$$n \nabla \left(\frac{1}{2} |\nabla S|^2 + \log n - V - \frac{\varepsilon^2}{6} \frac{\Delta \sqrt{n}}{\sqrt{n}} \right) = 0.$$

Assuming that $n > 0$, we infer that

$$\frac{1}{2} |\nabla S|^2 + \log n - V - \frac{\varepsilon^2}{6} \frac{\Delta \sqrt{n}}{\sqrt{n}} = 0. \quad (157)$$

The integration constant can be assumed to vanish by choosing a reference point for the electric potential. This formulation allows us to write the stationary quantum hydrodynamic equations, together with a self-consistent electric potential, as a system of second-order differential equations:

$$\begin{aligned} \text{div} (n \nabla S) &= 0, \quad \lambda_D^2 \Delta V = n - C(x), \\ \frac{\varepsilon^2}{6} \Delta \sqrt{n} &= \frac{1}{2} \sqrt{n} |\nabla S|^2 + \sqrt{n} \log n - \sqrt{n} V. \end{aligned}$$

Thus, we need boundary conditions for the functions S , n , and V .

The boundary $\partial\Omega$ is assumed to consist of two parts: the Dirichlet part Γ_D and the insulating part Γ_N , where $\Gamma_D \cup \Gamma_N = \partial\Omega$ and $\Gamma_D \cap \Gamma_N = \emptyset$. We suppose that the normal derivatives of the variables vanish on the insulating boundary,

$$\nabla n \cdot \eta = \nabla S \cdot \eta = \nabla V \cdot \eta = 0 \quad \text{on } \Gamma_N,$$

where η denotes the exterior unit normal vector on $\partial\Omega$. On the Dirichlet part, the boundary data are assumed to be the superposition of the thermal equilibrium functions $(n_{\text{eq}}, S_{\text{eq}}, V_{\text{eq}})$ and the applied potential U :

$$n = n_{\text{eq}}, \quad S = S_{\text{eq}} + U, \quad V = V_{\text{eq}} + U \quad \text{on } \Gamma_D.$$

The thermal equilibrium is defined by $J = 0$ or (as n is positive) $S = \text{const}$. By fixing the reference point for S , we can suppose that $S_{\text{eq}} = 0$. We assume further that

- the total space charge $C - n_{\text{eq}}$ vanishes on the boundary and
- no quantum effects occur on the boundary, i.e. $\Delta\sqrt{n_{\text{eq}}}/\sqrt{n_{\text{eq}}} = 0$.

Then we obtain from (157):

$$\frac{1}{2}|\nabla S_{\text{eq}}|^2 + \log n_{\text{eq}} - V_{\text{eq}} = 0$$

and, since $S_{\text{eq}} = 0$, $V_{\text{eq}} = \log n_{\text{eq}}$ on Γ_D . Therefore, the Dirichlet boundary conditions are given by

$$n = C, \quad S = U, \quad V = \log C + U \quad \text{on } \Gamma_D.$$

These conditions were employed to prove the existence and uniqueness of solutions for subsonic flow in [30].

7.3 Quantum Maxwellians

The quantum Maxwellian is defined by that Wigner function which maximizes the quantum entropy subject to the constraint that its moments are given. This idea is due to Degond and Ringhofer [20]. In order to define the quantum Maxwellian, we use the Wigner transform $W(\hat{\rho})$ of an operator $\hat{\rho}$ on $L^2(\mathbb{R}^3)$ with integral kernel ρ (satisfying certain regularity assumptions). Then we can write

$$(\hat{\rho}\phi)(x) = \int_{\mathbb{R}^3} \rho(x, y)\phi(y) dy, \quad \phi \in L^2(\mathbb{R}^3).$$

We recall that the *Wigner transform* of $\hat{\rho}$ is defined as the Fourier transform of the transformed function ρ :

$$W(\hat{\rho})(x, p) = \int_{\mathbb{R}^3} \rho\left(x + \frac{\varepsilon}{2}\eta, x - \frac{\varepsilon}{2}\eta\right) e^{-i\eta \cdot p} d\eta.$$

Its inverse W^{-1} , also called Weyl quantization, is defined as an operator on $L^2(\mathbb{R}^3)$,

$$(W^{-1}(f)\phi)(x) = \frac{1}{(2\pi\varepsilon)^3} \int_{\mathbb{R}^3 \times \mathbb{R}^3} f\left(\frac{x+y}{2}\right) \phi(y) e^{ip \cdot (x-y)/\varepsilon} dp dy, \quad \phi \in L^2(\mathbb{R}^3).$$

With these definitions, we are able to introduce as in [20] the *quantum exponential* Exp and the *quantum logarithm* Log formally by

$$\text{Exp } f = W(\exp W^{-1}(f)), \quad \text{Log } f = W(\log W^{-1}(f)),$$

where \exp and \log are the operator exponential and logarithm, respectively, defined by their corresponding spectral decomposition. The quantum exponential and logarithm have the following formal properties.

Lemma 7.3 (Properties of Exp and Log). *The quantum logarithm is the inverse of the quantum exponential. Furthermore, Exp and Log are formally (Fréchet) differentiable and*

$$\frac{d}{dw} \text{Log } w = \frac{1}{w}, \quad \frac{d}{dw} \text{Exp } w = \text{Exp } w.$$

Proof. The first assertion follows from the formal computation

$$\text{Log}(\text{Exp } w) = W(\exp W^{-1}(W(\log W^{-1}(w)))) = W(\exp(\log W^{-1}(w))) = w.$$

Since the Wigner transform and its inverse are linear operations, the second assertion follows from the properties of the operator exponential and logarithm (see [20, Lemma 3.3] or [19, Theorem 1] for a more precise argument). \square

Let a quantum mechanical state be described by the Wigner function w solving the Wigner-Boltzmann equation (142). The scaled *quantum entropy* or *von Neumann entropy* of the quantum mechanical state is given by

$$S(w) = -\frac{2}{(2\pi\varepsilon)^3} \int_{\mathbb{R}^3 \times \mathbb{R}^3} w(x, p, \cdot) \left((\text{Log } w)(x, p, \cdot) - 1 + \frac{|p|^2}{2} - V(x, \cdot) \right) dx dp, \quad (158)$$

where V is the electric potential. 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 set

$$\langle g(p) \rangle = \frac{2}{(2\pi\varepsilon)^3} \int_{\mathbb{R}^3} w(x, p, t) g(p) dp$$

for functions $g = g(p)$. The above notation is consistent with the notation from Section 3, $\langle f(k) \rangle = \int f(k) dk / 4\pi^3$, since in scaled variables, it holds $p = \varepsilon k$. Let some weight functions $\kappa(p) = (\kappa_0(p), \dots, \kappa_N(p))$ be given.

Lemma 7.4. *Let $w = w(x, p, t)$ be given and let the moments $m = (m_0, \dots, m_N)$ of w defined by*

$$m_j(x, t) = \langle w(x, p, t) \kappa_j(p) \rangle, \quad j = 0, \dots, N.$$

The formal solution of the constrained maximization problem

$$S(M[w]) = \max \{ S(f) : \langle f(x, p, t) \kappa(p) \rangle = m(x, t) \text{ for all } x \in \mathbb{R}^3, t > 0 \}, \quad (159)$$

if it exists, is given by

$$M[w] = \text{Exp}\left(\tilde{\lambda} \cdot \kappa + V - \frac{|p|^2}{2}\right),$$

where $\tilde{\lambda} = (\tilde{\lambda}_0, \dots, \tilde{\lambda}_N)$ are some Lagrange multipliers.

We call $M[w]$ the *quantum Maxwellian* of w . If we assume that $w_0(p) = 1$ and $w_2(p) = \frac{1}{2}|p|^2$, setting $\lambda_0 = \tilde{\lambda}_0 + V$, $\lambda_2 = \tilde{\lambda}_2 - 1$, and $\lambda_j = \tilde{\lambda}_j$ otherwise, we can write the quantum Maxwellian more compactly as

$$M[w] = \text{Exp}(\lambda \cdot \kappa(p)).$$

Proof. We define for $\tilde{\lambda} = (\tilde{\lambda}_0, \dots, \tilde{\lambda}_N)$ and $m = (m_0, \dots, m_N)$ the Lagrange functional

$$F(w, \tilde{\lambda}) = S(w) + \int_{\mathbb{R}^3} \tilde{\lambda}(x) \cdot (m - \langle w(x, p, t) \kappa(p) \rangle) dx.$$

Using Lemma 7.3, the derivative of the quantum entropy is given by

$$\left(\frac{d}{dw} S(w)\right)(u) = -\frac{2}{(2\pi\varepsilon)^3} \int_{\mathbb{R}^3 \times \mathbb{R}^3} \left(\text{Log } w + \frac{|p|^2}{2} - V\right) u(x, p) dx dp.$$

Therefore, the necessary condition for an extremal point reads as

$$\begin{aligned} 0 &= \left(\frac{d}{dw} F(w^*, \tilde{\lambda}^*)\right)(u) \\ &= \int_{\mathbb{R}^3 \times \mathbb{R}^3} \left(\text{Log } w + \frac{|p|^2}{2} - V - \tilde{\lambda}^*(x) \cdot \kappa(p)\right) u(x, p) dx dp \end{aligned}$$

for all functions $u(x, p)$. This implies that

$$\text{Log } w^* + \frac{|p|^2}{2} - V(x, t) - \tilde{\lambda}^*(x) \cdot \kappa(p) = 0$$

and finally,

$$w^* = \text{Exp}\left(\tilde{\lambda}^* \cdot \kappa + V - \frac{|p|^2}{2}\right),$$

finishing the proof. □

Example 7.5. We give an example of a quantum Maxwellians which is used in the following sections. We define, for given w , the local particle density n , mean velocity u , and energy density ne by

$$\begin{pmatrix} n \\ nu \\ ne \end{pmatrix} (x, t) = \frac{2}{(2\pi\varepsilon)^3} \int_{\mathbb{R}^3} w(x, p, t) \begin{pmatrix} 1 \\ p \\ \frac{1}{2}|p|^2 \end{pmatrix} dp.$$

□

The quantum Maxwellian is a nonlocal operator. It can be made more explicit when expanding it in terms of the scaled Planck constant ε , which appears in the definition of the Wigner transform. We only mention that

$$\text{Exp}(f) = \exp f + \mathcal{O}(\varepsilon^2).$$

The $\mathcal{O}(\varepsilon^2)$ -contribution can be made explicit but the formula is rather cumbersome and we refer to the literature, e.g., [31, Lemma 12.4].

7.4 Wigner-Boltzmann Equations and Quantum Hydrodynamics

The quantum hydrodynamic model of the previous section does not include collisional effects since the Schrödinger equation only models ballistic transport. In order to allow for collisional phenomena, we employ a (scaled) Wigner-Boltzmann equation

$$\partial_t w + p \cdot \nabla_x w + \theta[V]w = Q(w), \quad t > 0, \quad w(x, p, 0) = w_I(x, p), \quad (x, p) \in \mathbb{R}^6$$

(see Section 6.4 for a discussion of Wigner-Boltzmann models). The electric potential V is assumed to be a solution of the Poisson equation

$$\lambda_D^2 \Delta V = \frac{2}{(2\pi\varepsilon)^3} \int_{\mathbb{R}^3} w \, dp - C(x), \quad x \in \mathbb{R}^3. \quad (160)$$

The following presentation is based on [20] and [32]. We assume that the collision operator $Q(w)$ is the sum of two operators Q_0 and Q_1 . We employ as in Section 5 a hydrodynamic scaling and replace x by x/α and t by t/α , where $\alpha > 0$ is the ratio of the mean free paths corresponding to Q_0 and Q_1 , respectively. We assume that Q_0 models collisions which occur more frequently than those described by Q_1 which implies that $\alpha \ll 1$. Then we can write the Wigner-Boltzmann equation as

$$\alpha \partial_t w + \alpha(p \cdot \nabla_x w + \theta[V]w) = Q_0(w) + \alpha Q_1(w), \quad w(\cdot, \cdot, 0) = w_I. \quad (161)$$

The collisions modeled by Q_0 are supposed to conserve mass, momentum, and energy,

$$\langle Q_0(w) \kappa_j(p) \rangle = 0 \quad \text{for all } w, \quad j = 0, 1, 2, \quad (162)$$

where

$$\kappa_0(p) = 1, \quad \kappa_1(p) = p, \quad \kappa_2(p) = \frac{1}{2}|p|^2$$

are the weight functions. The collision operator Q_1 remains unspecified. For the moment, we only suppose that Q_1 conserves mass:

$$\langle Q_1(w) \rangle = 0 \quad \text{for all } w. \quad (163)$$

We also assume that the kernel of Q_0 consists exactly of the quantum Maxwellians. We need to specify this notion.

Let w be given. By Examples 7.5, the quantum Maxwellian as the maximizer of the quantum entropy under the constraints

$$\frac{2}{(2\pi\varepsilon)^3} \int_{\mathbb{R}^3} w(x, p, t) \begin{pmatrix} 1 \\ p \\ \frac{1}{2}|p|^2 \end{pmatrix} dp = \begin{pmatrix} n \\ nu \\ ne \end{pmatrix} (x, t), \quad x \in \mathbb{R}^3, t > 0, \quad (164)$$

where $n = \langle w \rangle$, $nu = \langle pw \rangle$, and $ne = \langle \frac{1}{2}|p|^2 w \rangle$, is (if it exists) given by

$$M[w](x, t) = \text{Exp} \left(A(x, t) - \frac{|p - v(x, t)|^2}{2T(x, t)} \right). \quad (165)$$

The Lagrange multipliers A , v , and T are uniquely determined by the moments of w . In the classical setting, they correspond to the logarithm of the particle density, the velocity, and the temperature, respectively. Thus, the assumption on the kernel of Q_0 can be formulated as

$$Q_0(w) = 0 \quad \text{if and only if} \quad w = M[w]. \quad (166)$$

We need the following result on the moments of the potential operator.

Lemma 7.6 (Moments of the potential operator). *Let the operator $\theta[V]$ be defined by (133). Then, for all functions $w = w(x, p, t)$,*

$$\langle \theta[V]w \rangle = 0, \quad \langle p\theta[V]w \rangle = -n\nabla_x V, \quad (167)$$

$$\langle \frac{1}{2}|p|^2 \theta[V]w \rangle = -\langle pw \rangle \cdot \nabla V, \quad (168)$$

$$\langle \frac{1}{2}p|p|^2 \theta[V]w \rangle = -(\langle p \otimes pw \rangle + \langle \frac{1}{2}|p|^2 w \rangle \text{Id}) \nabla V + \frac{\varepsilon^2}{8} \langle w \rangle \nabla \Delta V. \quad (169)$$

where $n = \langle w \rangle$.

Proof. We notice that an integration of the Fourier inversion formula

$$\phi(x, p, t) = \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} (\mathcal{F}(\phi))(x, \eta, t) e^{ip \cdot \eta} d\eta$$

over \mathbb{R}^3 with respect to p gives

$$(\mathcal{F}(\phi))(x, 0, t) = \int_{\mathbb{R}^3} \phi(x, p, t) dp = \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3 \times \mathbb{R}^3} (\mathcal{F}(\phi))(x, \eta, t) e^{ip \cdot \eta} d\eta dp. \quad (170)$$

With this expression we compute

$$\begin{aligned} \langle \theta[V]w \rangle &= \frac{2}{(2\pi\varepsilon)^3} \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3 \times \mathbb{R}^3} (\delta V)(x, \eta, t) (\mathcal{F}(w))(x, \eta, t) e^{ip \cdot \eta} d\eta dp \\ &= \frac{2}{(2\pi\varepsilon)^3} (\delta V)(x, 0, t) (\mathcal{F}(w))(x, 0, t) \\ &= \frac{2}{(2\pi\varepsilon)^3} \frac{i}{\varepsilon} \left[V \left(x + \frac{\varepsilon}{2} \eta, t \right) - V \left(x - \frac{\varepsilon}{2} \eta, t \right) \right]_{\eta=0} (\mathcal{F}(w))(x, 0, t) = 0. \end{aligned}$$

Furthermore, since $pe^{ip\cdot\eta} = -i\nabla_\eta e^{ip\cdot\eta}$, integration by parts yields

$$\begin{aligned}\langle p\theta[V]w \rangle &= \frac{2}{(2\pi\varepsilon)^3} \frac{i}{(2\pi)^3} \\ &\quad \times \int_{\mathbb{R}^3 \times \mathbb{R}^3} ((\nabla_\eta \delta V)\mathcal{F}(w) + (\delta V)\nabla_\eta \mathcal{F}(w))(x, \eta, t) e^{ip\cdot\eta} d\eta dp.\end{aligned}$$

Then the expression (170) implies that

$$\langle p\theta[V]w \rangle = 2i(2\pi\varepsilon)^{-3} ((\nabla_\eta \delta V)\mathcal{F}(w) + (\delta V)\nabla_\eta \mathcal{F}(w))(x, 0, t).$$

Employing $(\delta V)(x, 0, t) = 0$ and

$$(\nabla_\eta \delta V)(x, 0, t) = \frac{i}{2} \left[\nabla_x V \left(x + \frac{\varepsilon}{2} \eta, t \right) + \nabla_x V \left(x - \frac{\varepsilon}{2} \eta, t \right) \right]_{\eta=0} = i\nabla_x V(x, t)$$

finally yields

$$\langle p\theta[V]w \rangle = -2(2\pi\varepsilon)^{-3} \nabla_x V(x, t) (\mathcal{F}(w))(x, 0, t) = -\nabla_x V n,$$

proving (167).

We recall the formula (170):

$$\phi(x, 0, t) = \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3 \times \mathbb{R}^3} \phi(x, \eta, t) e^{ip\cdot\eta} d\eta dp$$

for all functions ϕ . Then, integrating by parts, we compute

$$\begin{aligned}\langle \frac{1}{2}|p|^2\theta[V]w \rangle &= \int_{\mathbb{R}^9} (\delta V)(x, \eta, t) w(x, p', t) e^{-ip'\cdot\eta} (-\Delta_\eta e^{ip\cdot\eta}) \frac{dp' d\eta dp}{(2\pi)^3(2\pi\varepsilon)^3} \\ &= - \int_{\mathbb{R}^9} \Delta_\eta (\delta V e^{-ip'\cdot\eta}) w(x, p', t) e^{ip\cdot\eta} \frac{dp' d\eta dp}{(2\pi)^3(2\pi\varepsilon)^3} \\ &= - \int_{\mathbb{R}^3} \Delta_\eta (\delta V e^{-ip'\cdot\eta}) \Big|_{\eta=0} w(x, p', t) \frac{dp'}{(2\pi\varepsilon)^3}.\end{aligned}$$

Since $(\delta V)(x, 0, t) = \Delta_\eta(\delta V)(x, 0, t) = 0$ and $\nabla_\eta(\delta V)(x, 0, t) = i\nabla V(x, t)$, the above expression becomes

$$\langle \frac{1}{2}|p|^2\theta[V]w \rangle = -2 \int_{\mathbb{R}^3} p' \cdot \nabla V(x, t) w(x, p', t) \frac{dp'}{(2\pi\varepsilon)^3} = -\langle pw \rangle \cdot \nabla V.$$

In a similar way, we can prove the second identity. Employing $\nabla_\eta \Delta_\eta(\delta V)(x, 0, t) = i(\varepsilon^2/4)\nabla\Delta V$, we obtain

$$\begin{aligned}\langle \frac{1}{2}p|p|^2\theta[V]w \rangle &= -i \int_{\mathbb{R}^9} \nabla_\eta \Delta_\eta (\delta V e^{-ip'\cdot\eta}) w(x, p', t) e^{ip\cdot\eta} \frac{dp' d\eta dp}{(2\pi)^3(2\pi\varepsilon)^3} \\ &= \int_{\mathbb{R}^3} \left(\frac{\varepsilon^2}{4} \nabla\Delta V - 2(p' \otimes p') \nabla V - |p'|^2 \nabla V \right) w(x, p', t) \frac{dp'}{(2\pi\varepsilon)^3} \\ &= \frac{\varepsilon^2}{8} \nabla\Delta V \langle w \rangle - \langle p \otimes pw \rangle \nabla V - \langle \frac{1}{2}|p|^2 w \rangle \nabla V.\end{aligned}$$

This finishes the proof. □

Derivation of the quantum hydrodynamic equations. The quantum hydrodynamic equations are now derived in the formal limit $\alpha \rightarrow 0$. Let w_α be a solution of the Wigner-Boltzmann equation (161) and V_α be a solution of the Poisson equation (160). The limit $\alpha \rightarrow 0$ in (161) gives $Q_0(w) = 0$, where $w = \lim_{\alpha \rightarrow 0} w_\alpha$, and hence, by assumption, $w = M[w]$. Multiplying (161) by the weight functions $\kappa_j(p)$ and integrating over $p \in \mathbb{R}^3$ yields the moment equations

$$\partial_t \langle \kappa_j w_\alpha \rangle + \operatorname{div}_x \langle p \kappa_j w_\alpha \rangle + \langle \kappa_j \theta[V] w_\alpha \rangle = \langle \kappa_j Q_1(w_\alpha) \rangle,$$

since $\langle \kappa_j Q_0(w_\alpha) \rangle = 0$ by assumption (162). The limit $\alpha \rightarrow 0$ in the moment equations then gives, by taking into account the constraints (164), the property (163) on Q_1 , and the moments of the potential operator, see Lemma 7.6,

$$\partial_t n - \operatorname{div} J_n = 0, \quad (171)$$

$$\partial_t J_n - \operatorname{div} \langle p \otimes p M[w] \rangle + n \nabla V = -\langle p Q_1(M[w]) \rangle, \quad (172)$$

$$\partial_t (ne) + \operatorname{div} \langle \frac{1}{2} |p|^2 p M[w] \rangle + J_n \cdot \nabla V = \langle \frac{1}{2} |p|^2 Q_1(M[w]) \rangle, \quad (173)$$

where $J_n = -nu$ is the current density. Defining the quantum stress tensor P and the quantum heat flux q by

$$P = \langle (p - u) \otimes (p - u) M[w] \rangle, \quad q = \langle \frac{1}{2} (p - u) |p - u|^2 M[w] \rangle, \quad (174)$$

we can simplify the integrals $\langle p \otimes p M[w] \rangle$ and $\langle \frac{1}{2} p |p|^2 M[w] \rangle$ slightly:

$$\langle p \otimes p M[w] \rangle = P + \frac{J_n \otimes J_n}{n}, \quad \langle \frac{1}{2} p |p|^2 M[w] \rangle = -(P + ne \operatorname{Id}) \frac{J_n}{n} + q.$$

The result is summarized in the following theorem.

Theorem 7.7 (Nonlocal quantum hydrodynamic equations). *Let the collision operator satisfy assumptions (162), (163), and (166). Let (w_α, V_α) be a solution of the Wigner-Boltzmann-Poisson system (160)-(161). Then, formally, as $\alpha \rightarrow 0$, $w_\alpha \rightarrow w$ and $V_\alpha \rightarrow V$, where $w = \operatorname{Exp}(A - |p - v|^2/2T)$, and (A, v, T, V) is a solution of the quantum hydrodynamic equations*

$$\partial_t n - \operatorname{div} J_n = 0, \quad (175)$$

$$\partial_t J_n - \operatorname{div} \left(\frac{J_n \otimes J_n}{n} + P \right) + n \nabla V = -\langle p Q_1(w) \rangle, \quad (176)$$

$$\begin{aligned} \partial_t (ne) - \operatorname{div} ((P + ne \operatorname{Id}) J_n - q) + J_n \cdot \nabla V &= \langle \frac{1}{2} |p|^2 Q_1(w) \rangle, \\ \lambda_D^2 \Delta V &= n - C(x), \end{aligned} \quad (177)$$

where the quantum stress tensor P and quantum heat flux q are introduced in (174). The initial data are given by

$$n(\cdot, 0) = \langle w_I \rangle, \quad J_n(\cdot, 0) = -\langle p w_I \rangle, \quad (ne)(\cdot, 0) = \langle \frac{1}{2} |p|^2 w_I \rangle,$$

and the Lagrange multipliers (A, v, T) are determined by

$$\begin{pmatrix} n \\ nu \\ ne \end{pmatrix} = \frac{2}{(2\pi\varepsilon)^3} \int_{\mathbb{R}^3} \text{Exp}\left(A - \frac{|p-v|^2}{2T}\right) \begin{pmatrix} 1 \\ p \\ \frac{1}{2}|p|^2 \end{pmatrix} dp,$$

where $J_n = -nu$ is the current density.

The quantum hydrodynamic model of the above theorem is rather involved and not easy to handle numerically. It can be made more explicit if we consider the isothermal situation. Below, we will expand the integrals in powers of ε^2 which yields another simplification.

Local quantum hydrodynamic equations. The quantum hydrodynamic model (175)-(177) is nonlocal since the stress tensor and heat flux depend implicitly on the moments through the Lagrange multipliers. These expressions can be expressed in powers of ε^2 in order to derive a local version of the model. Inserting the expansion of the quantum Maxwellian into the definition of the moments, we obtain after some lengthy computations (see [32, Lemma 3.4] for details):

$$\begin{aligned} n &= 2(2\pi\varepsilon^2)^{-3/2}e^A - \frac{\varepsilon^2}{12T}(2\pi\varepsilon^2)^{-3/2}e^A \left(-2\Delta A - |\nabla A|^2 \right. \\ &\quad \left. + \nabla \log T \cdot \nabla A - 2\Delta \log T + \frac{1}{4}|\nabla \log T|^2 + \frac{1}{2T}\text{Tr}(R^\top R) \right) + \mathcal{O}(\varepsilon^4), \end{aligned} \quad (178)$$

$$\begin{aligned} ne &= \frac{3}{2}nT + \frac{1}{2}n|u|^2 - \frac{\varepsilon^2}{24}n \left(\Delta \log n - \frac{1}{T}\text{Tr}(R^\top R) - \frac{3}{2}|\nabla \log T|^2 \right. \\ &\quad \left. - \Delta \log T - \nabla \log T \cdot \nabla \log n \right) + \mathcal{O}(\varepsilon^4), \end{aligned} \quad (179)$$

where the vorticity matrix $R = (R_{j\ell})$ is the antisymmetric part of the velocity derivatives, $R_{j\ell} = \partial u_j / \partial x_\ell - \partial u_\ell / \partial x_j$. Furthermore, the quantum stress tensor and quantum heat flux can be expanded as follows (see [32, Lemma 3.5]):

$$\begin{aligned} P &= nT \text{Id} + \frac{\varepsilon^2}{12}n \left(\frac{5}{2}\nabla \log T \otimes \nabla \log T - \nabla \log T \otimes \nabla \log n - \nabla \log n \otimes \nabla \log T \right. \\ &\quad \left. - (\nabla \otimes \nabla) \log(nT^2) + \frac{1}{T}R^\top R \right) + \frac{\varepsilon^2}{12}T \text{div} \left(\frac{n}{T}\nabla \log T \right) + \mathcal{O}(\varepsilon^4), \end{aligned} \quad (180)$$

$$q = -\frac{\varepsilon^2}{24}n \left(5R\nabla \log T + 2\text{div} R + 3\Delta u \right) + \mathcal{O}(\varepsilon^4). \quad (181)$$

The expansions simplify if we assume that the temperature varies slowly in the sense of $\nabla \log T = \mathcal{O}(\varepsilon^2)$. Then the expressions $\varepsilon^2 \nabla \log T$ are of order $\mathcal{O}(\varepsilon^4)$ and can be neglected in our approximation. We obtain, up to order $\mathcal{O}(\varepsilon^4)$:

$$\begin{aligned} P &= nT \text{Id} - \frac{\varepsilon^2}{12}n \left((\nabla \otimes \nabla) \log n - \frac{1}{T}R^\top R \right), \\ q &= -\frac{\varepsilon^2}{24}n(2\text{div} R + 3\Delta u), \\ ne &= \frac{3}{2}nT + \frac{1}{2}n|u|^2 - \frac{\varepsilon^2}{24}n \left(\Delta \log n - \frac{1}{T}\text{Tr}(R^\top R) \right). \end{aligned}$$

Equations (175)-(177), together with the above expansions, form a closed set of equations. The stress tensor consists of the classical pressure nT on the diagonal, the quantum pressure $(\varepsilon^2/12)n(\nabla \otimes \nabla) \log n$, and the vorticity correction $(\varepsilon^2/12)nR^\top R/T$. The quantum heat flux depends on the second derivatives of the velocity. Finally, the energy density consists of the thermal energy, kinetic energy, and quantum energy including a vorticity correction.

Further simplifications are obtained by assuming that the vorticity tensor R is small in the sense of $R = \mathcal{O}(\varepsilon^2)$. Notice that in one space dimension, this term vanishes.

Theorem 7.8 (Local quantum hydrodynamic equations). *Let the assumptions of Theorem 7.7 hold. We assume further that the temperature variations and the vorticity tensor are small in the sense of $\nabla \log T = \mathcal{O}(\varepsilon^2)$ and $R = \mathcal{O}(\varepsilon^2)$. Then the moments (n, J_n, ne) of the limit quantum Maxwellian solve the quantum hydrodynamic equations*

$$\partial_t n - \operatorname{div} J_n = 0, \quad (182)$$

$$\partial_t J_n - \operatorname{div} \left(\frac{J_n \otimes J_n}{n} \right) - \nabla(nT) + n \nabla V + \frac{\varepsilon^2}{6} n \nabla \left(\frac{\Delta \sqrt{n}}{\sqrt{n}} \right) = -\langle p Q_1(w) \rangle, \quad (183)$$

$$\partial_t(ne) - \operatorname{div} ((P + ne \operatorname{Id})u) - \frac{\varepsilon^2}{8} \operatorname{div} (n \Delta u) + J_n \cdot \nabla V = \langle \frac{1}{2} |p|^2 Q_1(w) \rangle, \quad (184)$$

where the energy density ne and the quantum stress tensor P are given by

$$P = nT \operatorname{Id} - \frac{\varepsilon^2}{12} n (\nabla \otimes \nabla) \log n, \quad ne = \frac{3}{2} nT + \frac{1}{2} n |u|^2 - \frac{\varepsilon^2}{24} n \Delta \log n. \quad (185)$$

The initial conditions for n , J_n , and ne are as in Theorem 7.7.

The quantum heat flux q (but not the vorticity tensor R) also appears in other quantum hydrodynamic derivations. Numerical results in [32] indicate that the dispersive term stabilizes the quantum hydrodynamic system numerically.

The above equations can be written in unscaled form as follows:

$$\begin{aligned} \partial_t n - \frac{1}{q} \operatorname{div} J_n &= 0, \quad x \in \mathbb{R}^3, \quad t > 0, \\ \partial_t J_n - \operatorname{div} \left(\frac{J_n \otimes J_n}{qn} \right) - \frac{qk_B}{m^*} \nabla(nT) + \frac{q^2}{m^*} n \nabla V + \frac{q\hbar^2}{6(m^*)^2} n \nabla \left(\frac{\Delta \sqrt{n}}{\sqrt{n}} \right) \\ &= -\frac{q}{\tau} \langle p Q_1(w) \rangle, \\ \partial_t(ne) - \operatorname{div} ((P + ne \operatorname{Id})u) - \frac{\hbar^2}{8m^*} \operatorname{div} (n \Delta u) + J_n \cdot \nabla V &= \frac{1}{\tau} \langle \frac{1}{2} |p|^2 Q_1(w) \rangle, \end{aligned}$$

where the unscaled pressure tensor and energy density read as

$$P = nk_B T \operatorname{Id} - \frac{\hbar^2}{12m^*} n (\nabla \otimes \nabla) \log n, \quad ne = \frac{3}{2} nk_B T + \frac{m^*}{2} n |u|^2 - \frac{\hbar^2}{24m^*} n \Delta \log n,$$

and the current density is given by $J_n = -qnu$.

References

- [1] R. Adler, A. Smith, and R. Longini. *Introduction to Semiconductor Physics*. John Wiley & Sons, New York, 1964.
- [2] L. Arkeryd. On the Boltzmann equation. *Arch. Rat. Mech. Anal.* 45 (1971), 1-34.
- [3] A. Arnold. The relaxation-time von Neumann-Poisson equation. In: O. Mahrenholtz and R. Mennicken (eds.), *Proceedings of ICIAM 95*, Hamburg. *Z. Angew. Math. Mech.* 76 Supp. 2 (1996), 293-296.
- [4] A. Arnold. Mathematical properties of quantum evolution equations. In: G. Allaire, A. Arnold, P. Degond, and T. Hou (eds.), *Quantum Transport – Modelling, Analysis and Asymptotics*, Lecture Notes Math. 1946, 45-110. Springer, Berlin, 2008.
- [5] D. Arnold. *Functional Analysis*. Lecture Notes, Penn State University, USA, 1997.
- [6] N. Ashcroft and N. Mermin. *Solid State Physics*. Sanners College, Philadelphia, 1976.
- [7] P. Bechouche, N. Mauser, and F. Poupaud. Semiclassical limit for the Schrödinger-Poisson equation in a crystal. *Commun. Pure Appl. Math.* 54 (2001), 851-890.
- [8] N. Ben Abdallah and P. Degond. On a hierarchy of macroscopic models for semiconductors. *J. Math. Phys.* 37 (1996), 3308-3333.
- [9] F. Bloch. Über die Quantenmechanik der Elektronen in Kristallgittern. *Z. Phys.* 52 (1928), 555-600.
- [10] L. Boltzmann. Weitere Studien über das Wärmegleichgewicht unter Gasmolekülen. *Sitzungsberichte Akad. Wiss. Wien* 66 (1872), 275-370. Translation: Further studies on the thermal equilibrium of gas molecules. In: S. Brush (ed.), *Kinetic Theory*, Vol. 2, 88-174. Pergamon Press, Oxford, 1966.
- [11] K. Brennan. *The Physics of Semiconductors*. Cambridge University Press, Cambridge, 1999.
- [12] A. Caldeira and A. Leggett. Path integral approach to quantum Brownian motion. *Physica A* 121 (1983), 587-616.
- [13] T. Carleman. Sur la théorie de l'équation intégró-différentielle de Boltzmann. *Acta Mathematica* 60 (1933), 91-146.
- [14] F. Castella, L. Erdős, F. Frommlet, and P. Markowich. Fokker-Planck equations as scaling limits of reversible quantum systems. *J. Stat. Phys.* 100 (2000), 543-601.
- [15] C. Cercignani, R. Illner, and M. Pulvirenti. *The Mathematical Theory of Dilute Gases*. Springer, New York, 1994.

- [16] C. Cohern-Tannoudji, J. Dupont-Roc, and G. Grynberg. *Processus d'interaction entre photons et atomes*. Savoirs actuels, Interditions/Editions du CNRS, 1988.
- [17] R. Dautray and J.-L. Lions. *Mathematical Analysis and Numerical Methods for Science and Technology*. Springer, Berlin, 1985.
- [18] J. Davies. *The Physics of Low-Dimensional Semiconductors*. Cambridge University Press, Cambridge, 1998.
- [19] P. Degond and C. Ringhofer. A note on quantum moment hydrodynamics and the entropy principle. *C. R. Acad. Sci. Paris, Sér. I* 335 (2002), 967-972.
- [20] P. Degond and C. Ringhofer. Quantum moment hydrodynamics and the entropy principle. *J. Stat. Phys.* 112 (2003), 587-628.
- [21] L. Diósi. On high-temperature Markovian equation for quantum Brownian motion. *Europhys. Letters* 22 (1993), 1-3.
- [22] R. DiPerna and P.-L. Lions. On the Cauchy problem for Boltzmann equations: global existence and weak stability. *Ann. Math.* 130 (1989), 321-366.
- [23] H. Federer. *Geometric Measure Theory*. Springer, New York, 1969.
- [24] I. Gasser and P. Markowich. Quantum hydrodynamics, Wigner transforms and the classical limit. *Asympt. Anal.* 14 (1997), 97-116.
- [25] I. Gasser, P. Markowich, D. Schmidt, and A. Unterreiter. Macroscopic theory of charged quantum fluids. In: *Mathematical Problems in Semiconductor Physics*, Pitman Res. Notes Math. Ser. 340, 42-75. Longman, Harlow, 1995.
- [26] F. Golse and F. Poupaud. Limite fluide des équations de Boltzmann des semiconducteurs pour une statistique de Fermi-Dirac. *Asympt. Anal.* 6 (1992), 135-160.
- [27] M. Grundmann. *The Physics of Semiconductors*. Springer, Berlin, 2006.
- [28] R. Hudson. When is the Wigner quasiprobability nonnegative? *Reports Math. Phys.* 6 (1974), 249-252.
- [29] K. Jackson and W. Schröter (eds.). *Handbook of Semiconductor Technology*, Vol. 1. Wiley-VCH, Weinheim, 2000.
- [30] A. Jüngel. A steady-state quantum Euler-Poisson system for semiconductors. *Commun. Math. Phys.* 194 (1998), 463-479.
- [31] A. Jüngel. *Transport Equations for Semiconductors*. Lecture Notes in Physics, Vol. 773. Springer, Berlin, 2009.

- [32] A. Jüngel, D. Matthes, and J.-P. Milišić. Derivation of new quantum hydrodynamic equations using entropy minimization. *SIAM J. Appl. Math.* 67 (2006), 46-68.
- [33] C. Kittel. *Introduction to Solid State Physics*. 7th edition, John Wiley & Sons, New York, 1996.
- [34] N. Kluksdahl, A. Kriman, D. Ferry, and C. Ringhofer. Self-consistent study of the resonant tunneling diode. *Phys. Rev. B* 39 (1989), 7720-7735.
- [35] P.-L. Lions and T. Paul. Sur les mesures de Wigner. *Rev. Mat. Iberoamer.* 9 (1993), 553-618.
- [36] M. Lundstrom. *Fundamentals of Carrier Transport*. 2nd edition, Cambridge University Press, Cambridge, 2000.
- [37] E. Madelung. Quantentheorie in hydrodynamischer Form. *Z. Physik* 40 (1927), 322-326.
- [38] P. Markowich, N. Mauser, and F. Poupaud. A Wigner-function approach to (semi) classical limits: electrons in a periodic potential. *J. Math. Phys.* 35 (1994), 1066-1094.
- [39] P. Markowich, C. Ringhofer, and C. Schmeiser. *Semiconductor Equations*. Springer, Vienna, 1990.
- [40] F. Poupaud. On a system of nonlinear Boltzmann equations of semiconductors physics. *SIAM J. Appl. Math.* 50 (1990), 1593-1606.
- [41] F. Poupaud. Diffusion approximation of the linear semiconductor Boltzmann equation: analysis of boundary layers. *Asympt. Anal.* 4 (1991), 293-317.
- [42] M. Reed and B. Simon. *Methods of Modern Mathematical Physics IV: Analysis of Operators*. Academic Press, New York, 1978.
- [43] C. Ringhofer. Computational methods for semiclassical and quantum transport in semiconductor devices. *Acta Numerica* (1997), 485-521.
- [44] U. Rössler. *Solid State Theory. An Introduction*. Springer, Berlin, 2004.
- [45] F. Scheck. *Theoretische Physik 2*. Springer, Berlin, 2006.
- [46] K. Seeger. *Semiconductor Physics. An Introduction*. Springer, Berlin, 2004.
- [47] M. Taylor. *Pseudodifferential Operators*. Princeton University Press, Princeton, 1981.
- [48] S. Weigert. How to determine a quantum state by measurements: the Pauli problem for a particle with arbitrary potential. *Phys. Rev. A* 53 (1996), 2078-2083.
- [49] W. Wenckebach. *Essentials of Semiconductor Physics*. John Wiley & Sons, Chichester, 1999.

- [50] W. van Roosbroeck. Theory of flow of electron and holes in germanium and other semiconductors. *Bell Syst. Techn. J.* 29 (1950), 560-607.
- [51] E. Wigner. On the quantum correction for the thermodynamic equilibrium. *Phys. Rev.* 40 (1932), 749-759.
- [52] C. Wilcox. Theory of Bloch waves. *J. d'Analyse Math.* 33 (1978), 146-167.
- [53] R. Wyatt. *Quantum Dynamics with Trajectories*. Springer, New York, 2005.
- [54] E. Zeidler. *Nonlinear Functional Analysis and Its Applications*, Vol. II. Springer, New York, 1990.