

A New Approach for the Derivation of Macroscopic Balance Equations beyond the Relaxation Time Approximation

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Abstract

A new method for the derivation of Hydrodynamic Equations has been developed. This new approach is more general than those based on the Relaxation Time Approximation (RTA) because it reproduces the equations of irreversible thermodynamics and especially ensures Onsager's Reciprocity Relations in the region of linear transport. Comparing the transport coefficients of this newly derived set of hydrodynamic equations with the conventional ones being based on the RTA yields conditions for the validity of the RTA which can be derived from stationary Monte Carlo bulk simulations.

In recent years the model of *Hydrodynamic Equations* (HDE) (see e. g. [1]) has attracted growing attention, since it appears to be a good compromise between the efficiency of the *Drift Diffusion Model* [2] and the accuracy of the Monte Carlo Model [3]. Such HDE are intended for a formulation of transport theory from a macroscopic point of view, which is much simpler than the microscopic description using *Boltzmann's transport equation* (BTE) [4]. The electrostatic potential ψ and the particle density n are the variables of Poisson's equation and the continuity equation for electrons. The information missing in both equations, but necessary for more detailed considerations in transport theory, is the knowledge of a selected set of scalar-like macroscopic expectation values $\langle X_\mu \rangle$; $\mu = 1, \dots, m$ like e. g. the components of mean drift velocity $\langle \vec{v} \rangle$, mean energy $\langle \epsilon \rangle$, or the components of the expectation value $\langle \epsilon \vec{v} \rangle$ related to energy flux density \vec{s} . This can be achieved from the solution of the BTE, that is the microscopic distribution function $h(\vec{r}, \vec{k})$, which is assumed to be normalized here [5]:

$$\langle X_\mu(\vec{r}) \rangle = \frac{2}{(2\pi)^3} \int d^3\vec{k} h(\vec{r}, \vec{k}) X_\mu(\vec{k}) \quad (1)$$

$$1 = \frac{2}{(2\pi)^3} \int d^3\vec{k} h(\vec{r}, \vec{k}) \quad (2)$$

$X_\mu(\vec{k})$ denotes the microscopic contribution of some electron state with crystal momentum $\hbar\vec{k}$. Both relations must be considered as *linear functionals* of the unknown distribution function $h(\vec{r}, \vec{k})$. The probability for finding some electron with crystal momentum $\hbar\vec{k}$ at point \vec{r} comes out to be $f(\vec{r}, \vec{k}) = n(\vec{r}) h(\vec{r}, \vec{k})$.

The structure of macroscopic balance equations for expectation values in stationary states cannot be derived from phenomenological theories like Maxwell equations. Usually these equations are derived from BTE by using the definition of expectation values according to (1) (see e. g. [1]). So far the derivation of all HDE being actually used for device modeling has been

based on the *Relaxation Time Approximation* (RTA) [6]. This approximation allows a simple model of the collision part of such macroscopic balance equations for stationary systems [7]:

$$\frac{1}{n} \nabla_{\vec{r}} \left\{ n \langle X_{\mu} \vec{v} \rangle \right\} = -e \vec{E} \cdot \left\langle \frac{1}{\hbar} \nabla_{\vec{k}} X_{\mu} \right\rangle - \tau_{X_{\mu}}^{-1} \left\{ \langle X_{\mu} \rangle - \langle X_{\mu} \rangle^{eq} \right\} \quad (3)$$

Since until now only very little is known about this approximation, recently attempts to clarify its validity have been started [8].

As will be shown in the first section of this paper, it is not necessary to inspect highly excited states for finding contradictions to the RTA. Such contradictions can be already found in the region of small external perturbations, that is in the region of *irreversible thermodynamics* [4], [9], [10] (compare figure 1). Therefore in this paper a more systematic derivation of HDE from BTE is proposed, which generalizes the approach of irreversible thermodynamics to high electric fields thus taking into account also hot electron effects. This new approach ensures that in the limit of weak electric fields the results of irreversible thermodynamics are reproduced. Besides the assumption of stationarity there are two further assumptions needed for this method which are in close agreement with those essential for the derivation of irreversible thermodynamics, and which will be discussed in sections 2 and 3. The new formulation of macroscopic balance equations will be discussed in section 4. It is not the goal of this paper to present the complete modeling of the extended version of a new set of HDE by Monte Carlo simulations. The result of this section will be a more general formulation of macroscopic balance equations and conditions for the validity of the RTA. Section 5 will focus on the discussion of some simple model, which can be handled by means of analytical techniques.

1 Failure of the Relaxation Time Approximation

The insufficiency of the RTA can be demonstrated by the theory of irreversible thermodynamics. This theory is well accepted and based on very fundamental physical principles. It considers only small local deviations from thermodynamic equilibrium ($\vec{E} = 0$), thus describing systems perturbed by weak electric fields and small spatial inhomogeneities in the region of linear transport. A consistent notation of the constitutive relations for current density \vec{i} and energy flux density \vec{s} under stationary conditions can be given with the linear expansion using *Onsager coefficients* L_{11} , L_{12} , L_{21} , and L_{22} . Most convenient for comparison with HDE is the form referring to the *electrochemical force* and *thermal force* as presented in [4]:

$$\vec{i} = L_{11} \left\{ e \nabla_{\vec{r}} \psi - T^{eq} \nabla_{\vec{r}} \left(\frac{\mu^{eq}}{T^{eq}} \right) \right\} + L_{12} \left\{ -\frac{1}{T^{eq}} \nabla_{\vec{r}} T^{eq} \right\} \quad (4)$$

$$\vec{s} = L_{21} \left\{ e \nabla_{\vec{r}} \psi - T^{eq} \nabla_{\vec{r}} \left(\frac{\mu^{eq}}{T^{eq}} \right) \right\} + L_{22} \left\{ -\frac{1}{T^{eq}} \nabla_{\vec{r}} T^{eq} \right\} \quad (5)$$

T^{eq} and μ^{eq} denote the temperature and chemical potential in thermal equilibrium. According to *Onsager's Reciprocity Relations* ($L_{12} = L_{21}$) the complete set of Onsager coefficients can be reduced to 3 independent ones which are in one-to-one correspondence with 3 independent phenomenological material parameters like e. g. electric and thermal conductivity and the thermoelectric power of the Seebeck effect, respectively [9]. But still the system's response to both thermodynamic forces must be modeled by different transport coefficients in every constitutive relation. This contradicts results based on the RTA. A detailed comparison for the

flux densities \vec{i} and \vec{s} as used in HDE [7], [11] shows that the Onsager coefficients must be identified with the following expressions:

$$\begin{pmatrix} L_{11} & L_{12} \\ L_{21} & L_{22} \end{pmatrix} = \frac{1}{m^*} \begin{pmatrix} \tau_i & \frac{5}{2} K_B T^{eq} \tau_i \\ \frac{5}{2} K_B T^{eq} \tau_s & \frac{35}{4} (K_B T^{eq})^2 \tau_s \end{pmatrix} \quad (6)$$

$\frac{1}{m^*}$ denotes the expectation value of the inverse effective mass tensor in the state of thermodynamic equilibrium. Usually both relaxation times τ_i and τ_s are determined independently from the field part of the corresponding balance equation under homogeneous conditions [7]. It is thus guaranteed that the system's response resulting from the electrochemical force is well modeled. But according to significant deviations of both relaxation times τ_i and τ_s in lowly doped silicon the RTA leads to a false modeling of the response to thermal forces and to a huge difference in L_{12} and L_{21} which contradicts Onsager's Reciprocity Relation $L_{12} = L_{21}$.

Figure 1 shows a schematic representation of Monte Carlo simulation results in silicon under homogeneous conditions at 300K lattice temperature. The region of linear transport was determined from the field dependency of the mobility in the Monte Carlo simulator. The region of RTA can be either obtained from simulation results of Onsager coefficients [11] or from the relation between both relaxation times τ_i and τ_s [7]. According to the results presented here the RTA is valid for the special case of highly doped semiconductors in the regime of rather weak electric field. In the case of MOSFET devices this situation occurs only in the region of *source-* and *drain contacts*. The channel region, which is of special interest in the simulation of sub- μ devices, is characterized by lower doping concentration and high electric fields, thus not complying the requirements of the RTA. This aspect should be taken into consideration, if deviations between results from Monte Carlo simulations and HDE based on the RTA are discussed.

2 Assumption of Local Transport Behavior

The first assumption needed for the more general approach is that of *local transport behavior*. Therefore all considerations will be restricted to systems including high field transport, but showing only weak spatial variations of macroscopic densities. This is the most general type of systems, for which it can be expected that their phenomenological properties and transport coefficients can be determined from Monte Carlo bulk simulations under stationary conditions. A simplified picture of this situation can be given by a 3-dimensional configuration space, which is spanned by 3 independent macroscopic densities, e. g. $\vec{i} \cdot \vec{E}$, T_e , and $\vec{s} \cdot \vec{E}$. $\vec{E} = -\nabla_{\vec{r}} \psi$ denotes the electric field and T_e the temperature of the electronic system. In general, however, a configuration space of higher dimension must be considered, built up from m different quantities. Figure 1 shows – as a 1-dimensional manifold – that subspace of states, which can be observed in stationary bulk systems with fixed doping concentration and lattice temperature under homogeneous electric field conditions. All typical states in inhomogeneous systems must be outside this manifold of homogeneous states. However states of systems with weak spatial inhomogeneities can be assumed to be close to this manifold. Hence for the latter cases the distribution functions can be derived from those of corresponding homogeneous bulk systems by some perturbation expansion taking into account the drift part of the BTE in lowest order.

For this purpose the usual derivation of HDE from the differential form of the BTE [4] is replaced by a new one based on the integral form similar to that proposed in [12]. If $h_{\vec{E}}^{hom}(\vec{k})$ denotes the stationary distribution function of a homogeneous bulk system with any electric

field strength \vec{E} , the stationary distribution function $h(\vec{r}, \vec{k})$ inside inhomogeneous systems can be approximately described as follows (integral form of the BTE):

$$n(\vec{r}) \left\{ h(\vec{r}, \vec{k}) - h_{\vec{E}(\vec{r})}^{hom}(\vec{k}) \right\} = - \int_0^{\infty} dt \frac{\Omega}{(2\pi)^3} \int d^3 \vec{k}_0 \Pi_{\vec{E}(\vec{r})}^{hom}(\vec{k}, \vec{k}_0; t) \vec{v}(\vec{k}_0) \cdot \nabla_{\vec{r}} \left[n(\vec{r}) h(\vec{r}, \vec{k}_0) \right] \quad (7)$$

$\frac{\Omega}{(2\pi)^3}$ denotes the density of states for Bloch wave functions within \vec{k} -space. The propagator $\Pi_{\vec{E}}^{hom}(\vec{k}, \vec{k}_0; t)$ is the probability that a particle in homogeneous systems with electric field \vec{E} is starting in some state with crystal momentum $\hbar \vec{k}_0$ and will reach some other state with crystal momentum $\hbar \vec{k}$ at time t later.

The new approach to HDE thus delivers a prescription how to account for the deviation $n(\vec{r}) \left\{ h(\vec{r}, \vec{k}) - h_{\vec{E}(\vec{r})}^{hom}(\vec{k}) \right\}$ by the evaluation of time integrals taking into account the dynamic response of the system. This response is induced by the perturbation of spatial inhomogeneities in the electron gas and vanishes for the case of homogeneous bulk systems. According to the approximation of local transport behavior the system's response is determined only from that small volume $\Delta V(\vec{r})$, where the desired distribution function $h(\vec{r}, \vec{k})$ is observed. Eq. (7) does not contain the deviations in response behavior resulting from surrounding volume elements with different physical specifications. Although this simplification is not valid in general the new approach is believed to be more accurate than the RTA.

3 Assumption of Minimum Information

This assumption necessary for our approach is primarily guided by the final goal of deriving a model of HDE itself. HDE can only deliver information for final sets of specified expectation values. Further quantities remain unknown. Therefore only distribution functions will be considered, which reproduce the particle density n together with m different scalar-like expectation values $\langle \Xi_{\nu} \rangle$; $\nu = 1, \dots, m$ similar to the set of $\langle X_{\mu} \rangle$ and additionally ensure minimum information I . The resulting method (well known as *maximum entropy method* [13]) is locally applied to small volumes $\Delta V(\vec{r})$ and does not account for nonlocal effects which is in agreement with the basic assumption of local transport behavior in this paper. The resulting distribution functions are known as generalized canonical distributions (GCD) [14].

The foundation of the mathematical framework for the solution of this problem is given by the relation between the local information I in volume $\Delta V(\vec{r})$ and the distribution function $h(\vec{r}, \vec{k})$. Contrary to the definition of expectation values the information I is defined as a *nonlinear functional*, being more sensitive to the analytical model of the distribution function:

$$I(\vec{r}) = \frac{2}{(2\pi)^3} \int d^3 \vec{k} h(\vec{r}, \vec{k}) \ln h(\vec{r}, \vec{k}) \quad (8)$$

Using the well-known variational method of Lagrange multipliers it is possible to find that distribution function $h(\vec{r}, \vec{k})$ which fulfills (1) and (2) and comprises minimum information I . The result can be denoted by a set of m space-dependent variational parameters α_{ν} ; $\nu = 1, \dots, m$ as follows:

$$h(\vec{r}, \vec{k}) = C(\vec{r}) \exp \left\{ - \sum_{\nu=1}^m \alpha_{\nu}(\vec{r}) \Xi_{\nu}(\vec{k}) \right\} \quad (9)$$

The normalization constant $C(\vec{r}) = C[\alpha_1(\vec{r}), \dots, \alpha_m(\vec{r})]$ is fixed according to (2). The GCD thus offers m different and independent parameters for best estimation of the inhomogeneous distribution function $h(\vec{r}, \vec{k})$. Therefore all expectation values can be formulated as ordinary functions of these variational parameters, that is $\langle Y(\vec{r}) \rangle = F_Y[\alpha_1(\vec{r}), \dots, \alpha_m(\vec{r})]$. The total change in real space of some expectation value $\langle Y(\vec{r}) \rangle$ can be determined from the change of all parameters α_ν using the static fluctuation-dissipation theorem [14]:

$$\nabla_{\vec{r}} \langle Y \rangle = \sum_{\nu=1}^m \frac{\partial \langle Y \rangle}{\partial \alpha_\nu} \nabla_{\vec{r}} \alpha_\nu = - \sum_{\nu=1}^m \langle \Delta \Xi_\nu \Delta Y \rangle \nabla_{\vec{r}} \alpha_\nu \quad (10)$$

The fluctuations $\langle \Delta \Xi_\nu \Delta Y \rangle$ describe the cross-correlation of the microscopic quantities $Y(\vec{k})$ and $\Xi_\nu(\vec{k})$ on the average. It is the physical meaning of the static fluctuation-dissipation theorem that these fluctuations show how sensitive the expectation value $\langle Y \rangle$ is with respect to changes of the α_ν . Eq. (10) is one of the key-features of the GCD for deriving conditions for the validity of the RTA in section 4.

4 Macroscopic Balance Equations

The derivation of macroscopic balance equations can be achieved from the deviation of expectation values $\langle X_\mu \rangle - \langle X_\mu \rangle_{\vec{E}}^{hom}$, which can be determined directly from (1) by inserting (7) for the distribution functions. The expectation value $\langle X \rangle_{\vec{E}}^{hom}$ refers to homogeneous systems with electric field \vec{E} and must be calculated from the distribution function $h_{\vec{E}}^{hom}(\vec{k})$ of appropriate homogeneous systems. The unknown derivative of the distribution function on the right hand side of (7) is approximately determined from the analytical formulation of the GCD in (9). The result for the balance equation can be denoted as a linear expansion using a complete set of thermodynamic forces in inhomogeneous systems:

$$\langle X_\mu \rangle - \langle X_\mu \rangle_{\vec{E}}^{hom} = -\vec{\gamma}_{\mu,o} \cdot \nabla_{\vec{r}} \ln n + \sum_{\nu=1}^m \vec{\gamma}_{\mu,\nu} \cdot \nabla_{\vec{r}} \alpha_\nu \quad (11)$$

$\nabla_{\vec{r}} \ln n$ denotes the thermodynamic force of the diffusion effect and all other forces are called conjugate to the expectation values $\langle \Xi_\nu \rangle$ mentioned above. The transport coefficients $\vec{\gamma}_{\mu,o}$ and $\vec{\gamma}_{\mu,\nu}$; $\nu = 1, \dots, m$ are space-dependent and can be determined from time integrals of microscopic correlation functions which are extracted from stationary Monte Carlo bulk simulations. The definition of correlation functions is already known from literature [15] and is related to the propagator $\Pi_{\vec{E}}^{hom}(\vec{k}, \vec{k}_0; t)$ of homogeneous systems in the following way:

$$\vec{g}_{\mu,\nu}(t) = \frac{2\Omega}{(2\pi)^6} \int d^3\vec{k} d^3\vec{k}_0 \Delta X_\nu(\vec{k}) \Pi_{\vec{E}}^{hom}(\vec{k}, \vec{k}_0; t) \Delta \left\{ \Xi_\nu(\vec{k}_0) \vec{v}(\vec{k}_0) \right\} h(\vec{r}, \vec{k}_0) \quad (12)$$

The correlation function $\vec{g}_{\mu,o}(t)$ corresponding to the transport coefficient $\vec{\gamma}_{\mu,o}$ can be deduced from this definition, if the set of microscopic quantities for the specification of the GCD is completed by the additional quantity $\Xi_o(\vec{k}) = 1$ and (12) is applied for the set $\nu = 0, 1, \dots, m$.

The balance equation (11) can be formulated much closer to that of the RTA in (3), if the expectation value $\langle X_\mu \rangle_{\vec{E}}^{hom}$ is related to that in thermodynamic equilibrium $\langle X_\mu \rangle^{eq}$. This can be achieved by the balance equation in homogeneous systems, which contains in addition the related field part:

$$\langle X_\mu \rangle_{\vec{E}}^{hom} - \langle X_\mu \rangle^{eq} = -\tau_{X_\mu} e \vec{E} \cdot \left\langle \frac{1}{\hbar} \nabla_{\vec{k}} X_\mu \right\rangle_{\vec{E}}^{hom} \quad (13)$$

τ_{X_μ} denotes that *phenomenological* relaxation time, which reproduces the field dependence of $\langle X_\mu \rangle_{\vec{E}}^{hom}$ together with that of $\langle \frac{1}{\hbar} \nabla_{\vec{k}} X_\mu \rangle_{\vec{E}}^{hom}$ and was already used in [7]. If in addition the expectation value $\langle \frac{1}{\hbar} \nabla_{\vec{k}} X_\mu \rangle_{\vec{E}}^{hom}$ is related to that in inhomogeneous systems $\langle \frac{1}{\hbar} \nabla_{\vec{k}} X_\mu \rangle$ by again applying the new approach for microscopic quantities $\frac{1}{\hbar} \nabla_{\vec{k}} X_\mu(\vec{k})$; $\mu = 1, \dots, m$, the resulting macroscopic balance equation is:

$$\langle X_\mu \rangle - \langle X_\mu \rangle^{eq} = -\tau_{X_\mu} e \vec{E} \cdot \langle \frac{1}{\hbar} \nabla_{\vec{k}} X_\mu \rangle - \vec{\Gamma}_{\mu,o} \cdot \nabla_{\vec{r}} \ln n + \sum_{\nu=1}^m \vec{\Gamma}_{\mu,\nu} \cdot \nabla_{\vec{r}} \alpha_\nu \quad (14)$$

All correlation functions necessary for the specification of this equation are modified by the additional contribution of the field part and are called *reduced* correlation functions here:

$$\begin{aligned} \vec{G}_{\mu,\nu}(t) &= \vec{g}_{\mu,\nu}(t) + \\ &+ \tau_{X_\mu} e \vec{E} \cdot \frac{2\Omega}{(2\pi)^6} \int d^3 \vec{k} d^3 \vec{k}_0 \Delta \left\{ \frac{1}{\hbar} \nabla_{\vec{k}} X_\mu(\vec{k}) \right\} \Pi_E^{hom}(\vec{k}, \vec{k}_0; t) \Delta \left\{ \Xi_\nu(\vec{k}_0) \vec{v}(\vec{k}_0) \right\} h(\vec{r}, \vec{k}_0) \end{aligned} \quad (15)$$

(ν is again completed to the set $\nu = 0, 1, \dots, m$.) They are used for the definition of *microscopic* relaxation times $\tau_{\mu,\nu}$ by integrating over time:

$$\int_0^\infty dt \vec{G}_{\mu,\nu}(t) = \tau_{\mu,\nu} \langle \Delta X_\mu \Delta \{ \Xi_\nu \vec{v} \} \rangle \quad (16)$$

In general the relaxation times $\tau_{\mu,\nu}$ must be regarded as 3-dimensional matrix-like quantities. This set of quantities contains very fundamental information on the dynamical properties of electron gases. The most simple case is given by reduced correlation functions $\vec{G}_{\mu,\nu}(t)$, which show an exponential decay in time with values starting from the cross-correlation $\langle \Delta X_\mu \Delta \{ \Xi_\nu \vec{v} \} \rangle$. $\tau_{\mu,\nu}$ thus denotes the *inverse decay constant* of the relaxation process in time, which appears for correlations between quantities $X_\mu(\vec{k})$ and $\Xi_\nu(\vec{k}) \vec{v}(\vec{k})$. Therefore the term “relaxation time” is much more appropriate for these quantities than for the phenomenological parameters τ_{X_μ} . All transport coefficients $\vec{\Gamma}_{\mu,o}$ and $\vec{\Gamma}_{\mu,\nu}$ can be obtained from the knowledge of these relaxation times:

$$\vec{\Gamma}_{\mu,o} = \tau_{\mu,o} \langle X_\mu \vec{v} \rangle \quad (17)$$

$$\vec{\Gamma}_{\mu,\nu} = \tau_{\mu,o} \langle \Delta \Xi_\nu \Delta \{ X_\mu \vec{v} \} \rangle + \{ \tau_{\mu,\nu} - \tau_{\mu,o} \} \langle \Delta X_\mu \Delta \{ \Xi_\nu \vec{v} \} \rangle \quad (18)$$

This method for the evaluation of transport coefficients is already known in a simpler form from the theory of irreversible thermodynamics (Compare *Kubo formula* based on correlation functions $\vec{g}_{\mu,o}(t)$, [16]), but was to the best knowledge of the authors not fully extended to the region of nonlinear transport so far. Up to now the only application beyond the region of linear transport was restricted to the determination of diffusion coefficients from velocity autocorrelation functions, which are described by $\vec{g}_{\mu,o}(t)$ for the special case of $X_\mu(\vec{k}) = v_i(\vec{k})$; $i = 1, 2, 3$. But with this approach every coefficient can be extracted independently in the region of nonlinear transport, thus delivering the complete knowledge of all phenomenological transport coefficients in HDE. One further crucial point, which has to be mentioned, is the fact, that the coefficients $\vec{\Gamma}_{\mu,o}$ and $\vec{\Gamma}_{\mu,\nu}$ are not determined from the correlation functions defined in (12), but from the reduced ones defined in (15). The analytical example of the Ornstein-Uhlenbeck process discussed in the following section clearly shows, that this distinction becomes necessary, if contradictions in the formulation of macroscopic balance equations ought to be avoided.

Using the mathematical framework of the GCD it is now possible to extract conditions for the validity of the RTA: We consider that special type of system, which leads to identical results for all microscopic relaxation times, that is $\tau_{\mu,o} = \tau_{\mu,\nu}$; $\mu, \nu = 1, \dots, m$. By use of (10) all parts containing thermodynamic forces $\nabla_{\vec{r}} \ln n$ and $\nabla_{\vec{r}} \alpha_\nu$ can be summed up to $\frac{1}{n} \nabla_{\vec{r}} \{n \langle X_\mu \vec{v} \rangle\}$, which is already known from (3). A complete identity with (3) is achieved, if in addition $\tau_{\mu,o}$ is identical to the phenomenological relaxation time τ_{X_μ} . The mathematical theorem proved in this section can thus be summarized as follows:

The validity of the Relaxation time approximation defined in (3) follows from the identity of all relaxation times $\tau_{X_\mu} = \tau_{\mu,o} = \tau_{\mu,1} = \dots = \tau_{\mu,m}$.

This condition is very restrictive and cannot be expected to be valid in the region of high electric fields. One way to improve the modeling of HDE therefore is to accept (14) as the basic relation and to derive the set of correlation functions from stationary Monte Carlo bulk simulations. Since (10) cannot be applied in pure form, a more sophisticated technique for analyzing correlation functions like that published in [15] becomes necessary. Following this approach both gradients $\nabla_{\vec{r}} n$ and $\nabla_{\vec{r}} \langle X_\mu \vec{v} \rangle$ in (3) are supplemented by a more general set $\nabla_{\vec{r}} \langle X_\nu \vec{v} \rangle$; $\nu \neq \mu$, describing transport properties in a more detailed manner.

5 Example: The Ornstein-Uhlenbeck Process

The *Ornstein-Uhlenbeck process* is a simple stochastic model for problems concerning *Brownian motion* of macroscopic particles with constant effective mass m in liquids. If this particle is assumed to carry the charge and effective mass of electrons, this process can be regarded as a very simple model of charge transport in semiconductors. The definition is given by the so-called *quasilinear Fokker-Planck equation*, which is similar to the BTE, but shows a much simpler modeling of the collision part:

$$\left\{ \frac{\partial}{\partial t} - \frac{e}{\hbar} \vec{E} \cdot \nabla_{\vec{k}} + \vec{v} \cdot \nabla_{\vec{r}} \right\} f(\vec{r}, \vec{k}, t) = \eta \left\{ \nabla_{\vec{k}} \cdot \vec{k} + \frac{m K_B T^{eq}}{\hbar^2} \Delta_{\vec{k}} \right\} f(\vec{r}, \vec{k}, t) \quad (19)$$

η is called the *friction constant* and turns out to be the basic constant for the description of transport properties. K_B denotes the Boltzmann constant and T^{eq} the temperature of the bath surrounding the particle under consideration. Related equations of motion for some macroscopic expectation values $\langle X_\mu \rangle$ can be simply obtained from the well-known procedure of multiplying (19) by the microscopic contribution $X(\vec{k})$ and integrating $\frac{2}{(2\pi)^3} \int d^3 \vec{k}$. The result for the collision part turns out to be identical with the RTA as defined in (3), if the balance equations of group velocity $\vec{v}(\vec{k})$ or band energy $\epsilon(\vec{k})$ are considered. The related relaxation times can be identified as *momentum relaxation time* $\tau_i = \frac{1}{\eta}$ and *energy relaxation time* $\tau_w = \frac{1}{2\eta}$.

In the following it will be demonstrated that the same result can be attained from our new approach based on (14). The matrix-like reduced correlation function $G_{\vec{v}, \Xi_\nu \vec{v}}(t)$ and the vector-like function $\vec{G}_{\epsilon, \Xi_\nu \vec{v}}(t)$ can be determined by use of analytical techniques from (19):

$$G_{\vec{v}, \Xi_\nu \vec{v}}(t) = \langle \Delta \vec{v} \Delta \{ \Xi_\nu \vec{v} \} \rangle e^{-\eta t} \quad (20)$$

$$\vec{G}_{\epsilon, \Xi_\nu \vec{v}}(t) = \langle \Delta \epsilon \Delta \{ \Xi_\nu \vec{v} \} \rangle e^{-2\eta t} + \frac{e \vec{E}}{\eta} \cdot \langle \Delta \vec{v} \Delta \{ \Xi_\nu \vec{v} \} \rangle e^{-\eta t} \{ 2e^{-\eta t} - 1 \} \quad (21)$$

The additional part in (21) leads to deviations from the simple model of exponential decay and results from the acceleration of particles in the electric field. It turns out, that both

relaxation times $\tau_{\vec{v}, \Xi, \nu} = \frac{1}{\eta}$ and $\tau_{\epsilon, \Xi, \nu} = \frac{1}{2\eta}$ are independent of the quantity $\Xi_\nu(\vec{k})\vec{v}(\vec{k})$ and thus fulfill the condition for the RTA proved in section 4. Furthermore they are identical to the phenomenological parameters τ_i and τ_w thus reproducing the result of valid RTA mentioned above. This result cannot be obtained, if the correlation functions $g_{\vec{v}, \Xi, \nu}(t)$ and $\tilde{g}_{\epsilon, \Xi, \nu}(t)$ are used instead of the reduced ones. Finally it should be mentioned, that the successful application of (14) is not only restricted to the more simple case of velocity and energy balance equation. More laborious calculations show, that the identity of the new approach based on the integral form of the BTE and the traditional one based on the differential form of the BTE can be proved for the balance equation of every expectation value.

6 Summary

A new approach for the derivation of hydrodynamic equations was presented, which is more general than those based on the relaxation time approximation. This approach reproduces the equations of irreversible thermodynamics in the region of weak electric fields and ensures Onsager's Reciprocity relations. The improvement was achieved by use of an integral form of Boltzmann's transport equation, which delivers a linear expansion of macroscopic balance equations based on general thermodynamic forces with transport coefficients $\vec{\Gamma}_{\mu, \nu}$ and $\vec{\Gamma}_{\mu, \nu}$; $\mu, \nu = 1, \dots, n$. These coefficients can be derived from stationary Monte Carlo bulk simulations by evaluation of a newly defined set of reduced correlation functions $\vec{G}_{\mu, \nu}$ and $\vec{G}_{\mu, \nu}$. The approximations necessary for this derivation are those of local transport behavior and of minimum information about the distribution function. No restrictive assumption must be made for the strength of the electric field, thus enhancing reliability for modeling hot electron effects. With respect to the conventional derivation of hydrodynamic equations conditions for the validity of the relaxation time approximation could be derived. These conditions can be examined with Monte Carlo bulk simulations by the evaluation of microscopic relaxation times $\tau_{\mu, \nu}$ from time integrals of the reduced correlation functions mentioned above. It was shown by means of analytical techniques, that these conditions are valid for the special case of momentum and energy balance equation of the Ornstein-Uhlenbeck process.

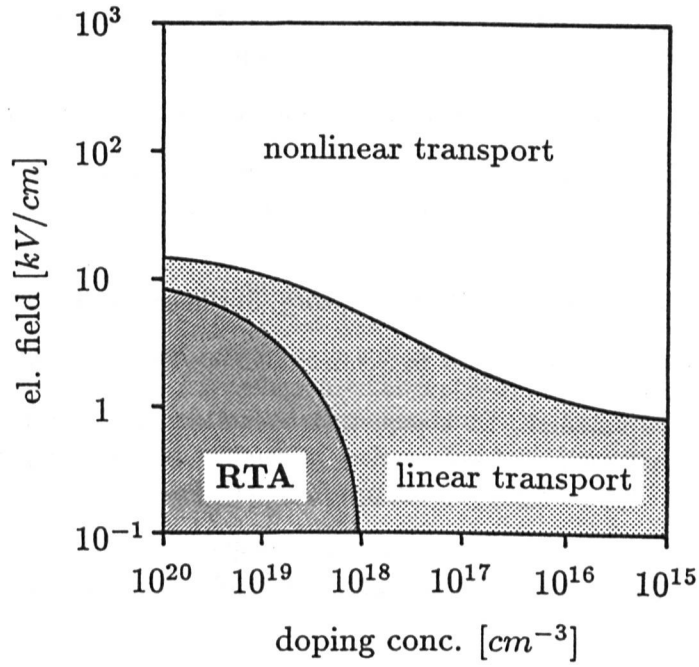


Figure 1: Schematic representation of Monte Carlo simulation results in silicon under homogeneous conditions at 300K lattice temperature.

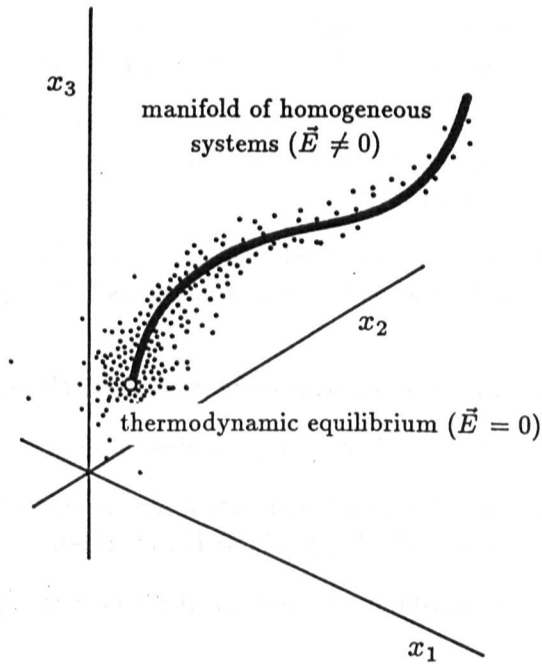


Figure 2: Simplified representation of the homogeneous situation as a 1-dimensional manifold in a 3-dimensional configuration space. All dots refer to local states in inhomogeneous systems.

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