

Extraction of Parameters for Balance Equations from Monte-Carlo Simulations

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Abstract

The Boltzmann transport equation (BTE) can be transformed in an equivalent balance equation system for an infinite number of moments. If this system is truncated, an approximate balance equation system is obtained. The equations consist of moments, space and time derivatives of the moments, and coefficients being functions of the moments. We show that the coefficients for a three-moment (hydrodynamic) model can easily be extracted from exact solutions of the BTE for homogeneous material. No approximations have to be made concerning the energy-momentum-relation or the shape of the distribution function. In principle, the method can be extended to higher order equations.

1. The Equivalent Moment Equations

The dynamics of the electron distribution function is described by the *Boltzmann-transport-equation* [1]:

$$\frac{\partial}{\partial t} f(\vec{x}, \vec{k}, t) = -\vec{u} \frac{\partial}{\partial \vec{x}} f - \dot{\vec{k}} \frac{\partial}{\partial \vec{k}} f - \hat{Q}[f]. \quad (1)$$

The electron distribution function may be expanded in any set of functions of the electron wave number \vec{k} which is complete. Elements of such a series are designated with $\hat{m}_\alpha(\vec{k})$. Insertion of this expansion in the BTE, multiplication with the functions \hat{m}_α and integration over the k -space yields an equation system for the coefficients of this series. In the following, we first consider electron transport in one-dimensional varying fields. The extension to more than one dimension will be discussed later. The series for the distribution function may be written in the form [2]

$$\frac{\partial}{\partial t} n \langle \hat{m}_\alpha \rangle = n \cdot \dot{\vec{k}} \langle \frac{\partial}{\partial \vec{k}} \hat{m}_\alpha \rangle - \frac{\partial}{\partial x} n \langle u \cdot \hat{m}_\alpha \rangle - n \cdot S^{(\alpha)} \quad (2)$$

with :

$$S^{(\alpha)} = \int d^3k \hat{m}_\alpha \cdot \hat{Q}(k), \quad \langle \hat{m}_\alpha \rangle = \frac{\int d^3k \hat{m}_\alpha \cdot f}{\int d^3k f} = \frac{1}{n} \int d^3k \hat{m}_\alpha \cdot f. \quad (3)$$

The functions $n \cdot \langle \hat{m}_\alpha \rangle$ are designated as *moments* of the distribution function. We can take the series (2) not to be an equation system for the coefficients of the

series expansion but for the moments themselves. If this series is truncated, a finite number of equations describes electron transport. The equations can be solved, if all terms in (2) are known as functions of the moments.

The moments have to be chosen so that the physical behaviour of the system is described with as few parameters as possible. A natural choice for the moments of zeroth, first and second order are n , $n \cdot v$ and $n \cdot w$. Here, n is the electron density, $v = \langle u \rangle$ the mean electron velocity and $w = \langle \epsilon \rangle$ the mean electron energy. Equation sets of this kind are called *hydrodynamic* models.

2. Introducing Physical Parameters

In equation (2), the physical significance of the coefficients is not obvious, and we now introduce expressions relating the coefficients to relaxation times, mobilities, and electron temperature. Relaxation times are defined by

$$\tau^{(\alpha)} = \frac{\langle \hat{m}_\alpha \rangle - \langle \hat{m}_\alpha \rangle_0}{S^{(\alpha)}}.$$

Note that these relaxation times may depend on any other moments. With

$$\delta \hat{m}_\alpha = \hat{m}_\alpha - \langle \hat{m}_\alpha \rangle \quad (4)$$

we define

$$\hat{C}^{(\alpha)} = \langle \delta u \cdot \delta \hat{m}_\alpha \rangle \quad \text{and} \quad \hat{D}^{(\alpha)} = \tau^{(\alpha)} \cdot \hat{C}^{(\alpha)}. \quad (5)$$

Then (2) can be rewritten in the form

$$\langle \hat{m}_\alpha \rangle = \hat{\mu}^{(\alpha)} \cdot \dot{k}_{\gamma'} + \hat{D}^{(\alpha)} \frac{\partial}{\partial x} n + \langle \hat{m}_\alpha \rangle_0. \quad (6)$$

Here, $\hat{\mu}^{(\alpha)}$ is the generalized mobility

$$\hat{\mu}^{(\alpha)} = \tau^{(\alpha)} \cdot \left[\langle \frac{\partial}{\partial k} \hat{m}_\alpha \rangle - \langle u \rangle \frac{\partial}{\partial x} \langle \hat{m}_\alpha \rangle + \frac{\partial}{\partial x} \hat{C}^{(\alpha)} + \frac{\partial}{\partial t} \langle \hat{m}_\alpha \rangle \right] \quad (7)$$

as well as $\hat{D}^{(\alpha)}$ is the generalized diffusivity. The coefficients $\hat{C}^{(\alpha)}$ are related to the electron temperature which is given by

$$k_B T = \langle \delta u \cdot m^*(\epsilon) \cdot \delta u \rangle. \quad (8)$$

For example, $\hat{C}^{(1)}$ can be rewritten as

$$\hat{C}^{(1)} = \frac{k_B}{\langle m^*(\epsilon) \rangle} [T + \delta T^{(1)}] \quad (9)$$

with :

$$k_B \delta T^{(1)} = 2 \cdot \langle u \rangle \langle m^*(\epsilon) \cdot \delta u \rangle - \langle u \cdot \delta m^*(\epsilon) \cdot u \rangle. \quad (10)$$

If $m^*(\epsilon) = \text{const.}$ one obtains $\delta T^{(1)} \Rightarrow 0$. Hence $\delta T^{(1)}$ is a correction term taking into account nonparabolicity. Similarly, $\hat{C}^{(2)}$ is given by

$$\hat{C}^{(2)} = \langle u \rangle \cdot k_B [T + \delta T^{(2)}] \quad (11)$$

with :

$$k_B \delta T^{(2)} = \frac{1}{2} \langle u \rangle \cdot \left(\langle \delta u \cdot m^*(\epsilon) \rangle + \frac{\langle \delta u \cdot m^*(\epsilon) \cdot \delta u^2 \rangle}{\langle u \rangle^2} \right). \quad (12)$$

The correction $\delta T^{(2)}$ disappears if the distribution function is symmetric with respect to $\langle u \rangle$. If this symmetry is not given, a contribution of $\delta T^{(2)}$ to heat conduction results [3].

To obtain a conventional hydrodynamic model, several of the following approximations usually are made (e. g. [4], [5]):

- The electrons have a constant effective mass
- The distribution function is symmetric with respect to $\langle u \rangle$
- The relaxation times depend only on the mean electron energy and are always given by their stationary values

3. Extraction of the Coefficients from Monte-Carlo Simulations

Usually, the coefficients in (2) are determined using some approximations yielding the v - and w -dependence. However, in principle these coefficients can be determined exactly by performing appropriate simulations. Here we simulate the reaction of an electron ensemble to square pulses of the electric field strength and store the coefficients occurring in (2) as functions of v and w . Fig. 1 shows that no ambiguities arise since the curves $w(v)$ belonging to different values of the height of the pulse do not intersect. Furthermore, any relevant combination of v and w occurs, thus yielding coefficients for any combination of v and w occurring during a simulation. The coefficients do not depend on n as far as electron-electron-interaction and Pauli-exclusion-principle are not taken into account.

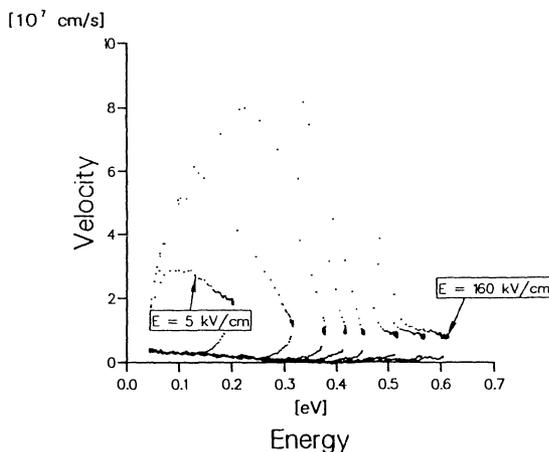


Figure 1: Mean electron velocity as a function of mean electron energy.

Fig. 2 shows the energy relaxation as function of electron energy and electron velocity $S^{(2)}(v, w)$. Usually, this function is taken to be a function of energy only $S^{(2)}(w_{stat})$. Hence a systematic error occurs if strongly nonstationary processes are simulated. The values tabulated in simulations of the one-dimensional case can also be used to perform two- or three-dimensional calculations. In these cases, one has to assume that the distribution function as a function of $|v|$ and w has the same shape as in the one-dimensional case. If heat conduction caused by gradients of the temperature is to be taken into account, higher order equations have to be studied. In principle, parameters can be calculated in a similar manner as described above.

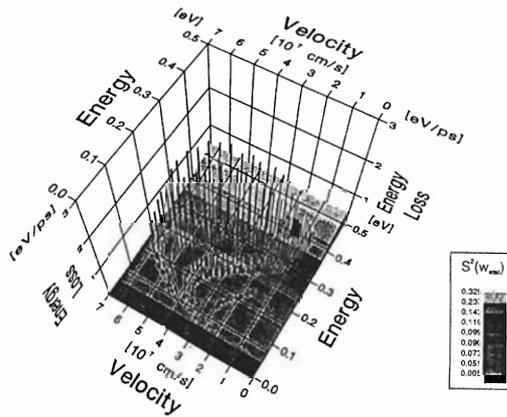


Figure 2: Mean electron energy loss $S^{(2)}(v, w)$ versus $S^{(2)}(w_{stat})$

4. Conclusions

We have developed a method for determining the coefficients in balance equations by appropriate Monte-Carlo simulations. Band structure effects can easily be taken into account. We arrived at an improved hydrodynamic transport model which yields in specific cases the exact nonstationary Monte-Carlo results.

References

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