

Thermodynamic derivation of the hydrodynamical model for charge transport in semiconductors

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(Received 6 November 1991; revised manuscript received 14 May 1992)

A thermodynamic derivation is given of the hydrodynamical model describing charge-carrier transport in semiconductors. The set of moment equations is closed by utilizing the principles of extended thermodynamics. The method of Maxwellian iteration yields, then, hydrodynamical-like equations with constitutive equations for the heat flux and anisotropic stresses.

I. INTRODUCTION

Lately, hydrodynamical models have been used in simulating charge-carrier transport in semiconductors particularly with regard to hot electrons and submicron devices.¹⁻⁹ The aim of these models is to incorporate higher-order effects than those included in the standard drift-diffusion equations, in order to be able to describe high-field transport in semiconductors.¹⁰

These models comprise the fundamental laws of balance of particle number, momentum, and energy for the charge carriers and are derived from the moment equations of the Boltzmann transport equation (BTE) by suitable approximations. In particular the right-hand sides of these equations, which represent the production of particles, momentum, and energy due to various interaction mechanisms (carrier-phonon, carrier-carrier, and carrier-impurity collisions) are modeled by relaxation-type terms (the distribution function is assumed to relax to an appropriate equilibrium distribution function). Moreover, anisotropic stress is ignored and a Fourier-like constitutive law is assumed for the heat flux vector.

The basic model, in which the various steps and approximations are derived and discussed in detail, is due to Blotekjaer.^{11,12} In Blotekjaer's model one considers the moment equations corresponding to particle number, momentum, stress tensor, and heat flow tensor (third-order off-center moment). In the latter equation the fourth-order moment appears. In order to close this set of balance equations Blotekjaer¹¹ assumes that the fourth-order moment has the value appropriate for a displaced Maxwellian. Furthermore, the source terms appearing on the right-hand sides of the aforementioned balance equations are calculated assuming a phenomenological relaxation-time approximation for the collision operator appearing in the Boltzmann transport equation (BTE) (i.e., writing it as a sum of relaxation-type terms according to each kind of interaction process).

A slightly different model has been proposed by Hänsch and Miura-Mattausch.¹ In their model the distribution function is expanded in Legendre polynomials and only the first two terms in the expansion are retained. Only the balance equations for particle number, momentum, and energy are considered and the closure is achieved by utilizing the Wiedemann-Franz law for the heat flux. Moreover, through the expansion of the distri-

bution function the collision term is expressed as a function of the moments.

Both the Blotekjaer and the Hänsch and Miura-Mattausch models are then further simplified in order to provide a manageable set of equations, suitable for device simulation. However, for more accurate results, the full models must be retained.

Akin to the approaches of Blotekjaer and of Hänsch and Miura-Mattausch are those recently proposed by Woolard *et al.*⁷ and by Thoma *et al.*,⁸ who, however, take into account the nonparabolicity of the band structure.

All these approaches have in common the assumption at the basis of the closure approximation, i.e., that some higher-order moment can be calculated by utilizing a displaced Maxwellian. Such an approximation is rather rough and imprecise and its range of validity needs to be assessed.¹⁰ More precisely, although it might be reasonable to expect the distribution function to be close to a drifted Maxwellian under strong electric fields, it is by no means clear what the magnitude of the error is when estimating some higher-order moment by utilizing such a distribution function. An assessment of the error could be obtained if one had a systematic (albeit formal) approximation procedure for solving the BTE for semiconductors, asymptotic with respect to some parameter, the leading term of which would be a drifted Maxwellian. Presently such a general approach does not seem to be available, probably due to the complexities of the collision terms. In fact only recently the collision operator for electron-phonon scattering has been investigated in detail, its collisional invariants classified and an "*H*-theorem" proved.¹³ The knowledge of the properties of the collision operator is essential in order to extend to the BTE for semiconductors the classical approximation methods used in rarefied gas dynamics, leading to the hydrodynamic limit (the methods of Hilbert, Chapman-Enskog, and Grad among others). An attempt has been made by Poupaud,^{14,15} trying to extend Hilbert's method to the BTE for semiconductors, assuming a collision operator in the form of a single relaxation term (which is definitely an unrealistic approximation to the complexities of the collision operator, and therefore not applicable for calculating, e.g., transport coefficients, among other things).

A more promising approach toward obtaining sensible hydrodynamical-like equations would be to resort to the Chapman-Enskog method. Extending it to the BTE for

semiconductors in a mathematically satisfactory way seems a far from trivial task. Another method suitable for deriving hydrodynamical-like equations is Grad's method of moments.¹⁶ This method yields, with an appropriate truncation, a set of evolution equations for the thirteen fields comprising, besides the five balance laws corresponding to particle number, momentum, and energy, rate-type equations for the heat flux and anisotropic stresses. These equations are known to describe dilute gases only near thermal equilibrium and fail drastically in nonequilibrium situations. This is the case of shock wave structure in which the Grad equations fail for a Mach number exceeding a critical value of order 2, while on the contrary the usual Navier-Stokes equations remain approximately valid up to much higher Mach numbers.¹⁷ However, the Grad method of moments can still be used in order to obtain hydrodynamical equations with constitutive equations of the Navier-Stokes and Fourier type, by successively applying to the Grad equations the Maxwellian iteration method (e.g., as formulated by Ikenberry and Truesdell).¹⁸ Although there is no general convergence proof this method seems to be preferable to the Chapman-Enskog one because it can be implemented much more straightforwardly in a systematic manner.¹⁸ In particular, the transport coefficients for heat conduction and viscous stresses can be obtained with much less effort and for this reason such a method is widely applied (e.g., in relativistic kinetic theory¹⁹).

In this paper we aim at the less ambitious approach of deriving the form of hydrodynamical-like equations for charge-carrier transport in semiconductors by utilizing the methods of extended thermodynamics.

Extended thermodynamics is a relatively recent approach to nonequilibrium thermodynamics,²⁰ and its main objective is the derivation of many fundamental results of the kinetic theory of gas from a limited number of general physical principles. More precisely, the Grad equations for the thirteen fields (density, velocity, energy, heat flux, and viscous stresses) can be obtained (apart from a numerical constant) from the general moment equations under the following general assumptions.

(i) The off-center fourth-order moment and the traceless third-order moment (which appear in the moment evolution equations for the anisotropic stresses and heat flux) are constitutive functions of the other moments, restricted only by the requirement of material frame indifference.²⁰

(ii) An entropy density and entropy flux can be defined, both constitutive functions of all the moments under consideration (the thirteen fields), which are also restricted only by the requirement of material frame indifference.

(iii) The entropy density and entropy flux satisfy a general entropy balance law (at this stage the requirement of positive entropy production is not enforced).

(iv) The constitutive functions for the off-center fourth moment and the traceless third-order moment, the entropy density, and entropy flux can be expanded around a state of local thermal equilibrium (the former two up to first order because one looks for linear constitutive relations, the entropy density, and entropy flux up to second order, although a higher-order analysis is also possible²⁰).

In this way one obtains the Grad equations of moments without resorting to approximation procedures for the distribution function, but on the basis of general physical principles. By imposing the restriction that the entropy production must be non-negative one then obtains restrictions on the coefficients which appear in the constitutive equations. By further applying the Maxwellian iteration procedure one recovers the usual Navier-Stokes and Fourier constitutive equations for a dilute gas, and the requirement of non-negative entropy production implies that the transport coefficients for heat conduction and viscosity are nonnegative.

In this article we adopt the approach of extended thermodynamics (suitably tailored to the problem under consideration) in order to derive hydrodynamical equations for carrier transport in semiconductors. This choice is motivated by the success obtained by extended thermodynamics in recovering the standard results of the Grad method for dilute gases.

The advantage of such an approach is that it generates constitutive laws for the appropriate higher moments of the distribution function (depending on the order of truncation) irrespective of detailed microscopic assumptions of the form of the distribution function.

Extended thermodynamics cannot provide numerical values for the parameters appearing in the source terms of the balance equations. However, it can yield useful restrictions in the form of inequalities among them.

In general, for practical applications, it will be necessary to treat the parameters appearing in the source terms as phenomenological quantities to be determined by experiments.

In Sec. II we recall the basic formalism of the moment equations. In Sec. III, after having selected the appropriate constitutive quantities, we impose the entropy principle (the salient feature of extended thermodynamics). We find that the results obtained by Liu and Müller²⁰ for the ideal classical gas are partially applicable to the case under consideration. Furthermore, we obtain physically interesting restrictions on the relaxation times arising from the source terms.

The set of moment equations we derive are still too complicated to be used in practical device simulation and, therefore, by utilizing a method akin to the Maxwellian iteration we obtain a reduced system (which is similar to the Navier-Stokes and Fourier equations of classical gas dynamics).

Finally, in Sec. IV we draw conclusions.

II. MOMENT EQUATIONS

For the sake of simplicity we assume a parabolic band structure for the solid.¹¹ Let $f(\mathbf{u}, \mathbf{x}, t)$ represent the density of charge carriers in phase space with position \mathbf{x} and velocity \mathbf{u} at time t .

Then the transport equation for one species of charge carriers, electrons, or holes, in an electric field, is

$$\frac{\partial f}{\partial t} + u^i \frac{\partial f}{\partial x^i} + \frac{q}{m} E^i \frac{\partial f}{\partial u^i} = \dot{f}_c, \quad (1)$$

where \mathbf{E} is the electric field, m is the effective mass (of electrons or holes), q the charge of a carrier (positive for holes and negative for electrons), \dot{f}_c the time rate of change of f due to collisions.

We define the number density of carriers

$$n = \int f d\mathbf{u} , \quad (2)$$

the mean carrier velocity

$$v_i(x,t) = \frac{1}{n} \int f u_i d\mathbf{u} , \quad (3)$$

and the pressure tensor

$$m_{ij} = m \int f (u_i - v_i)(u_j - v_j) d\mathbf{u} . \quad (4)$$

Furthermore we shall need three more moments, the heat-flow density tensor

$$m_{ijk} = m \int f (u_i - v_i)(u_j - v_j)(u_k - v_k) d\mathbf{u} , \quad (5)$$

and the fourth order off-center moment

$$m_{ijkl} = m \int f (u_i - v_i)(u_j - v_j)(u_k - v_k)(u_l - v_l) d\mathbf{u} \quad (6)$$

(the latter has no direct physical interpretation). The heat-flow vector \mathbf{q} is then defined as

$$q_i = \frac{1}{2} m_{iil} = \frac{m}{2} \int f (\mathbf{u} - \mathbf{v})^2 (u_i - v_i) d\mathbf{u} . \quad (7)$$

By multiplying Eq. (1) by 1, u_i , $u_i u_j$, $u_i (\mathbf{u})^2$, $(\mathbf{u})^4$, and integrating over velocity space we obtain the usual moment equations (in conservation form)

$$\frac{\partial n}{\partial t} + \frac{\partial}{\partial x^j} F^j = C , \quad (8)$$

$$\frac{\partial F^i}{\partial t} + \frac{\partial}{\partial x^j} F^{ij} = C^i + n \frac{q}{m} E^i , \quad (9)$$

$$\frac{\partial F^{ik}}{\partial t} + \frac{\partial}{\partial x^j} F^{ikj} = C^{ik} + 2n v^{(i} E^{k)} \frac{q}{m} , \quad (10)$$

$$\frac{\partial F^{ill}}{\partial t} + \frac{\partial}{\partial x^j} F^{ijll} = C^{ill} + \frac{q}{m} (2F^{il} E_l + F^{ll} E^i) , \quad (11)$$

where

$$F^i = n v^i , \quad F^{ij} = n v^i v^j + \frac{1}{m} m^{ij} ,$$

$$F^{ijk} = n v_i v_j v_k + \frac{1}{m} [3v_{(i} m_{jk)} + m_{ijk}] ,$$

$$F_{ijll} = n v_i v_j (v)^2 + \frac{1}{m} [m_{ll} v_i v_j + (v)^2 m_{ij} + 4v^k m_{k(i} v_{j)} + 2m_{ijl} v^l + m_{jll} v_i + m_{ill} v_j + m_{ijll}] ,$$

where round brackets around indices denote symmetrization. Here the quantities C , C^i , C^{ik} , C^{ill} appearing on the right-hand sides of Eqs. (8)–(11) are to be interpreted as production terms of the particle number, momentum, stress-energy, and energy-flow densities, respectively.

Now, following the approach of extended thermodynamics,²⁰ we consider Eqs. (8)–(11) as evolution equa-

tions in the 13 unknown independent variables n , v^i , m^{ij} , m^{ill} once the dependent variables

$$m^{(ijk)} = m^{ijk} - \frac{3}{5} m^{ll(i} \delta^{jk)} ,$$

$$m^{(jk)ll} = m^{ijll} - \frac{1}{3} m^{aall} \delta^{ij} ,$$

$$m^{aall} , C , C^i , C^{ik} , C^{ill}$$

are expressed as function of them. Here and in what follows for any set of indices $A^{(ijk\dots)}$ denotes the trace-free totally symmetric part of the tensor A .

The closure problem is to find expressions for $m^{(ijk)}$, $m^{(jk)ll}$, m^{aall} , C , C^i , C^{ik} , C^{ill} as constitutive functions of n , v^i , m^{ij} , m^{ill} on the basis of physically sensible assumptions. In the following section we shall obtain constitutive equations for $m^{(ijk)}$, $m^{(jk)ll}$, m^{aall} by assuming the objectivity (material frame indifference) and entropy principle.²⁰ Constitutive expressions for the production terms C , C^i , C^{ik} , C^{ill} can be obtained only at the cost of further assumptions (motivated by a relaxation-time representation for the collision term \dot{f}_c).

III. THE ENTROPY PRINCIPLE

This principle can be split into two parts. The first part amounts to assuming that a scalar function S (to be interpreted as entropy density) and a vector function S^k (to be interpreted as entropy flux) exist such that an entropy balance law holds. The second part states that the entropy production must be non-negative for all physicalizable states.

The entropy principle can be interpreted mathematically as a supplementary conservation law in the sense of Friedrichs and Lax.²¹ The equations of Newtonian and relativistic fluid dynamics and magnetofluid dynamics all admit the existence of such a supplementary conservation law with a convex entropy density, and this property implies that these theories can be described by symmetric hyperbolic systems.^{22,23}

Here we shall assume that such a principle applies to the system consisting of the solid and of the carrier components (say, electrons). *A priori* we cannot assume the entropy principle to hold for the electron component, because this would require an “ H theorem” under very general circumstances (see Ref. 13, where such a theorem is proved for the case of electron-optical phonon scattering). However, under the assumption that entropy density and entropy flux are additive functions of the variables describing each of the subsystems, we can obviously assume the first part of the entropy principle to hold also for the electron subsystem. The second part of the entropy principle will be treated separately in the sequel.

Let S and S^j now denote the electron gas-entropy density and entropy flux and g the entropy production. Then the first part of the entropy principle amounts to assuming that the following balance law:

$$\frac{\partial S}{\partial t} + \frac{\partial S^j}{\partial x^j} = g \quad (12)$$

holds for all solutions of the evolution Eqs. (8)–(11),

once the dependent variables $m^{(ijk)}$, $m^{(jk)ll}$, m^{aall} , C , C^i , C^{ik} , C^{ill} have been expressed as constitutive functions of the independent variables (n , v^i , m^{ij} , m^{ill}). Here we shall assume that these constitutive functions are objective, in the sense of material frame indifference.²² At variance with the case of an ideal gas treated in Ref. 20, in our case the velocity vector \mathbf{v} is an objective quantity, being the mean electron-gas velocity relative to the solid (assumed at rest). Therefore *a priori* there could be a dependence of S and the nonconvective part of S^j on \mathbf{v} . However, we exclude this because it would be inconsistent with our previous additivity assumption on the entropy density and entropy flux.

If we denote by

$$\frac{\partial F^A}{\partial t} + \frac{\partial}{\partial x_j} F^{Aj} = P^A, \quad A = 1, \dots, 13$$

the system of Eqs. (8)–(11), where F^A , F^{Aj} , P^A , denote the column vectors

$$F^A = (n, F^i, F^{ij}, F^{ill})^T,$$

$$F^{Aj} = (F^j, F^{ij}, F^{ikj}, F^{ijll})^T,$$

$$P^A = \left[C, C^i + \frac{nq}{m} E^i, C^{ik} + 2nv^{(i} E^{k)} \frac{q}{m}, C^{ill} + \frac{q}{m} (2F^{il} E_l + F^{ll} E^i) \right]^T$$

(with the superscript T denoting transportation) and use the general theorem of Liu,²⁴ we obtain the result that the entropy principle is equivalent to assuming the existence of multipliers Λ_A (usually called Lagrange multipliers because of their similarity to the familiar ones [22]) which are functions of the independent variables so that

$$\frac{\partial S}{\partial t} + \frac{\partial S^j}{\partial x^j} - \sum_A \Lambda_A \left[\frac{\partial F^A}{\partial t} + \frac{\partial}{\partial x_j} F^{Aj} \right] = 0 \quad (13)$$

for every value of the independent variables. We notice that the equality (13) involves only the left-hand sides of the evolution equations and therefore coincides with the corresponding equality obtained in the case of a simple gas.²¹

The most general solution satisfying (13) up to second order near thermal equilibrium (we remind the reader that thermal equilibrium corresponds to the vanishing of the heat-flow vector and the deviatoric part of the stress tensor, as well as zero relative velocity \mathbf{v}) has been found by Liu and Müller.²⁰ The solution found in Ref. 20 for this case reads

$$m^{(ijk)} = 0,$$

$$m^{(ij)ll} = m(7k_B T m^{-1} + 7mk_B^{-1} n^{-1} T^{5/2} a) m^{(ij)},$$

$$m^{aall} = m[5n(k_B T/m)^2 + 5aT^{5/2} + A],$$

$$S = S_0 + (S_1 m_{(kl)} m_{(kl)} + S_2 m_{ill} m_{ill}) \frac{1}{m^2}, \quad (14)$$

$$S_0 = k_B \frac{n}{m} \left[\ln(T^{3/2} \rho^{-1}) + D \right],$$

$$S_1 = -m(4nk_B T^2)^{-1},$$

$$S_2 = -m^2(20nk_B^2 T^3)^{-1},$$

with a , A , D arbitrary constants which must vanish for a nondegenerate gas.²⁰ Here T is the absolute temperature, k_B the Boltzmann constant, and the equation of state is the perfect gas law

$$m_{ll} = 3nk_B T.$$

Now we compute the entropy production g to second order in the deviation from thermodynamical equilibrium

$$g = \sum_A \Lambda_A P^A. \quad (15)$$

For this we cannot use the results in Ref. 20 because the production terms P^A in our case are quite different.

Equation (15) explicitly yields

$$g = \Lambda C + \Lambda_i \left[C^i + \frac{n}{m} q E^i \right] + \Lambda_{ik} \left[C^{ik} + 2nv^i E^k \frac{q}{m} \right] + \Lambda_{ill} \left[C^{ill} + 2 \frac{q}{m} F^{ip} E_p + \frac{q}{m} F^{pp} E^i \right]. \quad (16)$$

The Lagrange multipliers can be obtained from Eq. (13) and are

$$\Lambda = \frac{\partial S}{\partial n}; \quad \Lambda_i = \frac{\partial S}{\partial F_i}, \quad \Lambda_{ik} = \frac{\partial S}{\partial F_{ik}}; \quad \Lambda_{ill} = \frac{\partial S}{\partial F_{ill}}.$$

It is easy to check that the coefficient of the term $E^i q/m$ in Eq. (16) is

$$\frac{\partial S}{\partial F_i} n + 2 \frac{\partial S}{\partial F_{ik}} n v^k + \frac{\partial S}{\partial F_{kll}} (2F^{ki} + F^{pp} \delta^{ik}) = \frac{\partial S}{\partial v_i} = 0,$$

and therefore Eq. (16) reduces to

$$g = \Lambda C + \Lambda_i C^i + \Lambda_{ik} C^{ik} + \Lambda_{ill} C^{ill}. \quad (17)$$

If we define D^i , D^{ik} , D^{ill} by

$$C^i = C v^i + D^i,$$

$$C^{ik} = C v^i v^k + 2D^{(i} v^{k)} + D^{ik}$$

$$C^{ill} = C v^2 v^i + 2v^i v^j D_j + v^2 D^i + v^i D^{jj} + 2v_j D^{ij} + D^{ill},$$

then Eq. (17) becomes

$$\begin{aligned}
g &= C \left[\frac{\partial S}{\partial F} + \frac{\partial S}{\partial F_k} v^k + \frac{\partial S}{\partial F_{ik}} v^k v^i + \frac{\partial S}{\partial F_{kll}} v^k v^2 \right] + D^i \left[\frac{\partial S}{\partial F_i} + 2 \frac{\partial S}{\partial F_{ik}} v^k + \frac{\partial S}{\partial F_{kll}} (2v^k v^i + v^2 \delta^{ik}) \right] \\
&\quad + D^{ik} \left[\frac{\partial S}{\partial F_{ik}} + \frac{\partial S}{\partial F_{p ll}} (2v^k \delta^{ip} + v^p \delta^{ik}) \right] + D^{kpp} \frac{\partial S}{\partial F_{kll}} \\
&= C \frac{\partial S}{\partial n} + D^i n^{-1} \left[\frac{\partial S}{\partial v_i} - \frac{\partial S}{\partial m_{kll}} (2m^{ki} + m^{pp} \delta^{ik}) \right] + D^{ik} m \frac{\partial S}{\partial m_{ik}} + m D^{kpp} \frac{\partial S}{\partial m_{kll}} ,
\end{aligned}$$

or, equivalently,

$$g = \Lambda^I C + \Lambda_i^I D^i + \Lambda_{ij}^I D^{ij} + \Lambda_{ill} D^{ipp} , \quad (18)$$

where

$$\Lambda^I = \frac{\partial S_0}{\partial n} + m^{-2} \frac{\partial S_1}{\partial n} m_{\langle kl} m_{\rangle kl} + m^{-2} \frac{\partial S_2}{\partial n} m_{ill} m_{ipp} ,$$

$$\Lambda_i^I = -4m^{-2} n^{-1} (m^{\langle ki} + \frac{\xi}{6} m^{ll} \delta^{ik}) S_2 m_{kll} ,$$

$$\begin{aligned}
\Lambda_{ij}^I &= \left[\frac{\partial S_0}{\partial m_{ll}} m + m^{-1} \frac{\partial S_1}{\partial m_{ll}} m_{\langle kl} m_{\rangle kl} \right. \\
&\quad \left. + m^{-1} \frac{\partial S_2}{\partial m_{11}} m_{qll} m_{qpp} \right] \delta_{ij} + 2m^{-1} S_1 m_{\langle ij} ,
\end{aligned}$$

$$\Lambda_{ill} = 2m^{-1} S_2 m_{ill} .$$

In order to compute this entropy production g to second order (in the deviation from thermodynamical equilibrium) we need the representation of C , D^I to the second order and of D^i , $D^{\langle ij \rangle}$, D^{ipp} to the first order. For this we need explicit representations for these quantities as constitutive equations. Instead of proceeding in a general and systematic way (which would lead to cumbersome calculations), we make physically motivated assumptions on the basis of representations of the production terms as relaxation type quantities.

We remark that the choice of particular forms for the production terms is somehow ambiguous and can lead to different results. The procedure which we shall follow is that of the simplest generalization of the relaxation-form expression proposed by Baccarani and Wordeman²⁵ for energy. In particular the production terms for particle number, momentum density, and energy density are exactly those of Baccarani and Wordeman.²⁵ For the anisotropic stresses and energy flow we assume that the production terms can be written in the relation form, also taking into proper account convective stresses and convective energy flow. A justification of this procedure can be obtained in the simplistic case of a collision term \hat{f}_c in Eq. (1) of the single relaxation type.

Therefore, the simplest choice for C , C^i is

$$C = 0; \quad C^i = -\frac{nv_i}{\tau_p} , \quad (19)$$

with $\tau_p > 0$ the momentum relaxation time. This corresponds to the following expression for D^i :

$$D^i = -\frac{nv_i}{\tau_p} . \quad (20)$$

This choice has been motivated in Ref. 25 and used in Refs. 3–6 and is justified by the observation that for hot electrons recombination-generation processes are negligible and that C^i is given by a simple momentum relaxation expression. Notice that in this expression Galilean invariance is only apparently violated because v^i must be interpreted as relative velocity with respect to the lattice, considered as a rigid body at rest. In general the terms in v^i must be considered as velocities relative to the lattice and therefore are of first order in the deviation from thermodynamical equilibrium (in equilibrium $\mathbf{v} = 0$).

For C^{ik} we distinguish the trace C^{ll} and the trace-free part $C^{\langle ij \rangle}$, which might correspond to different relaxation processes.

The expression for C^{ll} corresponds to energy production and can be taken to be that proposed by Baccarani and Wordeman,²⁵

$$C^{ll} = \frac{-\frac{1}{2}nmv^2 + \frac{3}{2}nk_B(T_0 - T)}{\tau_w} , \quad (21)$$

where τ_w is to be interpreted as the relaxation time for energy and T_0 is the lattice equilibrium temperature. This yields the following expression for D^{ll} :

$$D^{ll} = \left[\frac{2n}{\tau_p} - \frac{n}{\tau_w} \right] v^2 + \frac{3nk_B}{\tau_w m} (T_0 - T) . \quad (22)$$

The expression for the trace-free part is needed only to first order in the deviation from thermal equilibrium and therefore can be taken to be

$$C^{\langle ik \rangle} = -\frac{1}{m\tau_\sigma} m^{\langle ik \rangle} , \quad (23)$$

where τ_σ is the shear stress relaxation time. (This is consistent with previous calculations, indicating the occurrence of anisotropic stresses in hot electrons in bulk semiconductor material.²⁶) Then this gives

$$D^{\langle ik \rangle} = -\frac{1}{m\tau_\sigma} m^{\langle ik \rangle} . \quad (24)$$

Also, C^{ill} is needed only to first order and therefore we can take

$$C^{ill} = -\frac{1}{m\tau_q} (m^{ill} + \frac{\xi}{3} v^i m^{pp}) , \quad (25)$$

which corresponds to a simple relaxation formula for the total-energy flow vector F^{ipp} (to first order away from thermal equilibrium), which is also the one used by Thoma *et al.*,⁸ τ_q being the corresponding relaxation time. This corresponds to the same expression for D^{ipp} ,

$$D^{ipp} = -\frac{1}{m\tau_q} (m^{ipp} + \frac{5}{3}v^i m^{pp}). \quad (26)$$

$$g = \frac{3nk_B(T-T_0)}{2\tau_w m T_0} + \frac{1}{20nk_B^2 T_0^3} \left[-20nk_B T q_i v_i \left(\frac{1}{\tau_p} - \frac{1}{\tau_q} \right) + 8 \frac{q^2}{\tau_q} \right] + \frac{n}{2T_0} \left[\frac{2}{\tau_p} - \frac{1}{\tau_w} \right] v^2 + \frac{3nk_B(T-T_0)^2}{2T_0^2 \tau_w} + \frac{m_{\langle ij \rangle} m_{\langle ij \rangle}}{5nk_B T_0^3 \tau_\sigma}.$$

Now the first order-term, which is linear in $T-T_0$, corresponds exactly to the rate of variation of the lattice entropy production (considering the solid as a rigid body) due to its thermal interaction with the electron gas. In fact it is just the ratio of the rate of the thermal energy exchanged between the electron gas and the solid, divided by the ambient temperature T_0 . The remaining second-order terms therefore represent the rate of entropy production due to the dissipative nature of the interaction of the electron gas with itself and with the phonons.

Now we can impose the second part of the entropy principle in the form that the quadratic part of the entropy production must be non-negative. This requirement implies the following inequalities:

We remark that the relaxation times τ_p, τ_w, τ_q , since they appear as multipliers of first-order nonequilibrium quantities, must be considered as functions of equilibrium variables.

The final expression for the entropy production g up to second order away from thermal equilibrium is

$$\tau_q > 0, \quad \tau_\sigma > 0, \quad 2\tau_w > \tau_p, \quad (27)$$

$$\left[\frac{1}{\tau_p} - \frac{1}{\tau_q} \right]^2 - \frac{4}{5\tau_q} \left[\frac{2}{\tau_q} - \frac{1}{\tau_w} \right] < 0.$$

From the inequalities appearing in (27), we immediately draw the conclusion that all the quantities

$$\tau_\sigma, \quad \tau_w, \quad \tau_q$$

are strictly positive (and this is necessary for stability).

Furthermore, a very important consequence is that τ_q cannot be arbitrary because it must satisfy the last inequality in (27).

Finally we write down explicitly the field equations. They are

$$\frac{\partial n}{\partial t} + v_i \frac{\partial n}{\partial x_i} + n \frac{\partial v_i}{\partial x_i} = 0, \quad (28)$$

$$\frac{\partial v_i}{\partial t} + v_j \frac{\partial v_i}{\partial x_j} + \frac{1}{mn} \frac{\partial m_{ij}}{\partial x_i} = \frac{q}{m} E^i + \frac{1}{n} D^i, \quad (29)$$

$$\frac{\partial m_{ij}}{\partial t} + v_k \frac{\partial m_{ij}}{\partial x_k} + m_{ij} \frac{\partial v_k}{\partial x_k} + \frac{1}{5} \delta_{ij} \frac{\partial m_{kll}}{\partial x_k} + \frac{1}{5} \frac{\partial m_{ill}}{\partial x_j} + \frac{1}{5} \frac{\partial m_{jll}}{\partial x_i} + 2m_{k(i} \frac{\partial v_{j)}}{\partial x_k} = m D_{ij}, \quad (30)$$

$$\frac{\partial m_{ill}}{\partial t} + v_j \frac{\partial m_{ill}}{\partial x_j} + \frac{7}{5} m_{ill} \frac{\partial v_k}{\partial x_k} - \left(\frac{5}{9} m_{ll}^2 m^{-1} n^{-2} \delta_{ik} + \frac{7}{3} m^{-1} n^{-2} m_{ll} m_{\langle ik \rangle} \right) \frac{\partial n}{\partial x_k} + \frac{2}{5} m_{jll} \frac{\partial v_j}{\partial x_i} + \frac{2}{3} m^{-1} n^{-1} m_{ll} \frac{\partial m_{\langle ik \rangle}}{\partial x_k} + \frac{5}{3} m^{-1} n^{-1} m_{\langle ik \rangle} \frac{\partial m_{ll}}{\partial x_k} + \frac{7}{5} m_{jll} \frac{\partial v_i}{\partial x_j} - 2 \frac{m_{\langle ij \rangle}}{mn} \frac{\partial m_{\langle jk \rangle}}{\partial x_k} + \frac{5}{9} \frac{m_{ll}}{mn} \frac{\partial m_{ll}}{\partial x_i} = m D_{ill} - n^{-1} D^j (m_{ll} \delta_{ij} + 2m_{ij}), \quad (31)$$

with D^i, D_{ij}, D_{ill} given by (20,22,24,26).

Drawing from the results of extended thermodynamics,²⁰ the convexity of the entropy density implies that the system (28)–(31) is equivalent to a symmetric hyperbolic system, at least in the neighborhood of thermal equilibrium. This is very comforting from the mathematical viewpoint because the initial value problem is well posed for symmetric hyperbolic systems.

However, the above system (28)–(31) is still too complicated to be used for device simulation and therefore

now we derive a reduced system, more akin to the usual hydrodynamical equations.

Following the approach proposed in Ref. 20, which is akin to the Maxwellian iteration, from Eqs. (28)–(31) we obtain, in the limit of short mean free path, constitutive equations for both $m_{\langle ij \rangle}$ and m_{ill} .

In this way Eqs. (28) and (29) and the trace of Eq. (30) will form a closed system in the independent variables n, v_i, m_{ll} , once $m_{\langle ij \rangle}$ and m_{ill} have been expressed as a function of them and of their derivatives.

The iteration works in the following way. We substitute in the left-hand sides of Eq. (31) and of the traceless part of Eq. (30) the s th iterates of $m_{\langle ij \rangle}$, m_{ill} . Then the right-hand sides of these equations yield the $(s+1)$ th iterates for $m_{\langle ij \rangle}$ and m_{ill} , once nonlinear terms of order higher than the s th in the deviations from thermodynamical equilibrium have been neglected.

The zeroth iterate is defined by the thermodynamical equilibrium values of $m_{\langle ij \rangle}$, m_{ill} , i.e.,

$$m_{\langle ij \rangle}^0 = 0, \quad m_{ill}^0 = 0.$$

In order to obtain the first iteration we notice that $m_{\langle ij \rangle}$ and m_{ill} must be considered to be of first order in the deviation from thermodynamical equilibrium, while their time or space derivatives are of second order. Likewise, the gradients of equilibrium quantities (n , v , T) are also considered to be of first order.

Finally, as stated before, in D^i , D^{ij} the terms in v^i must be considered as velocities relative to the lattice and therefore are of first order in the deviation from thermodynamical equilibrium (in equilibrium $v=0$).

The first iteration then gives

$$m_{\langle ij \rangle} = -nk_B T \tau_\sigma \left[\frac{\partial}{\partial x} v_i + \frac{\partial}{\partial x} v_j - \frac{2\partial}{3\partial x} v_k \delta_{ij} \right], \quad (32)$$

$$q_i = -\frac{5k_B^2 n T \tau_q}{2m} \frac{\partial}{\partial x_i} T + \frac{5}{2} nk_B T v_i \left[\frac{1}{\tau_p} - \frac{1}{\tau_q} \right] \tau_q. \quad (33)$$

We notice that the above constitutive equations are the usual Navier-Stokes equations for shear viscosity and a modified Fourier law for heat conduction (the difference with the usual Fourier law being due to a convective term). The total-energy flux obtained with the constitutive law (33) coincides with that proposed by Thoma *et al.*⁸

Finally the reduced system of equations we propose consists of the charge-carrier number conservation equation

$$\frac{dn}{dt} + n \frac{\partial v_i}{\partial x_i} = 0, \quad (34)$$

the momentum balance equation

$$\frac{dv_i}{dt} + \frac{1}{mn} \frac{\partial m_{\langle ij \rangle}}{\partial x_j} + \frac{1}{n} \frac{\partial p}{\partial x_i} = \frac{1}{m} q E_i - v_i / \tau_p, \quad (35)$$

and the energy balance equation

$$\begin{aligned} \frac{d}{dt} nk_B T + \frac{5}{3} nk_B T \frac{\partial}{\partial x_k} v_k + \frac{1}{3} \frac{\partial}{\partial x_k} m_{kll} + \frac{2}{3} m_{\langle ik \rangle} \frac{\partial v_i}{\partial x_k} \\ = \frac{2}{3} nm \left[\frac{1}{\tau_p} - \frac{1}{2\tau_w} \right] v^2 + \frac{mn}{2\tau_w} k_B (T_0 - T), \end{aligned} \quad (36)$$

supplemented by the constitutive equations (32) and (33) for $m_{\langle ij \rangle}$, q_i and where d/dt represents the convective derivative and p is the thermodynamical pressure $p = nk_B T/m$.

IV. CONCLUSIONS

In this paper we have found that the approach of extended thermodynamics can be applied to fluid modeling of hot electrons in semiconductors. It gives rise to a hydrodynamical model of more general nature than those proposed by Blotekjaer^{11,12} or Hänsch and Miura-Mattausch¹ on the basis of (more or less justifiable) assumptions on the distribution function.

Our model is also more satisfactory from the mathematical viewpoint (because it leads to an original system which is a symmetric hyperbolic system), and this could also be an advantage for numerical calculations. The range of physical applicability of the hyperbolic model remains to be investigated.

A better understanding of the model requires its testing *vis a vis* particular problems (e.g., the ballistic diode) and this will be the subject of future work.

ACKNOWLEDGMENT

Work partially supported by CNR (MMI-P.S. IPPMI, U.O. "Mathematical models of semiconductors").

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