

## Nonlinear effects in 3rd and 4th-order moments of transport-hydrodynamical models in semiconductors within Extended Thermodynamics

Ahmed Salhoumi <sup>(1)</sup>, Mohamed Zakari <sup>(2)</sup> and Yahia Boughaleb <sup>(1),\*</sup>

<sup>(1)</sup> *Faculté des Sciences Ben M'Sik, Département de Physique, L.P.M.C. B.P. 7955 Sidi Othman, Casablanca, Morocco.*

<sup>(2)</sup> *Universitat Autònoma de Barcelona, Departament de Física, Grup de Física Estadística, 08193 Bellaterra, Catalonia, Spain.*

In this paper, we treat the closure relations of hydrodynamical models in order to study electron transport in semiconductors. We adopt the Extended Thermodynamics theory in order to derive hydrodynamical equations for carrier transport and we try to close the system, i.e. to find constitutive equations for the third and fourth-order moments, by means of a generalized nonequilibrium distribution function.

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### I. INTRODUCTION

Hydrodynamical models have been used recently in simulating charge-carrier transport in semiconductors, particularly, with respect to hot electron and submicron devices [1-9]. These models 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]. Indeed, these models involve the fundamental laws of balance of particle number, momentum, and energy for the charge carriers and are derived from the moment equations of Boltzmann transport equation by appropriate approximations.

The basic model, in which the various steps and approximations are derived and discussed in detail, is due to Blotekjaer [11,12]. So as to close the set of balance equations considered by Blotekjaer [11], one assumes that higher-order moments have the value appropriate for a displaced Maxwellian. A slightly different model has been suggested 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 five balance equations for particle number, momentum and energy are considered and the closure is accomplished by means of the Wiedemann-Franz law for heat flux. Both the Blotekjaer and Hänsch and Miura-Mattausch models are then further simplified in order to provide a manageable set of equations appropriate for device simulation. However, for more accurate results, the full models must be registered. In the similar approaches of Blotekjaer and Miura-Mattausch, Woolard et al [7] and Thoma et al [8] have proposed models taking into account the nonparabolicity of the band structure of the crystal. All these approaches have in common the assumption at the basis of the closure approximation; i.e., that some higher moments can be calculated by means a displaced

Maxwellian. Such an approximation is rather rough and imprecise and its range of validity needs to be assessed [13].

Another method suitable for deriving hydrodynamical-like equations is Grad's method of moments [14]. This method yields, with an appropriate truncation, a set of evolution equations for the thirteen fields comprising, besides of the five balance laws corresponding to particle number, momentum, and energy, rate-type equations for heat flux and anisotropic viscous stresses. These equations are known to describe dilute gases only near thermal equilibrium and fail drastically in nonequilibrium situations. Extended Thermodynamics theories are relatively recent approaches to nonequilibrium thermodynamic phenomena [15], which, at variance with classical irreversible thermodynamics (CIT) [16] incorporates higher-order moments (to be interpreted as fluxes of fluxes) in the description of the thermodynamic state of the system. The main difference between Extended Thermodynamics [17] and Extended Irreversible Thermodynamics [18], which both include higher-order moments in the description of the thermodynamic state of the system, is that Extended Thermodynamics uses systematic and full exploitation of the entropy principle. Here, we adopt the Extended Thermodynamics theory in order to derive hydrodynamical equations for carrier transport in semiconductors and we try to close the system by means of a generalized distribution function. In fact, the closure relations were treated recently by Anile et al [13,19]. We report here their results and we calculate the third and fourth-order moments by expanding the generalized distribution function up to second order in Lagrange multipliers.

The plan of this contribution is as follows: in section II we recall the basic formalism of the moment equations. In section III, we treat the problem of closure relations within Extended Thermodynamics and by expanding the generalized distribution function up to second-order we calculate the third and fourth-order moments. Finally, we end with some concluding remarks.

\* Corresponding Author  
e-mail: salhoumi@mailcity.com

## II. GENERAL FORMALISM

Let  $f(\mathbf{x}, \mathbf{k}, t)$  represent the density of charge carriers in phase space with position  $\mathbf{x}$  and electron moment vector  $\mathbf{k}$ . Then, the transport equation (1) for one species of charge carriers, electrons or holes, in an electric field  $E$  is the semi-classical Boltzmann transport equation for one particle in the conduction band of semiconductors [10], where  $\mathbf{v}(\mathbf{k})$  denotes the electron group velocity given by  $\mathbf{v}(\mathbf{k}) = \nabla_{\mathbf{k}} \mathcal{E}$  and  $q$  the charge of a carrier (positive for holes and negative for electrons):

$$\frac{\partial f}{\partial t} + \mathbf{v}(\mathbf{k}) \cdot \nabla f - qE \cdot \nabla_{\mathbf{k}} f = P \quad (1)$$

For convenience, we shall use units such that Planck's constant  $\hbar = 1$ . The electron energy  $\mathcal{E}(\mathbf{k})$  is defined by the band structure of the crystal and  $P$  is the collision term due to the interaction of electron with phonons, impurities and among themselves [20]. In order to focus on the essential issues, we limit ourselves to the case when the effective mass approximation holds [21], i.e.

$$\mathcal{E}(\mathbf{k}) = \frac{\mathbf{k}^2}{2m^*}$$

$$\mathbf{v}(\mathbf{k}) = \frac{\mathbf{k}}{m^*}$$

with  $m^*$  is the effective electron mass.

For consistency, the boundary of the first Brillouin zone is moved towards infinity and the periodicity boundary condition on  $f(\mathbf{x}, \mathbf{k}, t)$  is replaced by the requirement that  $f$  vanishes sufficiently fast as  $\mathbf{k} \rightarrow \infty$ . Let us now define the particle density  $n(\mathbf{x}, t)$

$$n(\mathbf{x}, t) = \int d\mathbf{k} f(\mathbf{x}, \mathbf{k}, t)$$

and the mean velocity  $\mathbf{u}(\mathbf{x}, t)$  as

$$\mathbf{u}(\mathbf{x}, \mathbf{k}, t) = \int d\mathbf{k} \mathbf{v}(\mathbf{k}) f(\mathbf{x}, \mathbf{k}, t)$$

then the particle flux is

$$\mathbf{J} = n\mathbf{u}$$

By integrating equation (1) in  $\mathbf{k}$ -space we obtain, assuming as usual that  $f$  vanishes sufficiently fast at infinity, the particle continuity equation which is written as

$$\frac{\partial n}{\partial t} + \nabla \cdot (n\mathbf{u}) = 0 \quad (2)$$

Multiplying equation (1) by  $k^i$  and integrating it we obtain the momentum balance equation

$$\frac{\partial (nu^i)}{\partial t} + \frac{\partial \theta^{ij}}{\partial x^j} + \frac{nqE^i}{m^*} = P^i \quad (3)$$

where the pressure tensor  $\theta^{ij}$  and the production term  $P^i$  are given by

$$\theta^{ij} = \frac{\int d\mathbf{k} f k^i k^j}{m^{*2}} \quad \text{and} \quad P^i = \frac{\int d\mathbf{k} P k^i}{m^*}$$

Multiplying equation (1) by  $k^i k^j$  and integrating we obtain for the traceless part of the pressure tensor  $\theta_{ij}$

$$\frac{\partial \theta_{<ij>}}{\partial t} + \frac{\partial \theta_{<ij>r}}{\partial x^r} + \frac{2nqE_{<ij>}}{m^*} = P_{<ij>} \quad (4)$$

For any tensor  $T_{ij}$  the symbol  $T_{<ij>}$  denotes its trace-free symmetric part

$$T_{<ij>} = \frac{1}{2} (T_{ij} + T_{ji} - \frac{2}{3} T_k^k \delta_{ij})$$

then  $\theta_{ijr}$  and  $P_{ij}$  are given by

$$\theta_{ijr} = \frac{\int d\mathbf{k} f k_i k_j k_r}{m^{*3}} \quad \text{and} \quad P_{ij} = \frac{\int d\mathbf{k} P k_i k_j}{m^{*2}}$$

From the trace part of  $\theta_{ij}$  we obtain the energy balance equation

$$\frac{\partial W}{\partial t} + \nabla \cdot \mathbf{S} + nq\mathbf{E} \cdot \mathbf{u} = P_W \quad (5)$$

with  $W = \int d\mathbf{k} f \mathcal{E}(\mathbf{k})$  the energy density, the energy flux is  $\mathbf{S} = \int d\mathbf{k} f \mathcal{E}(\mathbf{k}) \mathbf{v}(\mathbf{k})$  and the energy rate of change due to collisions is written as  $P_W = \int d\mathbf{k} P \mathcal{E}(\mathbf{k})$ .

Furthermore, the energy flux equation is given by

$$\frac{\partial S_i}{\partial t} + \frac{\partial S_{ij}}{\partial x^j} + q(E_j \theta_{ij} + \frac{1}{m^*} W E_i) = \tilde{P}_i \quad (6)$$

where

$$S_{ij} = \frac{\int d\mathbf{k} f \mathcal{E}(\mathbf{k}) k_i k_j}{m^{*2}} \quad \text{and} \quad \tilde{P}_i = \frac{\int d\mathbf{k} P \mathcal{E}(\mathbf{k}) k_i}{m^*}$$

The tensor  $\theta_{ij}$  can be decomposed into its isotropic and anisotropic parts

$$\theta_{ij} = \frac{1}{3} \theta_{rr} \delta_{ij} + \theta_{<ij>}$$

with

$$\theta_{<ij>} = \frac{1}{2} (\theta_{ij} + \theta_{ji} - \frac{2}{3} \theta_{rr} \delta_{ij})$$

$$\theta_{rr} = \frac{d \mathbf{k} f \mathbf{k}^2}{m^{*2}} = \frac{2W}{m^*}$$

Therefore, equation (3) can be written as

$$\frac{\partial(nu^i)}{\partial t} + \frac{\partial(\frac{2W}{3m^*} \delta^{ij} + \theta^{<ij>})}{\partial x^r} + \frac{nqE^i}{m^*} = P^i$$

Likewise, we can decompose  $S_{ij}$  into its isotropic and anisotropic parts

$$S_{ij} = \frac{1}{3} S_{rr} \delta_{ij} + S_{<ij>}$$

Hence equation (6) can be written as

$$\frac{\partial S_i}{\partial t} + \frac{1}{3} \frac{\partial S_{rr}}{\partial x^i} + \frac{\partial S_{<ij>}}{\partial x^j} q \left( \frac{5WE_i}{3m^*} + E_j \theta_{<ij>} \right) = \tilde{P}_i$$

### III. CLOSURE RELATIONS AND EXTENDED THERMODYNAMICS

Let us rewrite the moments equations derived in the previous section. They are the continuity equation

$$\frac{\partial n}{\partial t} + \nabla \cdot (n\mathbf{u}) = 0 \quad (2)$$

the momentum balance equation

$$\frac{\partial(nu^i)}{\partial t} + \frac{\partial \theta^{ij}}{\partial x^j} + \frac{nqE^i}{m^*} = P^i \quad (3)$$

the stress equation for the traceless part of  $\theta_{ij}$

$$\frac{\partial \theta_{<ij>}}{\partial t} + \frac{\partial \theta_{<ij>r}}{\partial x^r} + \frac{2nqE_{<ij>}}{m^*} = P_{<ij>} \quad (4)$$

The energy equation for the trace of  $\theta_{ij}$

$$\frac{\partial W}{\partial t} + \nabla \cdot \mathbf{S} + nq\mathbf{E} \cdot \mathbf{u} = P_W \quad (5)$$

and the energy flux equation

$$\frac{\partial S_i}{\partial t} + \frac{\partial S_{ij}}{\partial x^j} + q(E_j \theta_{ij} + \frac{1}{m^*} W E_i) = \tilde{P}_i \quad (6)$$

It is convenient to introduce the random component  $\mathbf{c}$  of  $\mathbf{k}$  defined as  $\mathbf{k} = m^* (\mathbf{u} + \mathbf{c})$  and then we have

$$\theta^{ij} = nu^i u^j + d \mathbf{k} f c^i c^j$$

where the tensor  $\hat{\theta}^{ij} = d \mathbf{k} f c^i c^j$  is split into isotropic and traceless part as

$$\hat{\theta}^{ij} = \frac{1}{3} \hat{\theta}_k^k \delta^{ij} + \hat{\theta}^{<ij>}$$

with  $\hat{\theta}_k^k = d \mathbf{k} f c^2$ . Then

$$\theta^{ij} = nu^i u^j + \frac{1}{3} \hat{\theta}_k^k \delta^{ij} + \hat{\theta}^{<ij>} \quad (7)$$

If we define the electron temperature  $T$  as  $\hat{\theta}_k^k = \frac{3nk_B T}{m^*}$  then the energy density writes

$$W = \frac{m^*}{2} (n\mathbf{u}^2 + \hat{\theta}_k^k) = \frac{3nk_B T}{m^*} + \frac{nm^* \mathbf{u}^2}{2} \quad (8)$$

Furthermore, we can decompose the energy flow  $\mathbf{S}$  as

$$S_i = Wu_i + nk_B Tu_i + Q_i \quad (9)$$

where the  $i^{\text{th}}$  component of the heat flow vector  $Q_i$  is written as

$$\mathbf{Q} = \frac{m^*}{2} d \mathbf{k} f \mathbf{c}^2 \mathbf{c}$$

Finally, the flux of energy flux  $S_{ij}$  can be written as

$$\begin{aligned} S_{ij} = & Wu_i u_j + 2nk_B Tu_i u_j + \frac{1}{2} nk_B T \mathbf{u}^2 \delta_{ij} \\ & + \frac{m^*}{2} [u_i u_j \hat{\theta}_{<ir>} + u_i u_r \hat{\theta}_{<jr>} + \mathbf{u}^2 \hat{\theta}_{<ij>}] \\ & + u_j Q_i + u_i Q_j + u_r \hat{\theta}_{ijr} + \hat{\theta}_{ijrr} \end{aligned} \quad (10)$$

here

$$\hat{\theta}_{ijr} = \frac{m^*}{2} d\mathbf{k} f c_i c_j c_r \quad (11)$$

$$\hat{\theta}_{ijrs} = \frac{m^*}{2} d\mathbf{k} f c_i c_j c_r c_s \quad (12)$$

are the random parts of the third-order moment tensors and fourth-order moment tensor; the latter has no direct physical interpretation [13].

Therefore, we consider only the left-hand side of equations (2)-(6) assuming the right-hand-sides are known. Therefore, the variables appearing in the thirteen equations (2)-(6) are the thirteen variables  $n$ ,  $u^i$ ,  $T$ ,  $\hat{\theta}_{<ij>}$ ,  $Q_i$ , plus  $\hat{\theta}_{ijr}$ ,  $\hat{\theta}_{ijrr}$ . In order to get a closed system we need explicit expressions for  $\hat{\theta}_{ijr}$  and  $\hat{\theta}_{ijrr}$  which is the aim of this paper. Several authors have tried to solve the closure problem; to achieve such closure relations, there are two methods, one is based on drift-diffusion model [10,12,23] and another is based on Extended Thermodynamics [13,19,24,25]. We report here the results ensuing from the latter method. In fact, the critical assumption is that  $\hat{\theta}_{ijr}$  and  $\hat{\theta}_{ijrr}$  can be considered as functions of the lower order moments. As it stands, this is a more general and weaker assumption than that of a Maxwellian distribution function. To determine  $\hat{\theta}_{ijr}$  and  $\hat{\theta}_{ijrr}$ , Anile et al have applied the methods of Extended Thermodynamics and entropy principle [17,18], and they obtain the following constitutive equations up to second order around partial thermal equilibrium:

$$f_{neq} = A \exp\left(-\beta \frac{1}{2} m^* \mathbf{c}^2 - \gamma_i \left(\frac{1}{2} m^* \mathbf{c}^2 - \frac{5}{2\beta}\right) c_i - \Gamma_{<ij>} : m^* c_{<i} c_{>}\right) \quad (15)$$

where  $\beta$ ,  $\gamma$  and  $\Gamma$  are Lagrange multipliers and  $A$  is a normalization constant.

In fact, within the information theory we expand the distribution function up to second-order in Lagrange multipliers and we base ourselves on Extended Thermodynamics but with a slightly different interpretation of the inequalities arising from the second law of thermodynamics. The conditions imposed on the nonequilibrium distribution function are

$$d\mathbf{k} f_{neq} = d\mathbf{k} f_{eq} = n \quad (16)$$

$$d\mathbf{k} f_{neq} \mathbf{c} = d\mathbf{k} f_{eq} \mathbf{c} = 0 \quad (17)$$

$$\begin{aligned} \hat{\theta}_{<ijr>} &= \frac{2m^*}{15nk_B T} \left[ Q_i \hat{\theta}_{<jk>} + Q_j \hat{\theta}_{<ki>} + Q_k \hat{\theta}_{<ij>} \right] \\ &\quad - \frac{2m^*}{15nk_B T} Q_l \left[ \hat{\theta}_{<li>} \delta_{jk} + \hat{\theta}_{<lj>} \delta_{ki} + \hat{\theta}_{<lk>} \delta_{ij} \right] \end{aligned} \quad (13)$$

$$\begin{aligned} \hat{\theta}_{ijrr} &= \left[ \frac{5n(k_B T)^2}{2m^*} + \left( \sigma - \frac{2}{5nk_B T} \right) Q_i^2 \right] \delta_{ij} \\ &\quad + 2\sigma Q_i Q_j + \frac{7}{2} k_B T \hat{\theta}_{<ij>} + \frac{m^*}{n} \hat{\theta}_{<il>} \hat{\theta}_{<jl>} \end{aligned} \quad (14)$$

where  $\sigma$  is a free parameter to determine by means of Monte Carlo simulation.

In order to check the closure relation equations (13) and (14), Anile et al evaluated the quantities  $n$ ,  $u^i$ ,  $T$ ,  $\hat{\theta}_{<ij>}$ ,  $Q_i$ , by Monte Carlo simulation, and by using a fitting, they determined the free parameter  $\sigma$  (which is equal to -0.1321) appearing in the closure equation (14) [19].

Now, we deal with the closure relations; i.e. we want to express  $\hat{\theta}_{ijr}$  and  $\hat{\theta}_{ijrr}$  in terms of lower-order moments, by means of a generalized distribution function obtained from maximum-entropy arguments. So, the generalized distribution function describing a priori the nonequilibrium steady state of a system subjected to heat flux and viscous pressure takes the following expression,

$$d\mathbf{k} f_{neq} \left( \frac{1}{2} m^* \mathbf{c}^2 \right) = d\mathbf{k} f_{eq} \left( \frac{1}{2} m^* \mathbf{c}^2 \right) = \frac{3}{2} nk_B T \quad (18)$$

$$d\mathbf{k} f_{neq} \left( \frac{1}{2} m^* \mathbf{c}^2 - \frac{5}{2\beta} \right) c_i = Q_i \quad (19)$$

$$d\mathbf{k} f_{neq} c_{<i} c_{>} = \hat{\theta}_{<ij>} \quad (20)$$

where  $f_{eq}$  represents the local-equilibrium distribution corresponding to the particle density  $n$  and to the temperature  $T$ . To have  $Q_i$  perpendicular to the velocity we assume [14,26]

$$Q_i = B c_i \left( \frac{1}{2} m^* \mathbf{c}^2 - \frac{5}{2\beta} \right)$$

the last expression defines a compact form of a reduced heat flux.

The expansion of the nonequilibrium distribution function (15) up to the second-order in Lagrange multipliers gets the form

$$f_{neq} \approx A \left[ 1 - B(\mathbf{c}) \gamma_i c_i - \Gamma_{<jk>} : m^* c_{<j>} c_{<k>} \right. \\ \left. + \frac{1}{2} B(\mathbf{c}) (\gamma_i c_i)^2 + \frac{1}{2} (\Gamma_{<jk>} : m^* c_{<j>} c_{<k>})^2 \right. \\ \left. + m^* B(\mathbf{c}) \gamma_i c_i (\Gamma_{<jk>} : c_{<j>} c_{<k>}) \right] \exp\left(-\beta \frac{m^*}{2} \mathbf{c}^2\right) \quad (21)$$

where the Lagrange multipliers  $\beta$ ,  $\gamma$  and  $\Gamma$  are related to the restrictions (18), (19) and (20).  $A$  is obtained from equation (16). Thus, the Lagrange multiplier corresponding to the velocity has been written as  $-\frac{5}{2\beta}\gamma$ , a relation which, as it will be seen, satisfies the restriction (17). Therefore, the term  $(\frac{5}{2\beta})\gamma\mathbf{c}$  follows from the requirement that if the system is at rest then  $\langle \mathbf{c} \rangle = 0$  [26] and it behaves as  $(\frac{5}{2\beta})\mathbf{c} \approx (\frac{5}{2})k_B T \mathbf{c}$  near equilibrium.

We propose, at this moment, up to second order in  $Q_i$  and  $\hat{\theta}_{ij}$  the following expression for the third and fourth-order moment tensors, i.e.  $\hat{\theta}_{ijr}$  and  $\hat{\theta}_{ijrr}$ ,

$$\hat{\theta}_{<ijr>} = \hat{C}_1 [Q_i \hat{\theta}_{<jk>} + Q_j \hat{\theta}_{<ki>} + Q_k \hat{\theta}_{<ij>}] \\ + \hat{C}_2 Q_l [\hat{\theta}_{<li>} \delta_{jk} + \hat{\theta}_{<l>j>} \delta_{ki} + \hat{\theta}_{<lk>} \delta_{ij}] \quad (22)$$

$$\hat{\theta}_{ijrr} = \left[ \frac{5n}{2m^* \beta^2} + \hat{C}_3 Q^2 \right] \delta_{ij} + \hat{C}_4 Q_i Q_j \\ + \hat{C}_5 \hat{\theta}_{<ij>} + \hat{C}_6 \hat{\theta}_{<il>} \hat{\theta}_{<jl>} \quad (23)$$

where  $\hat{C}_i = \hat{C}_i(n, \beta, \gamma, \Gamma)$  (for  $i=1, \dots, 6$ ) are the coefficients to be determined within information theory by imposing several restrictions on  $Q_i$ ,  $\hat{\theta}_{<ij>}$ ,  $\hat{\theta}_{ijr}$  and  $\hat{\theta}_{ijrr}$  (more details of calculations are given in Ref [22]). After carrying out the calculations at the first order, we obtain the expressions

$$\hat{\theta}_{<ijr>} = \frac{2m^* \beta}{5n} [Q_i \hat{\theta}_{<jk>} + Q_j \hat{\theta}_{<ki>} + Q_k \hat{\theta}_{<ij>}] \\ - \frac{3m^* \beta}{5n} Q_l [\hat{\theta}_{<li>} \delta_{jk} + \hat{\theta}_{<l>j>} \delta_{ki} + \hat{\theta}_{<lk>} \delta_{ij}] \quad (24)$$

$$\hat{\theta}_{ijrr} = \left[ \frac{5n(k_B T)^2}{2m^*} + \frac{47}{25} \frac{\beta}{n} Q^2 \right] \delta_{ij} + \frac{119}{25} \frac{\beta}{n} Q_i Q_j \\ + \frac{7}{2} \frac{1}{\beta} \hat{\theta}_{<ij>} - \frac{21}{4} \frac{m^*}{n} \hat{\theta}_{<il>} \hat{\theta}_{<jl>} \quad (25)$$

Then, we obtain the same third and fourth-order moment constitutive equations as those of Anile et al [19] with a slight difference.

Thus, we can evaluate the free parameter  $\sigma$  appearing in equations (14), which we have reported here, by comparing it with the equation (25) established in information theory. So, we find that  $\sigma$  is proportional to  $1/nk_B T$  as

$$\sigma = 2.38 \frac{1}{nk_B T} \quad (26)$$

Consequently, we can cope with the difference appearing between our contribution and the results of Anile et al [19], which we think is a slight difference, by underlying that in contrast to the use of the usual heat-flux as in [19], i.e.

$$\mathbf{Q} = \left( \frac{1}{2} m^* \mathbf{c}^2 \right) \mathbf{c} \quad (27)$$

we have used the reduced heat flux, i.e.

$$\mathbf{Q} = \left( \frac{1}{2} m^* \mathbf{c}^2 - \frac{5}{2\beta} \right) \mathbf{c} \quad (28)$$

However, we should note that both definitions give the same average value for  $Q_i$ , but not for the moments of  $Q_i$ .

#### IV. CONCLUDING REMARKS

In this paper, we have been interested to calculate in the framework of extended thermodynamics the third and fourth-order moments in order to deal with the nonlinear effects in the closure relations of transport-hydrodynamical models. This is done for a nonequilibrium system under heat flux and viscous pressure by means of a generalized distribution function obtained from information theory.

Then, we have found the same constitutive equations of the third and fourth-order moments with a slight difference with regard to the results of Anile et al [19] and we have related this difference to the use of different microscopic definitions for the heat flux. Furthermore, we have expressed the free parameter  $\sigma$  appearing in the fourth-order moment equation (14) as a function of the density and the temperature.

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