PHYSICAL REVIEW E **91**, 063011 (2015)

Higher-order generalized hydrodynamics: Foundations within a nonequilibrium statistical ensemble formalism

Carlos A. B. Silva,[1] Clóves G. Rodrigues,[2,*] J. Galvão Ramos,[3] and Roberto Luzzi[3]
[1]*Departamento de Física, Instituto Tecnológico de Aeronáutica, 12228-901, São José dos Campos, São Paulo, Brazil*
[2]*Departamento de Física, Pontifícia Universidade Católica de Goiás, 74605-010 Goiânia, Goiás, Brazil*
[3]*Condensed Matter Physics Department, Institute of Physics "Gleb Wataghin" State University of Campinas-Unicamp, 13083-859 Campinas, São Paulo, Brazil*

(Received 19 February 2015; revised manuscript received 22 May 2015; published 22 June 2015)

Construction, in the framework of a nonequilibrium statistical ensemble formalism, of a higher-order generalized hydrodynamics, also referred to as mesoscopic hydrothermodynamics, that is, covering phenomena involving motion of fluids displaying variations short in space and fast in time—unrestricted values of Knudsen numbers, is presented. In that way, an approach is provided enabling the coupling and simultaneous treatment of the kinetics and hydrodynamic levels of descriptions. It is based on a complete thermostatistical approach in terms of the densities of matter and energy and their fluxes of all orders covering systems arbitrarily driven away from equilibrium. The set of coupled nonlinear integrodifferential hydrodynamic equations is derived. They are the evolution equations of the Gradlike moments of all orders, derived from a generalized kinetic equation built in the framework of the nonequilibrium statistical ensemble formalism. For illustration, the case of a system of particles embedded in a fluid acting as a thermal bath is fully described. The resulting enormous set of coupled evolution equations is of unmanageable proportions, thus requiring in practice to introduce an appropriate description using the smallest possible number of variables. We have obtained a hierarchy of Maxwell times, associated to the set of all the higher-order fluxes, which have a particular relevance in the process of providing criteria for establishing the contraction of description.

DOI: 10.1103/PhysRevE.91.063011 PACS number(s): 67.10.Jn, 05.70.Ln, 68.65.−k, 81.05.Ea

I. INTRODUCTION

It has been noticed that one of the complicated problems of the nonequilibrium theory of transport processes in dense gases and liquids is the fact that their kinetics and hydrodynamics are intimately coupled, and must be treated simultaneously (e.g., see Refs. [1–6]). On this we may say that microscopic descriptions of hydrodynamics, that is, associated to a derivation of kinetic equations from classical or quantum mechanics and containing kinetic (transport) coefficients written in terms of correlation functions, is a long standing traditional problem. An important aspect is the derivation of constitutive laws which express thermodynamic fluxes (or currents, as those of matter and energy) in terms of appropriate thermodynamic forces (typically gradients of densities as those of matter and energy). In their most general form these laws are nonlocal in space and noninstantaneous in time. A first kinetic-hydrodynamic approach can be considered to be the so-called *classical* (or *Onsagerian*) *hydrodynamics*; it gives foundations to, for example, the classical Fourier's and Fick's diffusion laws. But it works under quite restrictive conditions, namely, local equilibrium; linear relations between fluxes and thermodynamic forces (meaning weak amplitudes in the motion) with Onsager's symmetry laws holding; near homogeneous and static movement (meaning that the motion can be well described with basically Fourier components with long wavelengths and low frequencies, and then involves only smooth variation in space and time); weak and rapidly regressing fluctuations [3–7].

Hence, more advanced approaches are required to lift these restrictions. Consider first near homogeneity, which implies validity in the limit of long wavelengths (or wave number Q approaching zero). To go beyond it is necessary to introduce a proper dependence on Q valid, in principle, for intermediate and short wavelengths (intermediate to large wave numbers). In phenomenological theories this corresponds to going from classical irreversible thermodynamics to extended irreversible thermodynamics [8–10].

A large extension of Onsagerian hydrodynamics to account for such situations consists of the so-called mesoscopic hydrothermodynamics (MHT for short, meaning thermal physics of fluid continua). MHT was initiated as a large expansion of extended irreversible thermodynamics, as given foundations and applications to a mesoscopic thermodynamic theory of fast phenomena [11], centering the analysis on heat propagation.

A construction of a MHT at the statistical mechanical level is highly desirable for covering a large class of hydrodynamic situations obtaining an understanding of the physics involved from the microscopic level, and in the last instance gaining insights into technological and industrial processes as in, for instance, hydraulic engineering, food engineering, soft-matter engineering, oil production, and petrochemistry, etc., which have a largely associated economic interest.

It can be noticed that nowadays two approaches appear to be the most favorable for providing very satisfactory methods to deal with hydrodynamics within an ample scope of nonequilibrium conditions. They are nonequilibrium molecular dynamics (NMD) [12] and the kinetic theory based on the far reaching generalization of Gibbs' ensemble formalism, namely the nonequilibrium statistical ensemble formalism (NESEF for short) [13–17]. NMD is a computational method created for modeling physical systems at the microscopic level, being a

---

[*] cloves@pucgoias.edu.br

good technique to study the molecular behavior of several physical processes. Together with the so-called Monte Carlo method is part of what is known as numeric simulation methods [18].

Here we present an extensive derivation of a MHT on the basis of the kinetic theory founded on NESEF, quite appropriate to deal with systems in far-from-equilibrium conditions involving the development of ultrafast relaxation processes, and displaying nonlinear behavior leading, eventually, to instabilities and synergetic self-organization [19–21]. Within the framework of NESEF, but in a different approach to the one used here, an alternative MHT was introduced by Zubarev and Tishchenko [22,23].

It may be noticed that the formalism can be extended to deal with the so-called nonconventional hydrodynamics which is associated to disordered media [24], consisting of systems showing a complex structure of a fractal-like (self-affine in average) characteristics, whose range of applicability and of physical interest is large [25]. Belong to this problem the case of the distinctive behavior of polyatomic structures such as colloidal particles, surfactant micelles, and polymers and biopolymers (as DNA) in liquid solutions, which are classical examples of what is presently referred to as soft-condensed matter [26]. One particular case of apparently unusual behavior is the one associated to hydrodynamic motion leading to a so-called non-Fickian diffusion, described by a time evolution following a kind of fractional-power law [27]. The nonequilibrium statistical thermomechanical aspects of complex systems including illustrations is reported elsewhere [28]; a case involving hydrothermodynamics is given in Ref. [29].

In the present paper the conventional NESEF-based MHT is described in the next section, accompanied with the study of a system consisting of particles embedded in a fluid which acts as a thermal bath at rest and in thermal equilibrium with an external reservoir. The general theory for the MHT is built upon a generalization of Grad's moments method for solution of, in this case, a generalized kinetic equation derived in the context of NESEF [30].

II. THEORETICAL BACKGROUND

For building a nonlinear higher-order (generalized) hydrothermodynamics on a mechanical statistical basis, one needs to resort to a nonequilibrium statistical ensemble formalism (NESEF) for open systems. Such formalism was developed step by step along the past century by a number of renowned scientists whose contributions have been systematized and generalized in a close structure, as described in Refs. [13–17].

According to theory, immediately after the open system of N particles, in contact with external sources and reservoirs, has been driven out of equilibrium, the description of its nonequilibrium state requires us to introduce all its observables, their fluctuations, and, eventually, higher-order variances. In most cases it suffices to take a reduced set of observables, which implies having access to the so-called one-particle (or single-particle) $\hat{n}_1$ and two-particle $\hat{n}_2$ dynamical operators for any subset of the particles involved. This is so because all observable quantities can be expressed at the microscopic mechanical level in terms of these operators (e.g., Refs. [31] and [32]).

On the basis of the construction of the nonequilibrium statistical operator [13,14], and taking into account the noted above fact that a complete description of the nonequilibrium state of the system follows from the knowledge of the single- and two-particle density operators (or equivalently the associated reduced density matrices) which in classical mechanics are

$$\widehat{n}_1(\mathbf{r},\mathbf{p}) = \sum_{j=1}^{N} \delta(\mathbf{r}-\mathbf{r}_j)\delta(\mathbf{p}-\mathbf{p}_j), \tag{1}$$

$$\widehat{n}_2(\mathbf{r},\mathbf{p};\mathbf{r}',\mathbf{p}') = \sum_{j\neq k=1}^{N} \delta(\mathbf{r}-\mathbf{r}_j)\delta(\mathbf{p}-\mathbf{p}_j) \times\delta(\mathbf{r}'-\mathbf{r}_k)\delta(\mathbf{p}'-\mathbf{p}_k)\,, \tag{2}$$

where $\mathbf{r}_j$, $\mathbf{p}_j$ are the coordinate and momentum of the jth particle, and $\mathbf{r}$, $\mathbf{p}$ are called field variables, the most complete nonequilibrium statistical distribution [4,13–17] is the one built in terms of the auxiliary statistical operator

$$\bar{\mathcal{R}}(t,0) = \bar{\rho}(t,0)\rho_R, \tag{3}$$

where $\bar{\rho}$ refers to the system of N particles of mass m, and ρ_R is the one associated to a thermal bath of N_R particles of mass M taken in equilibrium at temperature T_0. The first one is given by

$$\bar{\rho}(t,0) = \exp\Big\{ -\phi(t) - \int d^3r d^3p\, F_1(\mathbf{r},\mathbf{p};t)\hat{n}_1(\mathbf{r},\mathbf{p}) - \int d^3r d^3p \int d^3r' d^3p'\, F_2(\mathbf{r},\mathbf{p},\mathbf{r}',\mathbf{p}';t) \times\hat{n}_2(\mathbf{r},\mathbf{p},\mathbf{r}',\mathbf{p}')\Big\}. \tag{4}$$

Hence, $\bar{\rho}(t,0)$ depends on the variables of the system of interest and ρ_R on the variables of the thermal bath; both distributions are taken as normalized, as it should, with $\phi(t)$ ensuring the normalization of $\bar{\rho}$, that is,

$$\phi(t) = \int d\Gamma\, \exp\Big\{ - \int d^3r d^3p\, F_1(\mathbf{r},\mathbf{p};t)\hat{n}_1(\mathbf{r},\mathbf{p}) - \int d^3r d^3p \int d^3r' d^3p'\, F_2(\mathbf{r},\mathbf{p},\mathbf{r}',\mathbf{p}';t) \times\hat{n}_2(\mathbf{r},\mathbf{p},\mathbf{r}',\mathbf{p}')\Big\}, \tag{5}$$

and F_1 and F_2 are the nonequilibrium thermodynamic variables conjugated to $\hat{n}_1$ and $\hat{n}_2$ meaning that

$$\frac{\delta \ln \overline{Z}(t)}{\delta F_1(\mathbf{r},\mathbf{p};t)} = -\mathrm{Tr}\{\widehat{n}_1(\mathbf{r},\mathbf{p})\bar{\rho}(t,0)\}, \tag{6}$$

$$\frac{\delta \ln \overline{Z}(t)}{\delta F_2(\mathbf{r},\mathbf{p},\mathbf{r}',\mathbf{p}';t)} = -\mathrm{Tr}\{\widehat{n}_2(\mathbf{r},\mathbf{p};\mathbf{r}',\mathbf{p}')\bar{\rho}(t,0)\}, \tag{7}$$

where $\ln \overline{Z}(t) = \phi(t)$ with $\overline{Z}(t)$ playing the role of a nonequilibrium partition function and δ stands for functional derivative, in complete analogy with the equilibrium case. Moreover, we introduce $\mathrm{Tr} \equiv \int d\Gamma$, where $d\Gamma$ is the element of volume in the phase space of the system, and for simplicity we have neglected to indicate the dependence on Γ of $\hat{n}_1$, $\hat{n}_2$, $\bar{\rho}$, $\bar{\mathcal{R}}$, and that ρ_R depends on the phase point Γ_R in the phase space of the bath.

We stress that $\bar{\rho}$ of Eq. (4) is not the statistical operator of the nonequilibrium system, but an auxiliary one—called the "instantaneously frozen quasiequilibrium statistical operator"—that allows the proper nonequilibrium statistical operator to be built, which needs to include *historicity and irreversibility* not present in $\bar{\rho}$, hence it does not account for dissipative processes, and besides it does not provide correct average values in the calculation of transport coefficients and response functions.

We recall that the nonequilibrium statistical operator is given by [4,13–17]

$$\mathcal{R}_\varepsilon(t) = \exp\left\{ \ln \bar{\rho}(t,0) - \int_{-\infty}^{t} dt' e^{\varepsilon(t'-t)} \frac{d}{dt'} \ln \bar{\rho}(t',t'-t) \right\} \times \rho_R \tag{8}$$

with $\bar{\rho}(t,0)$ of Eq. (4), and where

$$\bar{\rho}(t',t'-t) = \exp\{i(t-t')\mathcal{L}\}\bar{\rho}(t',0), \tag{9}$$

is the auxiliary operator carrying on the mechanical evolution of the system under Hamiltonian $\hat{H}$ ($\mathcal{L}$ is the Liouvillian operator of the system meaning $i\mathcal{L}\hat{A} = \{\hat{A},\hat{H}\}$). The system's Hamiltonian is separated out into two terms, namely,

$$\hat{H} = \hat{H}_0 + \hat{H}', \tag{10}$$

where $\hat{H}_0$ is the kinetic energy operator and

$$\hat{H}' = \hat{H}_1 + \hat{W} + \hat{H}_P \tag{11}$$

contains the internal interactions energy operator $\hat{H}_1$, while $\hat{W}$ accounts for the interaction of the system with the thermal bath, and $\hat{H}_P$ is the energy operator associated to the coupling of the system with external pumping sources. Finally, ε is an infinitesimal positive real number which is taken going to zero after the traces in the calculation of averages have been performed (it is present in a kernel that introduces irreversibility in the calculations, in a Krylov-Bogoliubov sense [13–15]). We stress that the second contribution in the exponent in Eq. (8) accounts for historicity and irreversible evolution from the initial time (taken in the remote past, $t_0 \to -\infty$, implying in adiabatic coupling of correlations (see for example Ref. [13]), or alternatively, can be seen as the adiabatic coupling of the interactions responsible for relaxation processes [33]). Moreover we notice that the time derivative in Eq. (8) takes care of the change in time of the thermodynamic state of the system (the first term in the argument, i.e., t') and of the microscopic mechanical evolution [second term in the argument, i.e., $t'-t$, see Eq. (9)], and that the initial value condition is $\varrho_\varepsilon(t_0) = \bar{\rho}(t_0,0)$ for $t_0 \to -\infty$.

The nonequilibrium thermodynamic space of states [34] associated with the basic dynamic variables $\hat{n}_1$ and $\hat{n}_2$ is composed by the one-particle and two-particle distribution functions

$$f_1(\mathbf{r},\mathbf{p};t) = \mathrm{Tr}\{\widehat{n}_1(\mathbf{r},\mathbf{p})\varrho_\varepsilon(t)\} = \mathrm{Tr}\{\widehat{n}_1(\mathbf{r},\mathbf{p})\overline{\rho}(t,0)\}, \tag{12}$$

$$\begin{aligned} f_2(\mathbf{r},\mathbf{p},\mathbf{r}',\mathbf{p}';t) &= \mathrm{Tr}\{\widehat{n}_2(\mathbf{r},\mathbf{p},\mathbf{r}',\mathbf{p}')\varrho_\varepsilon(t)\} \\ &= \mathrm{Tr}\{\widehat{n}_2(\mathbf{r},\mathbf{p},\mathbf{r}',\mathbf{p}')\overline{\rho}(t,0)\}, \end{aligned} \tag{13}$$

where we indicate that for the basic variables, and only for them, the average with the statistical operator ϱ_ε is equal to the one taken with the auxiliary operator $\overline{\rho}$ [13–15]. The trace operation Tr is in this classical approach to be understood as an integration over phase space; $\hat{n}_1$ and $\hat{n}_2$ are functions on phase space and $\overline{\rho}$ and ϱ_ε functionals of these two. The knowledge of the two distribution functions f_1 and f_2 allows us to determine the value and evolution of any observable of the system as well as of response functions and transport coefficients.

The knowledge of $f_1(\mathbf{r},\mathbf{p};t)$ implies complete information about the actual distribution of particles, and therefore of the physical properties of the system. Alternatively, knowing all the moments of the distribution allows us to have a complete knowledge of its characteristics. A knowledge of some moments is not sufficient to determine the distribution completely; it implies in only possessing partial knowledge of the characteristics of this distribution [35]. Grad noticed that the question of the general solutions of the standard Boltzmann equation can be tackled along two distinct lines. One is to attempt to solve the Boltzmann equation for the distribution f_1 itself in specific problems. The other is to obtain new phenomenological equations in an approach initiated by Maxwell [36] and continued by Grad [37,38] (it was called Grad's moments procedure [39]). These moments produce quantities with a clear physical meaning, namely, the densities of particles and of energy and the fluxes of particles of first and second order in a restricted 14-moments approach.

In brief, the rth-order moment is the flux of order r,

$$\mathbf{I}_s^{[r]}(\mathbf{r},t) = \int d^3p\, u_s^{[r]}(\mathbf{p}) f_1(\mathbf{r},\mathbf{p};t), \tag{14}$$

where $u_s^{[r]}$ is the r-rank tensor, $s \equiv n$ for particle motion, and $s \equiv h$ for energy motion,

$$\begin{aligned} u_n^{[r]}(\mathbf{p}) &= \left[\frac{\mathbf{p}}{m} \ldots (r \text{ times}) \ldots \frac{\mathbf{p}}{m}\right], \\ u_h^{[r]}(\mathbf{p}) &= \frac{p^2}{2m} u_n^{[r]}(\mathbf{p}), \end{aligned} \tag{15}$$

that is, the tensorial product of r times the vector $\mathbf{p}/m$; for $s \equiv n$, $r = 0$ stands for the density, $r = 1$ for the vector flux (or current), $r = 2$ for the flux of the flux which is related to the pressure tensor field, and $r > 2$ for all the other higher-order fluxes. For $s \equiv h$, $r = 0$ stands for the density of energy and $r \geqslant 1$ for the respective fluxes. The density of energy $h(\mathbf{r},t)$ follows from the trace of $m\mathbf{I}_n^{[2]}$, namely

$$h(\mathbf{r},t) = \int d^3p\, \frac{p^2}{2m} f_1(\mathbf{r},\mathbf{p};t). \tag{16}$$

The set composed by $n(\mathbf{r},t)$, $\mathbf{I}_n(\mathbf{r},t)$, $\mathbf{I}_n^{[2]}(\mathbf{r},t)$, and $h(\mathbf{r},t)$ is the one corresponding to Grad's 14-moments approach. It may be noticed that our moments approach is in terms of the mechanical quantities in a Galilean reference frame. The one of Grad is in a barycentric frame of reference with an admixture of mechanical and hydrothermodynamic variables. Finally, the hydrodynamic equations are

$$\frac{\partial}{\partial t}\mathbf{I}_s^{[r]}(\mathbf{r},t) = \int d^3p\, u_s^{[r]}(\mathbf{p})\frac{\partial}{\partial t} f_1(\mathbf{r},\mathbf{p};t), \tag{17}$$

with $r = 0,1,2,\ldots$, and where is to be introduced Eq. (27) shown below. Equations (17) consist of an enormous set of coupled nonlinear integrodifferential equations. Evidently, it can be handled only in a contracted version, introducing the hydrodynamics of order 0, 1, 2, etc...., thus classified according to the last flux that is retained in the contraction of the description. Criteria for deciding the order of the contraction must be established (see Ref. [40]). Hydrodynamics of order 0 leads for the density to satisfy Fick's standard diffusion equation, the one of order 1 to Maxwell-Cattaneo equation, and the other orders to generalized Burnett and super-Burnett-like equations.

To proceed further, and give a clear illustration of the functioning of the theory, we consider, as noticed, the case of a solution of N particles of mass m (the solute) in a fluid (the solvent) of N_R particles of mass M. The former is subjected to external forces—driving it out of equilibrium—and the latter (the thermal bath) is taken in a steady state of constant equilibrium with an external reservoir at temperature T_0. An analogous case, but at the quantum mechanical level, is the one of carriers embedded in the ionic lattice in doped or photoinjected semiconductors (see for example Refs. [41–48]).

We write for the Hamiltonian

$$\hat{H} = \hat{H}_S + \hat{H}_R + \hat{W} + \hat{H}_P, \tag{18}$$

where the first term on the right,

$$\hat{H}_S = \sum_{j=1}^{N}\frac{p_j^2}{2m} + \frac{1}{2}\sum_{j\neq k}^{N} V(|\mathbf{r}_j - \mathbf{r}_k|), \tag{19}$$

is the Hamiltonian of the particles in the solute, consisting of their kinetic energy and their pair interaction via a central force potential; the second term is

$$\hat{H}_R = \sum_{\mu=1}^{N_R}\frac{P_\mu^2}{2M} + \frac{1}{2}\sum_{\mu\neq\nu=1}^{N_R}\Phi_R(|\mathbf{R}_\mu - \mathbf{R}_\nu|), \tag{20}$$

which is the Hamiltonian of the particles in the solvent, acting as a thermal bath, consisting of their kinetic energy plus their pair interaction via a central force potential; moreover

$$\hat{W} = \sum_{j=1}^{N}\sum_{\mu=1}^{N_R} w(|\mathbf{r}_j - \mathbf{R}_\mu|) \tag{21}$$

is the interaction Hamiltonian of the particles with the thermal bath, and $H_P = \sum_i V_{\text{ext}}(\mathbf{r}_i,\mathbf{p}_i,t)$ is the Hamiltonian associated with the external force acting on the particles of the system.

Under the stated condition that the bath is in constant thermal equilibrium with an external reservoir at temperature T_0, its macroscopic state is characterized by the canonical distribution

$$\rho_R = Z^{-1}e^{-\beta_0\hat{H}_R}, \tag{22}$$

where $\beta_0 = [k_B T_0]^{-1}$ and Z is the corresponding partition function. The auxiliary nonequilibrium statistical operator of the whole system is the one of Eqs. (3) and (4). But, for simplicity, considering a dilute solution (large distance in average between the particles) or that the potential V is screened (e.g., molecules in an ionized saline solvent, e.g., [49]), we can disregard the influence of the two particle potential, and then ignore $\widehat{n}_2$, that is, taking $F_2 = 0$ in Eq. (4) retaining only $\widehat{n}_1$. In that case, we choose the single-particle reduced density, $\widehat{n}_1(\mathbf{r},\mathbf{p}\mid\Gamma)$, as the only relevant dynamical variable required. Hence, $\overline{\rho}(t,0)$, of Eq. (4), the auxiliary nonequilibrium statistical operator for the particles embedded in the bath, is

$$\begin{aligned}\overline{\varrho}(t,0) &= \exp\left\{-\phi(t) - \int d^3r d^3p F_1(\mathbf{r},\mathbf{p};t)\widehat{n}_1(\mathbf{r},\mathbf{p})\right\}\\ &= \prod_{j=1}^{N}\overline{\rho}_j(t,0),\end{aligned} \tag{23}$$

where

$$\begin{aligned}\overline{\rho}_j(t,0) = \exp\bigg\{ &-\phi_j(t) - \int d^3r d^3p F_1(\mathbf{r},\mathbf{p};t)\delta(\mathbf{r}-\mathbf{r}_j)\\ &\times\delta(\mathbf{p}-\mathbf{p}_j)\bigg\}\end{aligned} \tag{24}$$

is a probability distribution for an individual particle, with $\phi(t)$ and $\phi_j(t)$ ensuring the normalization conditions of $\overline{\rho}$ and $\overline{\rho}_j$.

The nonequilibrium equation of state [34], that is, the one relating the variables $f_1(\mathbf{r},\mathbf{p};t)$ and $F_1(\mathbf{r},\mathbf{p};t)$, is

$$f_1(\mathbf{r},\mathbf{p};t) = \text{Tr}\{\widehat{n}_1(\mathbf{r},\mathbf{p})\overline{\rho}(t,0)\} = \exp\{-F_1(\mathbf{r},\mathbf{p};t)\}, \tag{25}$$

or

$$F_1(\mathbf{r},\mathbf{p};t) = -\ln f_1(\mathbf{r},\mathbf{p};t). \tag{26}$$

On the other hand, the evolution equation for f_1 following from the NESEF-based kinetic theory, derived as shown in Ref. [30], is the generalized kinetic equation

$$\begin{aligned}\frac{\partial}{\partial t}f_1(\mathbf{r},\mathbf{p};t) &+ \frac{\mathbf{P}(\mathbf{r},\mathbf{p};t)}{m}\cdot\nabla f_1(\mathbf{r},\mathbf{p};t)\\ &+\mathbf{F}(\mathbf{r},\mathbf{p};t)\cdot\nabla_{\mathbf{p}}f_1(\mathbf{r},\mathbf{p};t) - B(\mathbf{p})f_1(\mathbf{r},\mathbf{p};t)\\ &- A_2^{[2]}(\mathbf{p})\odot[\nabla_{\mathbf{p}}\nabla]f_1(\mathbf{r},\mathbf{p};t)\\ &- B_2^{[2]}(\mathbf{p})\odot[\nabla_{\mathbf{p}}\nabla_{\mathbf{p}}]f_1(\mathbf{r},\mathbf{p};t) = 0,\end{aligned} \tag{27}$$

obtained in the Markovian approximation [13,15,50,51], where

$$\frac{\mathbf{P}(\mathbf{r},\mathbf{p};t)}{m} = \frac{\mathbf{p}}{m} - \mathbf{A}_1(\mathbf{p}), \tag{28}$$

$$\mathbf{F}(\mathbf{r},\mathbf{p};t) = -\nabla V_{\text{ext}}(\mathbf{r},\mathbf{p};t) - \mathbf{B}_1(\mathbf{p}) - \mathbf{F}_{\text{NL}}(\mathbf{r};t), \tag{29}$$

with the explicit expressions, for the vectorial quantities $\mathbf{A}_1(\mathbf{p})$, $\mathbf{B}_1(\mathbf{p})$, $\mathbf{F}_{\text{NL}}(\mathbf{r};t)$, the second-rank tensors $A_2^{[2]}(\mathbf{p})$, $B_2^{[2]}(\mathbf{p})$, and the scalar $B(\mathbf{p})$, together with a description of the physical meaning of the several contributions, given in Ref. [30]. We also wrote the symbol $\odot$ for full contraction of tensors.

The distribution $f_1(\mathbf{r},\mathbf{p};t)$ that follows solving Eq. (27) provides a complete information about the actual distribution of particles, and therefore of the physical properties of the system. As previously noticed, if one knows all the moments of the distribution we do have a knowledge of its characteristics. This is related to Tchebychef's procedure for obtaining characteristics of a probability distribution when we do possess the moments of successive order, e.g., [52]. On this Grad noticed that the question of the general solutions of the standard Boltzmann kinetic equation can be tackled obtaining new phenomenological equations which generalize the usual (classical-Onsagerian) fluid dynamical equations. The object is to show the transition from the Boltzmann equation in which a state is described by $f_1(\mathbf{r},\mathbf{p};t)$ to the conventional fluid description in which a state is given by the density $n(\mathbf{r},t)$, the velocity field $\mathbf{v}(\mathbf{r},t)$, and the stress tensor $T^{[2]}(\mathbf{r},t)$, in a sufficient generality to cover a broad class of problems. This approach was initiated by Maxwell [36] and continued by Grad [37] (it was called Grad's 14-moments procedure) [39].

We perform here an extensive generalization of the moments procedure, consisting of introducing the full set of moments of $f_1(\mathbf{r},\mathbf{p};t)$, of Eq. (27), in the variable $\mathbf{p}$. These moments produce quantities with a clear physical meaning, namely, the densities of particles and of energy and their fluxes of all orders: the two vectorial fluxes, or currents, the tensorial fluxes, beginning with the second-order one which is the flux of the first-order flux (the current of particles) which is related to the pressure tensor, and all the other higher-order fluxes. In that way we obtain a quite generalized *mesoscopic hydrodynamics* coupled to a *nonequilibrium thermodynamics*, all together in the kinetic approach provided by NESEF, as described in the next section.

III. MESOSCOPIC HYDRO-THERMODYNAMICS IN NESEF

Let us introduce, in the variable $\mathbf{p}$, the moments of the distribution $f_1(\mathbf{r},\mathbf{p};t)$, namely

$$n(\mathbf{r},t) = \int d^3p\, f_1(\mathbf{r},\mathbf{p};t), \tag{30}$$

which is the density of particles;

$$\mathbf{I}_n(\mathbf{r},t) = \int d^3p\, \mathbf{u}(\mathbf{p}) f_1(\mathbf{r},\mathbf{p};t), \tag{31}$$

where

$$\mathbf{u}(\mathbf{p}) = \mathbf{p}/m, \tag{32}$$

with $\mathbf{I}_n$ being the flux (current) of particles;

$$I_n^{[2]}(\mathbf{r},t) = \int d^3p\, \mathbf{u}^{[2]}(\mathbf{p}) f_1(\mathbf{r},\mathbf{p};t), \tag{33}$$

where $\mathbf{u}^{[2]} = [\mathbf{uu}]$ is the tensorial product of vectors $\mathbf{u}$, with $I_n^{[2]}$ being the second-order flux (or flux of the first flux), a rank-2 tensor, which multiplied by the mass is related to the pressure tensor, and

$$I_n^{[l]}(\mathbf{r},t) = \int d^3p\, \mathbf{u}^{[l]}(\mathbf{p}) f_1(\mathbf{r},\mathbf{p};t) \tag{34}$$

are the higher-order fluxes of order $l \geqslant 3$ [the previous three of Eqs. (30), (31), and (33) are those for $l = 0$, 1, and 2 respectively), where $u^{[l]}$ is the l-rank tensor consisting of the tensorial product of l vectors $\mathbf{u}$ of Eq. (32), that is,

$$\mathbf{u}^{[l]}(\mathbf{p}) = \left[\frac{\mathbf{p}}{m}\frac{\mathbf{p}}{m} \ldots (l \text{ times}) \ldots \frac{\mathbf{p}}{m}\right]. \tag{35}$$

We do have what can be called the *family of hydrodynamical variables describing the material motion*, i.e., the set

$$\left\{n(\mathbf{r},t), \mathbf{I}_n(\mathbf{r},t), \{I_n^{[l]}(\mathbf{r},t)\}\right\}, \tag{36}$$

with $l = 2,3,\ldots$.

On the other hand, we have the *family of hydrodynamical variables describing the thermal motion*, consisting of

$$h(\mathbf{r},t) = \int d^3p\, \frac{p^2}{2m} f_1(\mathbf{r},\mathbf{p};t), \tag{37}$$

$$\mathbf{I}_h(\mathbf{r},t) = \int d^3p \frac{p^2}{2m}\frac{\mathbf{p}}{m} f_1(\mathbf{r},\mathbf{p};t), \tag{38}$$

$$I_h^{[l]}(\mathbf{r},t) = \int d^3p \frac{p^2}{2m} \mathbf{u}^{[l]}(\mathbf{p}) f_1(\mathbf{r},\mathbf{p};t), \tag{39}$$

with $l = 2, 3, \ldots$; that is, in compact form those in the set

$$\left\{h(\mathbf{r},t), \mathbf{I}_h(\mathbf{r},t), \left\{I_h^{[l]}(\mathbf{r},t)\right\}\right\}, \tag{40}$$

which are, respectively, the density of energy, its first vectorial flux (current), and the higher-order tensorial fluxes. It can be noticed that in this case of a parabolic type energy-momentum dispersion relation, $E(p) = p^2/2m$, the set of Eq. (40) is encompassed in the previous one: in fact

$$h(\mathbf{r},t) = \frac{m}{2}\mathrm{Tr}\left\{I_n^{[2]}(\mathbf{r},t)\right\}, \tag{41}$$

$$\mathbf{I}_h(\mathbf{r},t) = \frac{m}{2}\mathrm{Tr}_2\left\{I_n^{[3]}(\mathbf{r},t)\right\}, \tag{42}$$

where Tr_2 stands for the contraction of two indexes, and, in general

$$I_h^{[l]}(\mathbf{r},t) = \frac{m}{2}\mathrm{Tr}_2\left\{I_n^{[l+2]}(\mathbf{r},t)\right\}, \tag{43}$$

for all the other higher-order fluxes of energy. Hence, any flux of energy of order l is contained in the flux of matter of order $l+2$. In what follows we concentrate the attention on the study of the hydrodynamic motion of the particles, with heat transport to be dealt with in a future communication in this series.

IV. MHT EVOLUTION EQUATIONS IN NESEF

We proceed now to the derivation of the MHT equations, that is, the equations of evolutions for the basic macrovariables of the family of material motion, i.e., those in the set of Eq. (36).

Let us consider the flux of order l ($l = 0,1,2,\ldots$); its evolution equation is

$$\frac{\partial}{\partial t} I_n^{[l]}(\mathbf{r},t) = \int d^3p\, u^{[l]}(\mathbf{p}) \frac{\partial}{\partial t} f_1(\mathbf{r},\mathbf{p};t). \tag{44}$$

Using Eq. (27), but excluding a dependence on $\mathbf{p}$ of the external force, after lengthy but straightforward calculations we arrive at the general set of coupled equations for the density, $l = 0$, the current, $l = 1$, and all the other higher-order fluxes, $l \geqslant 2$, given by

$$\frac{\partial}{\partial t} I_n^{[l]}(\mathbf{r},t) + \nabla \cdot I_n^{[l+1]}(\mathbf{r},t) = \frac{1}{m} \sum_{s=1}^{l} \wp(1,s)[\boldsymbol{\mathcal{F}}_{\text{ext}}(\mathbf{r},t) I_n^{[l-1]}(\mathbf{r},t)] + J_\tau^{[l]}(\mathbf{r},t) + J_L^{[l]}(\mathbf{r},t) + J_{\text{NL}}^{[l]}(\mathbf{r},t), \tag{45}$$

where $\wp(1,s)$ means that we must take a permutation of the first free index (1) with the sth ($s = 1,2,3,\ldots,l$) free index of the Cartesian tensor $[\boldsymbol{\mathcal{F}}_{\text{ext}}(\mathbf{r},t) I_n^{[l-1]}(\mathbf{r},t)]$, when written in the indicial notation. Observe that the number of terms in the sum is given by the number of all permutations of l symbols in which $l - 1$ is repeated. All this ensures the correct symmetry of this contribution, that is, a fully symmetrical tensor of order l.

The several terms on the right of Eq. (45) are

$$\boldsymbol{\mathcal{F}}_{\text{ext}}(\mathbf{r},t) = -\nabla V_{\text{ext}}(\mathbf{r};t), \tag{46}$$

that is the applied external force, created by the action of the potential V_{ext}, and the terms with $\mathbf{A}_1(\mathbf{p})$, $\mathbf{B}_1(\mathbf{p})$, and $\mathbf{F}_{\text{NL}}(\mathbf{r};t)$ present in Eqs. (28) and (29) are encompassed in $J_\tau^{[l]}$, $J_L^{[l]}$, and $J_{\text{NL}}^{[l]}$, which are described in Appendix A: they have cumbersome expressions which we do not include in the main text to facilitate the reading of the paper.

According to the results presented in Appendix A we can see that the expressions for $J_\tau^{[l]}$ and $J_L^{[l]}$ are linear in the hydrodynamic basic variables of the set of Eq. (36) with tensorial coefficients $\Lambda^{[r]}$. The first one contains contributions of a relaxation character, and the second involves local couplings with the different fluxes. On the other hand $J_{\text{NL}}^{[l]}$, nonlinear (bilinear) in the fluxes, accounts for nonlocal correlations involving all of them. Next, we reorganize these expressions evidencing the contributions that contain the neighboring fluxes to the one of order l, namely $I_n^{[l-1]}(\mathbf{r},t)$ and $I_n^{[l+1]}(\mathbf{r},t)$, that is, arising out of the terms with $k = 0$ and $k = 1$ in the sum over k in Eqs. (A11) and (A12), to rewrite Eq. (45) in the form

$$\begin{aligned}\frac{\partial}{\partial t} I_n^{[l]}(\mathbf{r},t) &+ \nabla \cdot I_n^{[l+1]}(\mathbf{r},t) \\ &= \frac{1}{m} \sum_{s=1}^{l} \wp(1,s)\big[\boldsymbol{\mathcal{F}}_{\text{ext}}(\mathbf{r},t) I_n^{[l-1]}(\mathbf{r},t)\big] - \theta_l^{-1} I_n^{[l]}(\mathbf{r},t) \\ &\quad + a_{L0} \sum_{s=1}^{l} \wp(1,s)\big[\nabla I_n^{[l-1]}(\mathbf{r},t)\big] + 2l a_{L1} \nabla \cdot I_n^{[l+1]}(\mathbf{r},t) \\ &\quad + b_{\tau 0}\big\{\widehat{\wp}_l\big[\mathbf{1}^{[2]} I_n^{[l-2]}(\mathbf{r},t)\big]\big\} + J_{\text{NL}}^{[l]}(\mathbf{r},t) + S_n^{[l]}(\mathbf{r},t).\end{aligned} \tag{47}$$

The last term on the right of Eq. (47) is given by

$$\begin{aligned}S_n^{[l]}(\mathbf{r},t) = {}& b_{\tau 1} \frac{2}{m} \big\{\widehat{\wp}_l\big[\mathbf{1}^{[2]} I_h^{[l-2]}(\mathbf{r},t)\big]\big\} + 3l a_{\tau 1} \frac{2}{m} I_h^{[l]}(\mathbf{r},t) \\ & + a_{L1} \frac{2}{m} \sum_{s=1}^{l} \wp(1,s)\big[\nabla I_h^{[l-1]}(\mathbf{r},t)\big] + R_n^{[l]}(\mathbf{r},t),\end{aligned} \tag{48}$$

where $R_n^{[l]}(\mathbf{r},t)$, given in Appendix A, contains the contributions of the fluxes of order higher than $l + 2$, and the kinetic coefficients $a_{\tau 1}$, a_{L0}, a_{L1}, $b_{\tau 0}$, $b_{\tau 1}$ are given in Appendix B. The first three contributions on the right of Eq. (48) are associated with the fluxes of energy of orders $l - 2$, $l - 1$, and l, terms that can be considered consisting of thermostriction effects and which, then, couple these equations with the set of kinetic equations describing the motion of energy, i.e., the hydrodynamical variables of the set of Eq. (40). However it can be noticed, as already mentioned, that the fluxes of energy can be given in terms of those of particles, namely, $I_h^{[l]} = (m/2) Tr_2\{I_n^{[l+2]}\}$, [cf. Eqs. (41)–(43)]. Moreover,

$$\theta_l^{-1} = l[|a_{\tau 0}| + (l-1)|b_{\tau 1}|], \tag{49}$$

with θ_l playing the role of a Maxwell-characteristic time associated to the lth flux.

We stress that $l = 0$ corresponds to the density $n(\mathbf{r},t)$, $l = 1$ to the first flux (current) $\mathbf{I}_n(\mathbf{r},t)$, $l = 2$ to the second flux $I_n^{[2]}(\mathbf{r},t)$ which, as already stated, multiplied by the mass m is related to the pressure tensor $P^{[2]}(\mathbf{r},t)$], and $l > 2$ to the other higher-order fluxes. Hence, Eq. (47) represents the coupled set of evolution equations involving the density and all its fluxes in its most general form. It must be noticed that it is linear in the basic variables; no approximation has been introduced. Nonlinearities should arise out of the interparticle interaction which we have disregarded in the present paper (the case of a dilute solution). However, as already noticed, such a set of equations is intractable, and, of course, we need to look in each case at how to find the best description using the smallest possible number of variables, in other words to introduce an appropriate—for each case—contraction of description: *this contraction implies retaining the information considered as relevant for the problem in hand, and to disregard nonrelevant information* [53].

Elsewhere [40] we have discussed the question of the contraction of description (reduction of the dimensions of the nonequilibrium thermodynamic space of states). As shown in Ref. [40], a criterion for justifying the different levels of contraction can be derived: It depends on the range of wavelengths and frequencies which are relevant for the characterization, in terms of normal modes, of the hydrothermodynamic motion in the nonequilibrium open system. Maxwell times have a particular relevance and we proceed to analyze them.

V. HIERARCHY OF MAXWELL CHARACTERISTIC TIMES

Let us now analyze Maxwell characteristics times of Eq. (49) to show that they follow a hierarchy of values. First we note that, using Eq. (B7) in Eq. (49) and the definition in Eq. (B1) we can write

$$\theta_l^{-1} = l\left[1 + \frac{1}{5}\frac{M}{m+M}(l-1)\right]\theta_1^{-1}, \tag{50}$$

which tells us that any characteristic time for $l \geqslant 2$ is proportional to the one of $l = 1$, that is the one for the first flux which multiplied by the mass m is the linear momentum density and then all are proportional to the linear momentum relaxation time. On the other hand we do have that

$$\frac{\theta_{l+1}}{\theta_l} = \frac{l}{l+1}\,\frac{5(1+x)+l-1}{5(1+x)+l}, \tag{51}$$

for $l = 1,2,3,\dots$ and where $x = m/M$, and then the ordering sequence

$$\theta_1 > \theta_2 > \theta_3 > \cdots > \theta_l > \theta_{l+1} > \cdots \tag{52}$$

is verified, and we can see that $\theta_l \to 0$ as $l \to \infty$. Moreover according to Eq. (50) it follows that

$$\theta_l = \frac{5(1+x)}{l[5(1+x)+(l-1)]}\theta_1. \tag{53}$$

Comparing with the second flux ($l = 2$), the one related to the pressure tensor, it follows that for the Brownian particles ($x \gg 1$) $\theta_2 \simeq \theta_1/2$ and for the Lorentz particles ($x \ll 1$) $\theta_2 \simeq 5\theta_1/12$. A comparison with the third flux leads to the results that $\theta_3 \simeq \theta_1/3$ and $\theta_3 \simeq 5\theta_1/21$ for the Brownian and Lorentz particles respectively. For any l we do have approximately

(1) for the Brownian particle ($m/M \gg 1$)

$$\theta_l \simeq \theta_1/l, \tag{54}$$

(2) for the Lorentz particle ($m/M \ll 1$)

$$\theta_l \simeq [5/(4+l)l]\theta_1, \tag{55}$$

or $\theta_l \simeq 5\theta_1/l^2$ for large l.

Moreover according to Eq. (51) as the order of flux largely increases, its characteristic Maxwell time approaches zero, and $\theta_{l+1}/\theta_l \simeq 1$, with both being practically null. In Fig. 1 is displayed the ratio of characteristic Maxwell times, for flux of order ℓ, with the momentum relaxation time, as a function of m/M, i.e., the quotient of the masses m of the particles in the system and M of those in the thermal bath.

It can be noticed that in Fig. 1 the quotient of masses has little effect on θ_l/θ_1 but it varies significantly with the order ℓ of the flux and plays a particular relevance in the criteria for establishing the contraction of description discussed next.

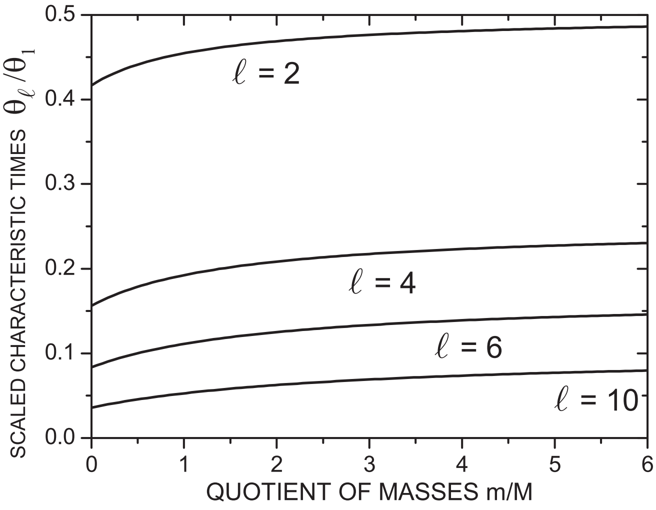

FIG. 1. The quotient between several Maxwell characteristic times and the one of the first flux as a function of m/M.

VI. CRITERION OF CONTRACTED DESCRIPTION AND AN APPLICATION

Returning to the question of the contracted description it can be shown [40] that a truncation criterion can be derived, which *rests on the characteristics of the hydrodynamic motion that develops under the given experimental procedure.*

Since inclusion of higher and higher-order fluxes implies describing a motion involving increasing Knudsen numbers per hydrodynamic mode (that is governed by smaller and smaller wavelengths—larger and larger wave numbers—accompanied by higher and higher frequencies), in a qualitative manner, we can say that, as a general “thumb rule,” the criterion indicates that *a more and more restricted contraction can be used when the prevalent wavelengths in the motion are larger and larger.* Therefore, in simpler words, when the motion becomes more and more smooth in space and time, the more reduced can be the dimension of the basic macrovariables space to be used for the description of the nonequilibrium thermodynamic state of the system.

As shown elsewhere [40], we can conjecture a general contraction criterion, namely, a contraction of order r (meaning keeping the densities and their fluxes up to order r) can be introduced, once we can show that in the spectrum of wavelengths, which characterize the motion, predominate those larger than a “frontier” one, $\lambda^2_{(r,r+1)} = v^2\theta_r\theta_{r+1}$, where v is of the order of the thermal velocity and θ_r and θ_{r+1} are the corresponding Maxwell times. We shall try to illustrate the matter using a contraction of order 2.

Let us first write down the equations of evolution [whose general expression is given in Eq. (47) corresponding to the density and its fluxes of all order] for $\ell = 0$: the density, for $\ell = 1$: the first flux of the density, $\ell = 2$: the flux of the first flux which multiplied by m is related to the pressure tensor field, and $\ell = 3$: the flux of the pressure. We do have, respectively,

$$\frac{\partial}{\partial t}n(\mathbf{r},t) + \nabla \cdot \mathbf{I}_n(\mathbf{r},t) = 0, \tag{56}$$

$$\begin{aligned}\frac{\partial}{\partial t}\mathbf{I}_n(\mathbf{r},t) &+ \nabla \cdot I_n^{[2]}(\mathbf{r},t)\\ &= \frac{n(\mathbf{r},t)}{m}\mathcal{F}(\mathbf{r},t) - \theta_1^{-1}\mathbf{I}_n(\mathbf{r},t) + a_{L0}\nabla n(\mathbf{r},t)\\ &\quad + 2a_{L1}\nabla \cdot I_n^{[2]}(\mathbf{r},t) + \mathbf{S}_n(\mathbf{r},t),\end{aligned} \tag{57}$$

$$\begin{aligned}\frac{\partial}{\partial t}I_n^{[2]}(\mathbf{r},t) &+ \nabla \cdot I_n^{[3]}(\mathbf{r},t)\\ &= \frac{1}{m}\{[\mathcal{F}(\mathbf{r},t)\mathbf{I}_n(\mathbf{r},t)] + [\mathbf{I}_n(\mathbf{r},t)\mathcal{F}(\mathbf{r},t)]\}\\ &\quad - \theta_2^{-1}I_n^{[2]}(\mathbf{r},t) + a_{L0}\{\nabla\mathbf{I}_n(\mathbf{r},t) + [\nabla\mathbf{I}_n(\mathbf{r},t)]^{\mathrm{tr}}\}\\ &\quad + 4a_{L1}\nabla \cdot I_n^{[3]}(\mathbf{r},t) + b_{\tau 0}n(\mathbf{r},t)\mathbf{1}^{[2]} + S_n^{[2]}(\mathbf{r},t),\end{aligned} \tag{58}$$

$$\begin{aligned}\frac{\partial}{\partial t}I_n^{[3]}(\mathbf{r},t) &+ \nabla \cdot I_n^{[4]}(\mathbf{r},t)\\ &= \frac{1}{m}\sum_{s=1}^{3}\wp(1,s)\big[\mathcal{F}(\mathbf{r},t)I_n^{[2]}(\mathbf{r},t)\big] - \theta_3^{-1}I_n^{[3]}(\mathbf{r},t)\end{aligned}$$

$$+a_{L0}\sum_{s=1}^{3}\wp(1,s)\big[\nabla I_n^{[2]}(\mathbf{r},t)\big]+6a_{L1}\nabla\cdot I_n^{[4]}(\mathbf{r},t)$$
$$+b_{\tau0}\{\widehat{\wp}_3[\mathbf{1}^{[2]}\mathbf{I}_n(\mathbf{r},t)]\}+S_n^{[3]}(\mathbf{r},t), \tag{59}$$

where $\boldsymbol{\mathcal{F}}(\mathbf{r},t)$ and the expressions for $\mathbf{S}_n(\mathbf{r},t)$, $S_n^{[2]}(\mathbf{r},t)$, and $S_n^{[3]}(\mathbf{r},t)$ are given in Appendix C. The Maxwell times θ_1 and θ_2 are obtained from Eq. (49) respectively for $l = 1$, 2, and 3. Moreover, as noticed, if we multiply Eq. (58) by the mass m, we do have an equation for the pressure field tensor,

$$P^{[2]}(\mathbf{r},t)=mI_n^{[2]}(\mathbf{r},t), \tag{60}$$

composed of the hydrostatic contribution (the diagonal terms) and the shear stress (the nondiagonal terms) and the convective pressure. We also mention that taking into account Eq. (74) below relating $\mathbf{I}_n(\mathbf{r},t)$ with the barycentric velocity $\mathbf{v}(\mathbf{r},t)$, Eq. (57) can be transformed in an evolution equation for the latter to obtain a generalized Navier-Stokes equation (future publication).

Let us now, for illustration, consider the case when we can perform a truncation in a second order, that is, to consider as basic variables $n(\mathbf{r},t)$ its flux $\mathbf{I}_n(\mathbf{r},t)$ and the pressure tensor $mI_n^{[2]}(\mathbf{r},t)$. In this contracted description we consider Eqs. (56) and (57) but with the further restrictions of neglecting (1) the shear stress contribution, more precisely introducing the trace of the pressure tensor which is proportional to the energy density $h(\mathbf{r},t)$, that is,

$$\mathrm{Tr}\{P^{[2]}(\mathbf{r},t)\}=2h(\mathbf{r},t), \tag{61}$$

where convective pressure has been disconsidered, cf. Eq. (75) below; (2) the terms with coefficients a_L whose origin is in self-energy corrections, which simply would renormalize the kinetic coefficients; and (3) the terms $\mathbf{S}_n(\mathbf{r},t)$ and $S_n^{[2]}(\mathbf{r},t)$ which contain the energy density $h(\mathbf{r},t)$ and its flux $\mathbf{I}_h(\mathbf{r},t)$ thus disregarding thermostriction effects.

The evolution equations for the chosen hydrodynamic variables, $n(\mathbf{r},t)$, $\mathbf{I}_n(\mathbf{r},t)$, and $I_n^{[2]}(\mathbf{r},t)$, in the conditions stated above, take the form

$$\frac{\partial}{\partial t}n(\mathbf{r},t)+\nabla\cdot\mathbf{I}_n(\mathbf{r},t)=0, \tag{62}$$

$$\frac{\partial}{\partial t}\mathbf{I}_n(\mathbf{r},t)+\nabla\cdot I_n^{[2]}(\mathbf{r},t)=\frac{n(\mathbf{r},t)}{m}\boldsymbol{\mathcal{F}}(\mathbf{r},t)-\theta_1^{-1}\mathbf{I}_n(\mathbf{r},t), \tag{63}$$

$$\frac{\partial}{\partial t}I_n^{[2]}(\mathbf{r},t)+\nabla\cdot I_n^{[3]}(\mathbf{r},t)$$
$$=b_{\tau0}n(\mathbf{r},t)\mathbf{1}^{[2]}-\theta_2^{-1}I_n^{[2]}(\mathbf{r},t)$$
$$+\frac{1}{m}\{[\boldsymbol{\mathcal{F}}(\mathbf{r},t)\mathbf{I}_n(\mathbf{r},t)]+[\mathbf{I}_n(\mathbf{r},t)\boldsymbol{\mathcal{F}}(\mathbf{r},t)]\}. \tag{64}$$

Deriving in time Eq. (62) and, next, in the ensuing result inserting $\partial\mathbf{I}_n(\mathbf{r},t)/\partial t$, and using Eq. (63) we arrive at the hyperbolic (Maxwell-Cattaneo type) evolution equation for $n(\mathbf{r},t)$

$$\frac{\partial^2}{\partial t^2}n(\mathbf{r},t)+\frac{1}{\theta_1}\frac{\partial}{\partial t}n(\mathbf{r},t)$$
$$=\nabla\cdot\nabla\cdot I_n^{[2]}(\mathbf{r},t)-\nabla\cdot\left[\frac{n(\mathbf{r},t)}{m}\boldsymbol{\mathcal{F}}(\mathbf{r},t)\right]. \tag{65}$$

Furthermore, deriving in time this Eq. (65) and using Eq. (64) it follows that

$$\frac{\partial^3}{\partial t^3}n(\mathbf{r},t)+\left[\frac{1}{\theta_1}+\frac{1}{\theta_2}\right]\frac{\partial^2}{\partial t^2}n(\mathbf{r},t)+\frac{1}{\theta_1\theta_2}\frac{\partial}{\partial t}n(\mathbf{r},t)$$
$$=b_{\tau0}\nabla^2n(\mathbf{r},t)-\nabla\cdot\nabla\cdot\nabla\cdot I_n^{[3]}(\mathbf{r},t)$$
$$-\frac{1}{\theta_2}\nabla\cdot\left[\frac{n(\mathbf{r},t)}{m}\boldsymbol{\mathcal{F}}(\mathbf{r},t)\right]$$
$$+\frac{1}{m}\nabla\cdot\nabla\cdot\{[\boldsymbol{\mathcal{F}}(\mathbf{r},t)\mathbf{I}_n(\mathbf{r},t)]+[\mathbf{I}_n(\mathbf{r},t)\boldsymbol{\mathcal{F}}(\mathbf{r},t)]\}$$
$$-\frac{\partial}{\partial t}\nabla\cdot\left[\frac{n(\mathbf{r},t)}{m}\boldsymbol{\mathcal{F}}(\mathbf{r},t)\right]. \tag{66}$$

The divergence of the third-order flux, $\nabla\cdot I_n^{[3]}$, in terms of the basic variables, is evaluated on the basis of Eq. (64), the evolution equation for the second-order flux which, we recall, is related to the pressure tensor [cf. Eq. (60)]. For that purpose we consider conditions such that the pressure is changing slowly in time ($\theta_2\partial I_n^{[2]}/\partial t\ll I_n^{[2]}$ or $\omega\ \theta_2\ll1$ along the evolution), and then from Eq. (64) it follows that

$$\nabla\cdot I_n^{[3]}(\mathbf{r},t)=b_{\tau0}n(\mathbf{r},t)\mathbf{1}^{[2]}-\theta_2^{-1}I_n^{[2]}(\mathbf{r},t)$$
$$+\frac{1}{m}\{[\boldsymbol{\mathcal{F}}(\mathbf{r},t)\mathbf{I}_n(\mathbf{r},t)]+[\mathbf{I}_n(\mathbf{r},t)\boldsymbol{\mathcal{F}}(\mathbf{r},t)]\}, \tag{67}$$

and using this result in Eq. (66) we arrive at the equation

$$\frac{\partial^3}{\partial t^3}n(\mathbf{r},t)+\left[\frac{1}{\theta_1}+\frac{1}{\theta_2}\right]\frac{\partial^2}{\partial t^2}n(\mathbf{r},t)+\frac{1}{\theta_1\theta_2}\frac{\partial}{\partial t}n(\mathbf{r},t)$$
$$=\frac{1}{\theta_2}\nabla\cdot\nabla\cdot I_n^{[2]}(\mathbf{r},t)-\frac{1}{\theta_2}\nabla\cdot\left[\frac{n(\mathbf{r},t)}{m}\boldsymbol{\mathcal{F}}(\mathbf{r},t)\right]$$
$$-\frac{\partial}{\partial t}\nabla\cdot\left[\frac{n(\mathbf{r},t)}{m}\boldsymbol{\mathcal{F}}(\mathbf{r},t)\right]. \tag{68}$$

To close this Eq. (68) it is necessary to evaluate $I_n^{[2]}$ which, we recall, is given by

$$I_n^{[2]}(\mathbf{r},t)=\int d^3p\left[\frac{\mathbf{p}}{m}\frac{\mathbf{p}}{m}\right]f_1(\mathbf{r},\mathbf{p};t). \tag{69}$$

We resort now to the use of Eq. (25) and for $F_1(\mathbf{r},\mathbf{p},t)$ we use an expansion in variable $\mathbf{p}$, namely

$$F_1(\mathbf{r},\mathbf{p},t)$$
$$=F_{1n}(\mathbf{r},t)+\left.\frac{\partial F_1(\mathbf{r},\mathbf{p},t)}{\partial\mathbf{p}}\right|_0\cdot\mathbf{p}+\frac{1}{2}\left.\frac{\partial^2F_1(\mathbf{r},\mathbf{p},t)}{\partial p^2}\right|_0\frac{p^2}{2m}$$
$$+\frac{1}{2}\left.\frac{\partial^2F_1(\mathbf{r},\mathbf{p},t)}{\partial\mathbf{p}\partial\mathbf{p}}\right|_0\odot[\overset{\circ}{\mathbf{pp}}]+\cdots, \tag{70}$$

where lower-index 0 indicates that the derivative is taken at $\mathbf{p}=\mathbf{0}$, and $[\overset{\circ}{\mathbf{pp}}]$ is the traceless part of the tensor. We rewrite F_1 in the form

$$F_1(\mathbf{r},\mathbf{p},t)\simeq\varphi_n(\mathbf{r},t)+\mathbf{F}_n(\mathbf{r},t)\cdot\frac{\mathbf{p}}{m}+F_h(\mathbf{r},t)\frac{p^2}{2m}, \tag{71}$$

that is, keeping terms up to second order in $\mathbf{p}$. This is consistent with the contracted description we used, and of disregarding the shear stress, and where φ_n, $\mathbf{F}_n$ and F_h are the nonequilibrium thermodynamic variables conjugated to the density, the flux, and the trace of $I_n^{[2]}$ which is proportional to the energy. Moreover, introducing the alternative forms

$$\mathbf{F}_n(\mathbf{r},t) \equiv -m\beta(\mathbf{r},t)\mathbf{v}(\mathbf{r},t), \tag{72}$$

$$F_h(\mathbf{r},t) \equiv \beta(\mathbf{r},t), \tag{73}$$

it follows that

$$\mathbf{I}_n(\mathbf{r},t) = n(\mathbf{r},t)\mathbf{v}(\mathbf{r},t), \tag{74}$$

defining the barycentric velocity $\mathbf{v}(\mathbf{r},t)$. From Eqs. (30), (31), and (33) there follows that

$$\begin{aligned} h(\mathbf{r},t) &= \frac{m}{2}\mathrm{Tr}\{I_n^{[2]}(\mathbf{r},t)\} \\ &= \frac{3}{2}n(\mathbf{r},t)\beta^{-1}(\mathbf{r},t) + \frac{m}{2}n(\mathbf{r},t)\mathrm{v}^2(\mathbf{r},t), \end{aligned} \tag{75}$$

where we can write $\beta^{-1}(\mathbf{r},t){=}k_BT^*(\mathbf{r},t)$ introducing a nonequilibrium temperature (called quasitemperature [54,55]), as well as

$$\mathbf{I}_h(\mathbf{r},t) = \frac{5}{2}n(\mathbf{r},t)\beta^{-1}(\mathbf{r},t)\mathbf{v}(\mathbf{r},t) + \frac{m}{2}n(\mathbf{r},t)\mathrm{v}^2(\mathbf{r},t)\mathbf{v}(\mathbf{r},t), \tag{76}$$

and

$$I_n^{[2]}(\mathbf{r},t) = \frac{1}{m}\beta^{-1}(\mathbf{r},t)n(\mathbf{r},t)\mathbf{1}^{[2]} + n(\mathbf{r},t)\mathbf{v}(\mathbf{r},t)\mathbf{v}(\mathbf{r},t). \tag{77}$$

Introducing Eq. (77) in Eq. (68), if

$$\nabla\cdot\left[\frac{n(\mathbf{r},t)}{m}\mathcal{F}(\mathbf{r},t)\right] \gg \theta_2\frac{\partial}{\partial t}\nabla\cdot\left[\frac{n(\mathbf{r},t)}{m}\mathcal{F}(\mathbf{r},t)\right]$$

we finally arrive at

$$\begin{aligned} &\theta_1\theta_2\frac{\partial^3}{\partial t^3}n(\mathbf{r},t) + [\theta_1+\theta_2]\frac{\partial^2}{\partial t^2}n(\mathbf{r},t) + \frac{\partial}{\partial t}n(\mathbf{r},t) \\ &\quad = -\nabla\cdot\mathbf{j}_n(\mathbf{r},t), \end{aligned} \tag{78}$$

where

$$\mathbf{j}_n(\mathbf{r},t) = -\mathcal{D}^{[2]}(\mathbf{r},t)\cdot\nabla n(\mathbf{r},t) - n(\mathbf{r},t)\mathbf{V}(\mathbf{r},t) \tag{79}$$

plays the role of a generalized flux with at the right being present a generalized thermodynamic force, and where

$$\mathcal{D}^{[2]}(\mathbf{r},t) = \theta_1\left[\frac{k_BT^*(\mathbf{r},t)}{m}\mathbf{1}^{[2]} + [\mathbf{v}(\mathbf{r},t)\mathbf{v}(\mathbf{r},t)]\right] \tag{80}$$

is playing the role of a generalized diffusion tensor (composed of two parts, a first one of thermal origin and a second associated to the drift kinetic energy) and

$$\mathbf{V}(\mathbf{r},t) = \theta_1\left[\nabla\left(\frac{k_BT^*(\mathbf{r},t)}{m}\right)\right] + \theta_1\left[\nabla\cdot[\mathbf{v}\mathbf{v}] - \frac{1}{m}\mathcal{F}(\mathbf{r},t)\right], \tag{81}$$

composed of three terms, one of thermal origin another coming from the drifting movement and a third from the applied force.

Moreover, in the steady state ($\partial n/\partial t = 0$ and then $\mathbf{j} = 0$) there follows that the density satisfies the equation

$$\mathcal{D}^{[2]}(\mathbf{r})\cdot\nabla n(\mathbf{r}) = -n(\mathbf{r})\mathbf{V}(\mathbf{r}). \tag{82}$$

Returning to Eq. (78), its Fourier transform reads

$$i\omega[-\omega^2\theta_1\theta_2 - i\omega(\theta_1+\theta_2) + 1]n(\mathbf{Q},\omega) = i\mathbf{Q}\cdot\mathbf{j}_n(\mathbf{Q},\omega), \tag{83}$$

which give us an illustration on the criterion of contraction of description: (1) In conditions such that $\omega^2\theta_1\theta_2 \ll 1$, the term with the third time derivative can be neglected and the evolution equation acquires the form of a generalized hyperbolic Maxwell-Cattaneo one. (2) If further $\omega(\theta_1+\theta_2) \ll 1$ the second time derivative also can be neglected and we are left with a generalized parabolic diffusionlike equation, and in that way there follows a chain of increasing contractions of description of the hydrodynamic motion.

Finally, to perform numerical calculations and analyze the results we introduce a central force interaction between particles in the system with those in the bath of the Gaussian form, called the Gaussian core model (GCM) [56],

$$w(r) = \frac{U}{\sqrt{2\pi r_0^2}}e^{-r^2/r_0^2}, \tag{84}$$

with the open parameters U and r_0 (r_0 is a length scale playing the role of a range length and U/r_0 being the interaction strength). It has been noticed that this kind of potential belongs to the class of interactions which do not diverge at the origin, i.e., are bounded. They are potentials corresponding to effective interactions between the centers of mass of soft, flexible macromolecules such as polymer chains [57], dendrimers [58], and others. The centers of mass of two macromolecules can coincide without violation of the excluded volume conditions, hence implying a bounded interaction [59]. Several studies of this potential can be consulted, for example, in Refs. [60–63].

It can be noticed that GCM of Eq. (84) roughly mimics a hard sphere potential with radius r_0, and that in the limit of r_0 going to zero goes over a contact potential $U\delta(r)$. The Fourier transform is

$$\psi(\mathbf{Q}) = \frac{\pi}{\sqrt{2}}Ur_0^2e^{-r_0^2Q^2/4}. \tag{85}$$

In terms of these results we find that

$$\theta_1^{-1} = \frac{\sqrt{\pi}}{6\sqrt{2}}\frac{n_R}{M^{1/2}}\frac{M}{m}\left(1+\frac{M}{m}\right)\beta_0^{3/2}U^2, \tag{86}$$

which tells us that the momentum relaxation time becomes very large for the Brownian particle when $m \gg M$, and very small for the Lorentz particle when $m \ll M$. Furthermore, θ_1 increases with the power 3/2 of the temperature T_0 and, as expected, with the reciprocal of the density of scattering centers.

Moreover, it can also be noticed that in the limit of a contact potential ($r_0 \to 0$), the quantity

$$\frac{1}{\kappa} = \frac{\sqrt{\pi}}{2^{3/2}}\left[1+\frac{m}{M}\right]^{-1}r_0 \tag{87}$$

tells us that κ^{-1} goes to zero and then [cf. Eqs. (B4) and (B8)] the kinetic coefficients a_{L0} and a_{L1} approach zero, i.e., $J_L(\mathbf{r},t)$ does not contribute.

VII. SUMMARY OF SOME APPLICATIONS

An interesting application of MHT, that provides a good illustration of the formalism at work, is in the study of the the so-called thermal-laser stereolithography. This is a process which allows solid physical parts to be made directly and rapidly from computer data without the necessity of tooling or cutting machining. A first apparatus for industrial use was patented in 1987 by 3D-Systems Inc. It enables the production of complex three-dimensional models by the successive solidifying of layers of liquids resin. The liquid plastic hardens only where touched by the laser beam, and the model is built layer by layer. The metamorphic transition from computer designed models to physical parts takes place in a short time and, hence, the process is sometimes called rapid phototyping, a better denomination than the rather metaphoric use of the term lithography. More details are in Ref. [64].

Presently, thermal lithography is used to transcribe patterns or images to a surface at the micro- or nanoscale, and in the fabrication of nanomaterials, as well as in bone implant in three dimensions [65,66]. The thermal prototyping method was based on the use of a CO_2 laser (photon wavelength of 10.6 μm) which introduces local heating of the thermosensible resin inducing surface curing. The sintering process results in a localized solidification which can be quite rapid.

Experimental observations of thermal-laser phototyping, a study to probe quality characteristics in different experimental protocols, was interpreted in terms of MHT, more precisely in a contracted description of order 1 (i.e., the one which includes the densities of matter and of energy, and their fluxes of first order. The detailed study is present in Ref. [64].

The experimental observations studied, in the framework of a MHT of order 1 as noticed, led to obtaining for the motion of matter and heat a damped wave propagation (solutions of the hyperbolic form of the equations of evolution in a generalized aspect of a Maxwell-Cattaneo equation). It may be noticed that the wave propagation of matter may be simply observed by the eye using an amplifying lens (sometimes by the unaided eye), and the propagation of heat through interpretation of the curing (sintering) process.

The experimental results showed that the resulting models that were at first quite imperfect were improved using a modification of the texture of the thermally sensible resin, consisting of adding to it silica powder (this is shown in Fig. 4 in Ref. [64]). This fact was a result, as shown in [64], that the addition of impurities modifies (decreases) Maxwell time for the flux (current) of energy (and then of nonequilibrium temperature) thus modifying the frontier that separates the damped wave and the diffusion regimes, characterized by the wave number $k_M = [c_h \theta_{I_h}]^{-1}$ (c_h the velocity of propagation of the flux—of the order of the thermal velocity—and the flux-Maxwell time θ_{I_h}). Depending on the domain of relevant values of wave numbers k contributing to the movement, for $k > k_M$ the motion is basically a damped oscillatory one, while for $k < k_M$ there follows overdamped movement, i.e., a diffusive one (see Fig. 2 in [64]). Thus, with the predominance of the diffusive motion the heat generated at the spot of the laser illumination there remains localized at sufficient times to get cooled in the impurified resin.

As already stated this technoindustrial process provides a good illustration of the working of MHT, with a, say, visual characterization of the question of contraction of description in MHT [67], as well as the important role of Maxwell time for determining the character of the motion [68].

Furthermore, MHT has been used in the study of optical and transport properties in polar semiconductors, then at a quantum mechanical level. But electrons, in conditions in which they are in electronic and optoelectronic devices, behave as classical fluids, that is, are well described by a Maxwell-Boltzmann distribution. No description is given here, and we simply refer the reader to the publications on the subject (for example Refs. [69,70]. It may be noticed that the change of description from the standard one to the MHT of order 1 shows that when the latter one is used it is evidenced an extreme modification (orders of magnitude decrease) in the thermal conductivity when the size of the sample approaches the nanometric space scale.

Moreover, as noticed in the Introduction, nonequilibrium molecular dynamics [12,18] is an alternative formalism based on computing modeling, and a comparison with the present one is reported in Ref. [71] involving studies of electron conductivity in doped polar semiconductors where is reported a good agreement between the results obtained in both formalisms, and with experimental data when available.

VIII. CONCLUDING REMARKS

We have here shown that a statistical nonequilibrium ensemble formalism (applicable to the study of systems even in conditions far from equilibrium) provides a microscopic foundation for a higher-order generalized hydrodynamics (HOGH). Its description is based on the set of hydrodynamic variables consisting of the densities of energy and matter (particles) and their fluxes of all orders.

The construction of this HOGH was based on the use of the moments method for the solution of the single-particle kinetic equation (generalization of Boltzmann equation [72] in a way akin to Grad's 14-moments approach. In our theory are in principle involved the moments of all order. Moreover we recall, as noticed in the main text, that we deal at a purely mechanical level in a Galilean frame of reference. In Grad's 14-moments approach is used a barycentric frame of reference, and the evolution equation presents an admixture of mechanical and hydrothermodynamical variables.

It may be noticed that our construction is in the spirit of Truesdell's principle of equipresence [73], namely, in the evolution equation for the density appears the divergence of the first flux which then is to be incorporated as a basic variable, in the evolution equation for this first flux is present the divergence of the second flux which then it is incorporated as a basic variable, and so on and so forth.

There follows a set consisting of an enormous number of coupled evolution equations for all the fluxes, which is of unmanageable proportions. A contraction of description is required [40,53] that is, to keep a small number of fluxes as basic variables. What is involved is that introduction of an ever increasing number of fluxes is necessary to describe hydrodynamic motion characterized by smaller and smaller wavelengths (accompanied by larger and larger frequencies).

We may say that this is in the spirit of the Burnett approach [74]. For large wavelengths a HOGH of order 0 can be applied, and the moments follow a diffusionlike parabolic equation; when increasing wavelengths are involved a HOGH of order 1 is required, and the movement follows a hyperbolic Maxwell-Cattaneo-like equation. When ever increasing wavelengths are involved HOGH of order 2 and higher would be required, and the evolution equations are of order 3 and higher in time.

All these hydrodynamic variables are the average value over the nonequilibrium ensemble of the corresponding microscopic mechanical operators. Once the complete set of macrovariables is given we can obtain the nonlinear hydrodynamic equations, which are the average value over the nonequilibrium ensemble of Hamilton equations of motion (in the classical level or Heisenberg equations at the quantum level) of the basic microvariables (mechanical observables). Once all these hydrodynamical variables, cf. Eqs. (30)–(34) and (37)–(39), involve the single-particle distribution function $f_1(\mathbf{r},\mathbf{p};t)$, their evolution equations follow from the evolution equation for f_1 [cf. Eq. (27)]. The set of evolution equations given in Eq. (45) is obtained: $l = 0$ for the density, $l = 1$ for the first (vectorial) flux, $l \geqslant 2$ for the higher-order tensorial fluxes, all of which are coupled together.

These generalized hydrodynamic equations on the left side present the conserving part of the corresponding quantity, and on the right-hand side present the collision integrals which include the action of external sources and the contributions of scattering processes responsible for dissipative effects.

In that way we do have a quite generalized hydrodynamics under any arbitrary condition of excitation, which, as noticed, can be referred to as *mesoscopic hydrothermodynamics.*

ACKNOWLEDGMENTS

We acknowledge financial support from Fundação de Amparo à Pesquisa do Estado de São Paulo. C.A.B.S. acknowledges a leave of absence granted by the Brazilian Technological Institute of Aeronautics, and is grateful to the Condensed Matter Physics Department at the University of Campinas for the kind hospitality received there.

APPENDIX A: SCATTERING INTEGRALS IN EQ. (45)

The three scattering integrals $J_\tau^{[l]}$, $J_L^{[l]}$, and $J_{\rm NL}^{[l]}$ in Eq. (45) are

$$\begin{aligned} J_\tau^{[l]}(\mathbf{r},t) &= \frac{n_R}{\mathcal{V}}\frac{\sqrt{2\pi M\beta_o}}{m^2}\sum_{\mathbf{Q}}\frac{|\psi(Q)|^2}{Q} \\ &\quad\times\int d^3p\sum_P\big[\mathbf{QQu}^{[l-2]}(\mathbf{p})\big]e^{-\alpha[(\mathbf{Q}/Q)\cdot\mathbf{p}]^2}f_1(\mathbf{r},\mathbf{p};t) \\ &\quad-\frac{n_R}{\mathcal{V}}\frac{(M\beta_0)^{3/2}\pi}{\sqrt{2\pi}m^2}\sum_{\mathbf{Q}}\frac{|\psi(Q)|^2}{Q}\left(\frac{1}{M}+\frac{1}{m}\right)\int d^3p \\ &\quad\times\sum_P[\mathbf{Qu}^{[l-1]}(\mathbf{p})]\mathbf{Q}\cdot\mathbf{p}\,e^{-\alpha[(\mathbf{Q}/Q)\cdot\mathbf{p}]^2}f_1(\mathbf{r},\mathbf{p};t), \end{aligned} \tag{A1}$$

with $\alpha = M\beta_0/2m^2$; $\psi(Q)$ is the Fourier transform of the interaction potential between the particles and the thermal bath, i.e., Eq. (21), and according to Eq. (35)

$$[\mathbf{QQu}^{[l-2]}(\mathbf{p})] = \left[\mathbf{QQ}\frac{\mathbf{p}}{m}\dots\ (l-2)\text{ times}\ \dots\frac{\mathbf{p}}{m}\right], \tag{A2}$$

$$\begin{aligned} J_L^{[l]}(\mathbf{r},t) &= -\frac{n_R}{\mathcal{V}}\frac{M\beta_0}{m^2}\sum_{\mathbf{Q}}\frac{|\psi(Q)|^2}{Q^2}\mathbf{Q}\cdot\nabla\int d^3p \\ &\quad\times\sum_P\big[\mathbf{Qu}^{[l-1]}(\mathbf{p})\big]F(\mathbf{p},\mathbf{Q})f_1(\mathbf{r},\mathbf{p};t), \end{aligned} \tag{A3}$$

where

$$F(\mathbf{p},\mathbf{Q}) = 1+\sum_{n=1}^{\infty}\frac{(-1)^n}{(2n-1)!!}2^n\alpha^n\left(\frac{\mathbf{Q}}{Q}\cdot\mathbf{p}\right)^{2n}. \tag{A4}$$

$$J_{\rm NL}^{[l]}(\mathbf{r},t) = -\frac{1}{m}\sum_{s=1}^{l}\wp(1,s)\big[\mathbf{F}_{\rm NL}(\mathbf{r},t)I_n^{[l-1]}(\mathbf{r},t)\big], \tag{A5}$$

$$\mathbf{F}_{\rm NL}(\mathbf{r};t) = \int d^3r'\int d^3p'\mathbf{G}_{\rm NL}(\mathbf{r}'-\mathbf{r},\mathbf{p}')f_1(\mathbf{r}',\mathbf{p}';t), \tag{A6}$$

$$\begin{aligned} \mathbf{G}_{\rm NL}(\mathbf{r}'-\mathbf{r},\mathbf{p}') &= \frac{n_R\beta_0}{\mathcal{V}}\sum_{\mathbf{Q}}\mathbf{Q}|\psi(Q)|^2\Bigg\{iF(\mathbf{Q},\mathbf{p}') \\ &\quad+\left(\frac{M\beta_0}{2\pi}\right)^{1/2}\frac{\pi}{m}\frac{\mathbf{Q}\cdot\mathbf{p}'}{Q}e^{-\alpha(\frac{\mathbf{Q}}{Q}\cdot\mathbf{p}')^2}\Bigg\} \\ &\quad\times e^{i\mathbf{Q}\cdot(\mathbf{r}'-\mathbf{r})}. \end{aligned} \tag{A7}$$

The notation

$$\sum_P[\mathbf{Qu}^{[l-1]}(\mathbf{p})] \equiv \sum_P\left[\mathbf{Q}\frac{\mathbf{p}}{m}\dots\ (l-1)\text{ times}\ \dots\ \frac{\mathbf{p}}{m}\right] \tag{A8}$$

means that one has to sum all permutations of the vectors in order to ensure that the tensor has the same symmetry of the tensor $I_n^{[l]}$ on the left hand side of Eq. (45).

Next, making a Taylor series expansion of the exponential in both contributions in Eq. (A1) and in Eq. (A7), i.e.,

$$\exp\left[-\alpha\left(\frac{\mathbf{Q}}{Q}\cdot\mathbf{p}\right)^2\right] = \sum_{k=0}^{\infty}\frac{(-1)^k\alpha^k}{k!}\mathbf{Q}^{[2k]}\odot\mathbf{p}^{[2k]}, \tag{A9}$$

where $\mathbf{Q}^{[l]}$ stands for

$$\mathbf{Q}^{[l]} = [\mathbf{Q}\dots\ (l\text{ times})\dots\mathbf{Q}], \tag{A10}$$

and we recall that $\odot$ stands for full contraction of the two tensors of rank $2k$. Then using Eq. (A4) for $F(\mathbf{p},\mathbf{Q})$, we can rewrite Eqs. (A1), (A5), and (A3) in a closed form in terms of all the fluxes, namely

$$\begin{aligned} J_\tau^{[l]}(\mathbf{r},t) &= \sum_{k=0}^{\infty}\widehat{\wp}_l\big[\Lambda_{\tau0}^{[2k+2]}\odot I_n^{[2k+l-2]}(\mathbf{r},t)\big] \\ &\quad+\sum_{k=0}^{\infty}\sum_{s=1}^{l}\wp(1,s)\big[\Lambda_\tau^{[2k+2]}\odot I_n^{[2k+l]}(\mathbf{r},t)\big] \end{aligned} \tag{A11}$$

$$J_L^{[l]}(\mathbf{r},t) = \sum_{k=0}^{\infty}\sum_{s=1}^{l} \wp(1,s)\big[\Lambda_L^{[2k+2]} \odot \nabla I_n^{[2k+l-1]}(\mathbf{r},t)\big], \quad \text{(A12)}$$

$$\begin{aligned} J_{\mathrm{NL}}^{[l]}(\mathbf{r},t) = &-\frac{1}{m}\sum_{s=1}^{l}\wp(1,s)\sum_{k=0}^{\infty}\int d^3\mathbf{r}' \\ &\times\big\{\big[\big[\Lambda_{NL1}^{[2k+1]}(\mathbf{r}'-\mathbf{r})\odot I_n^{[2k]}(\mathbf{r}',t)\big]I_n^{[l-1]}(\mathbf{r},t)\big] \\ &+\big[\big[\Lambda_{NL2}^{[2k+2]}(\mathbf{r}'-\mathbf{r})\odot I_n^{[2k+1]}(\mathbf{r}',t)\big]I_n^{[l-1]}(\mathbf{r},t)\big]\big\}, \end{aligned} \quad \text{(A13)}$$

where

$$\widehat{\wp}_l = \sum_{s=2}^{l}\wp(2,s) + \sum_{r=3}^{l}\wp(1,r) + \sum_{r=3}^{l-1}\sum_{s=r+1}^{l}\wp(1,r;2,s) \quad \text{(A14)}$$

is an operator involving the set of permutations that ensures the proper symmetry of the tensor on which it acts. Here the operation $\Lambda^{[r]} \odot \Lambda^{[s]}$ indicates the contraction of some indexes in order to give the right tensorial order of the equation. For example in Eqs. (A11) and (A12) it indicates the contraction of $(r+s-l)/2$ indexes as to produce a tensor of rank l. The several tensorial kinetic coefficients of Eqs. (A11)–(A13) are

$$\Lambda_{\tau 0}^{[2k+2]} = \sum_{\mathbf{Q}} g_{\tau k}(Q)\mathbf{Q}^{[2k+2]}, \quad \text{(A15)}$$

$$\Lambda_{\tau}^{[2k+2]} = \sum_{\mathbf{Q}} f_{\tau k}(Q)\mathbf{Q}^{[2k+2]}, \quad \text{(A16)}$$

$$\Lambda_{L}^{[2k+2]} = \sum_{\mathbf{Q}} f_{Lk}(Q)\mathbf{Q}^{[2k+2]}, \quad \text{(A17)}$$

$$\begin{aligned}\Lambda_{NL1}^{[2k+1]}(\mathbf{r}'-\mathbf{r}) = &\, i\frac{n_R\beta_0}{\mathcal{V}}\sum_{\mathbf{Q}}|\psi(Q)|^2 e^{i\mathbf{Q}\cdot(\mathbf{r}'-\mathbf{r})} \\ &\times\frac{(-1)^k}{(2k-1)!!}\left(\frac{M\beta_0}{Q^2}\right)^k\mathbf{Q}^{[2k+1]}, \end{aligned}\quad \text{(A18)}$$

$$\begin{aligned}\Lambda_{NL2}^{[2k+2]}(\mathbf{r}'-\mathbf{r}) = &\,\frac{n_R\beta_0}{\mathcal{V}}\frac{(M\beta_0)^{1/2}\pi}{\sqrt{2\pi}}\sum_{\mathbf{Q}}\frac{|\psi(Q)|^2}{Q} \\ &\times e^{i\mathbf{Q}\cdot(\mathbf{r}'-\mathbf{r})}\frac{(-1)^k}{k!}\left(\frac{M\beta_0}{2Q^2}\right)^k\mathbf{Q}^{[2k+2]}. \end{aligned}\quad \text{(A19)}$$

where we have defined

$$g_{\tau k}(Q) = \frac{n_R}{\mathcal{V}}\frac{\sqrt{2\pi M\beta_0}}{m^2}\frac{|\psi(Q)|^2}{Q}\frac{(-1)^k}{k!}\left(\frac{M\beta_0}{2Q^2}\right)^k, \quad \text{(A20)}$$

$$\begin{aligned}f_{\tau k}(Q) = &\,\frac{n_R}{\mathcal{V}}\frac{(M\beta_0)^{3/2}\pi}{\sqrt{2\pi}m}\frac{|\psi(Q)|^2}{Q}\left(\frac{1}{M}+\frac{1}{m}\right) \\ &\times\frac{(-1)^{k+1}}{k!}\left(\frac{M\beta_0}{2Q^2}\right)^k, \end{aligned}\quad \text{(A21)}$$

$$f_{Lk}(Q) = \frac{n_R}{\mathcal{V}}\frac{M\beta_0}{m^2}\frac{|\psi(Q)|^2}{Q^2}\frac{(-1)^{k+1}}{(2k-1)!!}\left(\frac{M\beta_0}{Q^2}\right)^k. \quad \text{(A22)}$$

The last term on the right of Eq. (48) is given by

$$R_n^{[l]}(\mathbf{r},t) = J_\tau R^{[l]}(\mathbf{r},t) + J_{LR}^{[l]}(\mathbf{r},t), \quad \text{(A23)}$$

$$J_{LR}^{[l]}(\mathbf{r},t) = \sum_{k=2}^{\infty}\sum_{s=1}^{l}\wp(1,s)\big[\Lambda_L^{[2k+2]}\odot\nabla I_n^{[2k+l-1]}(\mathbf{r},t)\big], \quad \text{(A24)}$$

$$\begin{aligned}J_\tau R^{[l]}(\mathbf{r},t) = &\sum_{k=2}^{\infty}\sum_{s=1}^{l}\wp(1,s)\big[\Lambda_\tau^{[2k+2]}\odot I_n^{[2k+l]}(\mathbf{r},t)\big] \\ &+\sum_{k=2}^{\infty}\big\{\widehat{\wp}_l\big[\Lambda_{\tau 0}^{[2k+2]}\odot I_n^{[2k+l-2]}(\mathbf{r},t)\big]\big\}, \end{aligned}\quad \text{(A25)}$$

where the operators $\wp(1,s)$ and $\widehat{\wp}_l$ are defined in the main text.

APPENDIX B: KINETIC COEFFICIENTS IN EQS. (47) AND (48)

We do have that

$$a_{\tau 0} = \frac{\mathcal{V}}{(2\pi)^3}\frac{4\pi}{3}\int dQ\, Q^4 f_{\tau 0}(Q), \quad \text{(B1)}$$

with $k=0$ in Eq. (11), and

$$f_{\tau 0}(Q) = -\frac{n_R}{\mathcal{V}}\frac{(M\beta_0)^{3/2}\pi}{\sqrt{2\pi}m^2}\frac{|\psi(Q)|^2}{Q}\left(\frac{m}{M}+1\right), \quad \text{(B2)}$$

where $\psi(Q)$ is the Fourier transform of the potential energy $w(|\mathbf{r}_j - \mathbf{R}_\mu|)$, n_R is the density of particles in the thermal bath, $\mathcal{V}$ is the volume, and $\beta_0^{-1} = k_B T_0$. Moreover,

$$a_{\tau 1} = -\frac{M\beta_0}{10}a_{\tau 0}, \quad \text{(B3)}$$

$$a_{L0} = \sqrt{\frac{2}{M\beta_o\pi}}\frac{1}{\kappa}a_{\tau 0}, \quad \text{(B4)}$$

$$\frac{1}{\kappa} = \frac{\int dQ\, Q^2|\psi(Q)|^2}{\int dQ\, Q^3|\psi(Q)|^2\left(1+\frac{m}{M}\right)}, \quad \text{(B5)}$$

$$b_{\tau 0} = -\frac{2}{M\beta_0}a_{\tau 0}\left(1+\frac{m}{M}\right)^{-1}, \quad \text{(B6)}$$

$$b_{\tau 1} = \frac{a_{\tau 0}}{5}\left(1+\frac{m}{M}\right)^{-1}, \quad \text{(B7)}$$

$$a_{L1} = -\frac{1}{5\kappa}\sqrt{\frac{2M\beta_0}{\pi}}a_{\tau 0}. \quad \text{(B8)}$$

APPENDIX C: LAST TERMS OF EQS. (57)–(59)

The contributions present in Eqs. (57)–(59) in Sec. VI are

$$\boldsymbol{\mathcal{F}}(\mathbf{r},t) = -\nabla V_{\mathrm{ext}}(\mathbf{r};t) - \mathbf{F}_{\mathrm{NL}}(\mathbf{r};t), \quad \text{(C1)}$$

$$\mathbf{S}_n(\mathbf{r},t) = 3a_{\tau 1}\frac{2}{m}\mathbf{I}_h(\mathbf{r},t) + \frac{2}{m}a_{L1}\nabla h(\mathbf{r},t) + \mathbf{R}_n(\mathbf{r},t), \quad \text{(C2)}$$

$$S_n^{[2]}(\mathbf{r},t) = \frac{2}{m} b_{\tau 1} h(\mathbf{r},t)\mathbf{1}^{[2]} + 6a_{\tau 1}\frac{2}{m} I_h^{[2]}(\mathbf{r},t) + a_{L1}\frac{2}{m}\{\nabla \mathbf{I}_h(\mathbf{r},t) + [\nabla \mathbf{I}_h(\mathbf{r},t)]^{\mathrm{tr}}\} + R_n^{[2]}(\mathbf{r},t), \tag{C3}$$

where the upper index tr stands for transpose,

$$S_n^{[3]}(\mathbf{r},t) = b_{\tau 1}\frac{2}{m}\{\widehat{\wp}_3[\mathbf{1}^{[2]}\mathbf{I}_h(\mathbf{r},t)]\} + a_{L1}\frac{2}{m}\sum_{s=1}^{3}\wp(1,s)[\nabla I_h^{[2]}(\mathbf{r},t)] + 9a_{\tau 1}\frac{2}{m} I_h^{[3]}(\mathbf{r},t) + R_n^{[3]}(\mathbf{r},t). \tag{C4}$$

In which

$$\mathbf{R}_n(\mathbf{r},t) = \sum_{k=2}^{\infty}\{\Lambda_\tau^{[2k+2]} \odot I_n^{[2k+1]}(\mathbf{r},t) + \Lambda_L^{[2k+2]} \odot \nabla I_n^{[2k]}(\mathbf{r},t)\}, \tag{C5}$$

$$R_n^{[2]}(\mathbf{r},t) = \sum_{k=2}^{\infty}\{\Lambda_{\tau 0}^{[2k+2]} \odot I_n^{[2k]}(\mathbf{r},t) + \Lambda_\tau^{[2k+2]} \odot I_n^{[2k+2]}(\mathbf{r},t) + I_n^{[2k+2]}(\mathbf{r},t) \odot \Lambda_\tau^{[2k+2]} + \Lambda_L^{[2k+2]} \odot \nabla I_n^{[2k+1]}(\mathbf{r},t) + [\Lambda_L^{[2k+2]} \odot \nabla I_n^{[2k+1]}(\mathbf{r},t)]^{\mathrm{tr}}\}, \tag{C6}$$

$$R_n^{[3]}(\mathbf{r},t) = J_{\tau R}^{[3]}(\mathbf{r},t) + J_{LR}^{[3]}(\mathbf{r},t), \tag{C7}$$

$$J_{LR}^{[3]}(r,t) = \sum_{k=2}^{\infty}\sum_{s=1}^{3}\wp(1,s)[\Lambda_L^{[2k+2]} \odot \nabla I_n^{[2k+2]}(\mathbf{r},t)], \tag{C8}$$

$$J_{\tau R}^{[3]}(\mathbf{r},t) = \sum_{k=2}^{\infty}\widehat{\wp}_3[\Lambda_{\tau 0}^{[2k+2]} \odot I_n^{[2k+1]}(\mathbf{r},t)] + \sum_{k=2}^{\infty}\sum_{s=1}^{3}\wp(1,s)[\Lambda_\tau^{[2k+2]} \odot I_n^{[2k+3]}(\mathbf{r},t)]. \tag{C9}$$

The several kinetic tensorial coefficients $\Lambda^{[r]}$ are given in Appendix A.

---

[1] Yu. L. Klimontovich, A unified approach to kinetic description of processes in active systems, in *Statistical Theory of Open Systems* (Kluwer Academic, Dordrecht, The Netherlands, 1995), Vol. 1.

[2] J. P. Boon and S. Yip, *Molecular Hydrodynamics* (McGraw-Hill, New York, 1980; reprinted by Dover, New York, 1991).

[3] H. J. Kreuzer, *Nonequilibrium Thermodynamics and its Statistical Foundations* (Clarendon, Oxford, UK, 1981).

[4] D. N. Zubarev, V. G. Morosov, and G. Röpke, *Statistical Mechanics of Nonequilibrium Processes*, Vol. 1: *Basic Concepts, Kinetic Theory*, Vol. 2: *Relaxation and Hydrodynamics Processes* (Akademie Verlag - Wiley VCH, Berlin, 1996).

[5] S. K. Belyaev, Hydrodynamics: problems and paradoxes, Phys. Usp. **38**, 287 (1995).

[6] D. N. Zubarev, V. G. Morosov, I. P. Omelyan, and M. V. Tokarchuk, Unification of the kinetic and hydrodynamic approaches in the theory of dense gases and liquids, Theor. Math. Phys+ **96**, 997 (1993).

[7] H. G. B. Casimir, On Onsager's principle of microscopic reversibility, Rev. Mod. Phys. **17**, 343 (1945).

[8] D. Jou, J. Casas-Vazquez, and G. Lebon, *Extended Irreversible Thermodynamics*, 4th enlarged edition (Springer, Berlin, 2010).

[9] I. Müller and T. Ruggeri, *Extended Thermodynamics* (Springer, Berlin, 1993).

[10] D. Jou, J. Casas-Vazquez, and G. Lebon, Extended irreversible thermodynamics, Rep. Prog. Phys. **51**, 1105 (1998); Extended irreversible thermodynamics revisited, **62**, 1035 (1999).

[11] T. Dedeurwaerdere, J. Casas-Vázquez, D. Jou, and G. Lebon, Foundations and applications of a mesoscopic thermodynamic theory of fast phenomena, Phys. Rev. E **53**, 498 (1996).

[12] B. J. Adler and D. J. Tildesley, *Computer Simulation in Liquids* (Oxford University Press, Oxford, 1987).

[13] R. Luzzi, A. R. Vasconcellos, and J. G. Ramos, *Predictive Statistical Mechanics: A Nonequilibrium Ensemble Formalism* (Kluwer Academic, Dordrecht, The Netherlands, 2002).

[14] R. Luzzi, A. R. Vasconcellos, and J. G. Ramos, The theory of irreversible processes: Foundations of a non-equilibrium statistical ensemble formalism, Riv. Nuovo Cimento **29**, 1 (2006).

[15] D. N. Zubarev, *Nonequilibrium Statistical Thermodynamics* (Plenum-Consultants Bureau, New York, 1974).

[16] A. L. Kuzemski, Statistical mechanics and the physics of many-particle model systems, Phys. Part. Nuclei **40**, 949 (2009).

[17] A. I. Akhiezer and S. V. Peletminskii, *Methods of Statistical Physics* (Pergamon, Oxford, 1981).

[18] M. H. Kalos and P. A. Whitlock, *Monte Carlo Methods* (Wiley Interscience, New York, 2007).

[19] G. Nicolis, *Introduction to Nonlinear Science* (Cambridge University Press, Cambridge, UK, 1995).

[20] H. Haken, *Synergetics* (Springer, Berlin, 1978).

[21] P. Glandsdorff and I. Prigogine, *Thermodynamic Theory of Structure, Stability and Fluctuations* (Wiley-Interscience, London, 1971).

[22] D. N. Zubarev and S. V. Tishchenko, Nonlocal hydrodynamics with memory, Physica **59**, 285 (1972).

[23] D. N. Zubarev, Theory of turbulent transport on the basis of nonequilibrium statistical thermodynamics, Theor. Math. Phys. **46**, 47 (1981).

[24] S. Havlin and D. Ben-Avraham, Diffusion in disordered media, Adv. Phys. **36**, 695 (1987).

[25] F. Family and T. Vicsek, *Dynamics of Fractal Surfaces* (World Scientific, Singapore, 1991).

[26] T. A. Witten, Insights from soft-condensed matter, Rev. Mod. Phys. (Supplement Centenary APS) **71**, S367 (1999); T. A. Witten and P. A. Pincus, *Structured Fluids: Polymers, Colloids, Surfactants* (Oxford University Press, Oxford, 2004); J. R. Dutcher and A. G. Marangoni, *Soft Materials* (Marcel Dekker, New York, 2005).

[27] J. Crank, *The Mathematics of Diffusion* (Oxford University Press, Oxford, 1975).

[28] R. Luzzi, A. R. Vasconcellos, and J. G. Ramos, Non-equilibrium statistical mechanics of complex systems: an overview, Riv. Nuovo Cimento **30**, 95 (2007).

[29] J. G. Ramos, A. Gorenstein, M. U. Kleinke, T. G. Souza Cruz, and R. Luzzi, Statistical approach to non-Fickian diffusion, Int. J. Mod. Phys. B **20**, 4821 (2006).

[30] C. A. B. Silva, J. G. Ramos, A. R. Vasconcellos, and R. Luzzi, Generalized Kinetic Equation for Far-from-Equilibrium Many-Body Systems, J. Stat. Phys. **143**, 1020 (2011).

[31] U. Fano, Description of states in quantum mechanics by density matrix and operator techniques, Rev. Mod. Phys. **29**, 74 (1957).

[32] N. N. Bogoliubov, *Lectures in Quantum Statistics* (Gordon and Breach, New York, 1967), Vol. 1.

[33] J. T. Alvarez-Romero and L. S. Garcia-Colin, The foundations of informational statistical thermodynamics revisited, Physica A **232**, 207 (1996).

[34] R. Luzzi, A. R. Vasconcellos, and J. G. Ramos, *Statistical Foundations of Irreversible Thermodynamics* (Teubner-Bertelsmann, Springer, Stuttgart, 2000); Irreversible thermodynamics in a nonequilibrium statistical ensemble formalism, Riv. Nuovo Cimento **24**, 1 (2001).

[35] F. Reif, *Foundations of Statistical and Thermal Physics* (McGraw-Hill, New York, 1965).

[36] J. C. Maxwell, On the Dynamical Theory of Gases, Philos. Trans. R. Soc. (London) **157**, 49 (1867).

[37] H. Grad, On the kinetic theory of rarefied gases, Commun. Pure Appl. Math. **2**, 331 (1949).

[38] H. Grad, Statistical mechanics, thermodynamics, and fluid dynamics of systems with an arbitrary number of integrals, Commun. Pure Appl. Math. **5**, 455 (1952).

[39] H. Grad, Principles of the Kinetic Theory of Gases, in *Handbuch der Physik*, edited by S. Flügge (Springer, Berlin, 1958), Vol. XII, pp. 205–294.

[40] J. G. Ramos, A. R. Vasconcellos, and R. Luzzi, A nonequilibrium ensemble formalism: Criterion for truncation of description, J. Chem. Phys. **112**, 2692 (2000).

[41] R. Luzzi and A. R. Vasconcellos, Ultrafast Transient Response of nonequilibrium plasma in semiconductors, in *Semiconductor Processes Probed by Ultrafast Laser Spectroscopy*, edited by R. R. Alfano (Academic, New York, 1984), Vol. 1.

[42] C. G. Rodrigues, A. R. Vasconcellos, R. Luzzi, and V. N. Freire, Urbach's tail in III-nitrides under an electric field, J. Appl. Phys. **90**, 1879 (2001).

[43] A. C. Algarte, A. R. Vasconcellos, and R. Luzzi, Kinetics of hot elementary excitations in photoexcited polar semiconductors, Phys. Status Solidi B **173**, 487 (1992).

[44] C. G. Rodrigues, A. R. Vasconcellos, and R. Luzzi, Ultrafast relaxation kinetics of photoinjected plasma in III-nitrides, J. Phys. D: Appl. Phys. **38**, 3584 (2005).

[45] A. R. Vasconcellos, R. Luzzi, and J. R. Madureira, Optical properties of semiconductors via pump-probe experiments: statistical-thermodynamical approach, hot plasma and coherent phonon states, J. Phys.: Condens. Matter **12**, 5325 (2000).

[46] C. G. Rodrigues, A. R. Vasconcellos, and R. Luzzi, Nonlinear transport in n-III-nitrides: selective amplification and emission of coherent LO phonons, Solid State Commun. **140**, 135 (2006).

[47] C. G. Rodrigues, A. R. Vasconcellos, R. Luzzi, and V. N. Freire, Transient transport in III-nitrides: interplay of momentum and energy relaxation times, J. Phys.: Condens. Matter **19**, 346214 (2007).

[48] C. G. Rodrigues, A. R. Vasconcellos, R. Luzzi, and V. N. Freire, Electron mobility in nitride materials, Braz. J. Phys. **32**, 439 (2002); C. G. Rodrigues, A. R. Vasconcellos, and R. Luzzi, Non-linear electron mobility in n-doped III-nitrides, *ibid.* **36**, 255 (2006).

[49] J. P. Bouchaud, A. Ott, D. Langevin, and W. Urbach, Anomalous diffusion in elongated micelles and its Lévy flight interpretation, J. Phys. II (France) **1**, 1465 (1991); A. Ott, J. P. Bouchaud, D. Langevin, and W. Urbach, Anomalous diffusion in "living polymers": A. genuine Levy flight?, Phys. Rev. Lett. **65**, 2201 (1990).

[50] A. L. Kuzemski, Theory of transport processes and the method of the nonequilibrium statistical operator, Int. J. Mod. Phys. B **21**, 2821 (2007).

[51] L. Lauck, A. R. Vasconcellos, and R. Luzzi, A nonlinear quantum transport theory, Physica A **168**, 789 (1990).

[52] G. Castelnuovo, *Calcolo delle Probabilità* (Zanichelli, Bologna, Italy, 1928); B. V. Gnedenko, *The Theory of Probability* (MIR, Moscow, 1969), Vol. 2.

[53] R. Balian, Y. Alhassed, and H. Reinhardt, Dissipation in many-body systems: A geometric approach based on information theory, Phys. Rep. **131**, 1 (1986).

[54] R. Luzzi, A. R. Vasconcellos, J. Casas-Vazquez, and D. Jou, Characterization and measurement of a nonequilibrium temperature-like variable in irreversible thermodynamics, Physica A **234**, 699 (1997); On the selection of the state space in nonequilibrium thermodynamics, **248**, 111 (1998).

[55] R. Luzzi, A. R. Vasconcellos, J. Casas-Vazquez, and D. Jou, Thermodynamic variables in the context of a nonequilibrium statistical ensemble approach, J. Chem. Phys. **107**, 7383 (1997).

[56] F. H. Stillinger, Phase transitions in the Gaussian core system, J. Chem. Phys. **65**, 3968 (1976).

[57] A. A. Louis, P. G. Bolhuis, J. P. Hansen, and E. J. Meijer, Can polymer coils be modeled as "soft colloids"? Phys. Rev. Lett. **85**, 2522 (2000).

[58] C. N. Likos, M. Schmidt, H. Löwen, M. Ballauff, D. Pötschke, and P. Lindner, Soft interaction between dissolved dendrimers: theory and experiment, arXiv:cond-mat/0010235.

[59] C. N. Likos, A. Lang, M. Watzlawek, and H. Löwen, Criterion for determining clustering versus reentrant melting behavior for bounded interaction potentials, Phys. Rev. E **63**, 031206 (2001).

[60] F. H. Stillinger and T. A. Weber, Study of melting and freezing in the Gaussian core model by molecular dynamics simulation, J. Chem. Phys. **68**, 3837 (1978).

[61] F. H. Stillinger and T. A. Weber, Lindemann melting criterion and the Gaussian core model, Phys. Rev. B **22**, 3790 (1980).

[62] F. H. Stillinger, High temperature expansion for the Gaussian core model, J. Chem. Phys. **70**, 4067 (1979).

[63] F. H. Stillinger, Duality relations for the Gaussian core model, Phys. Rev. B **20**, 299 (1979).

[64] R. Luzzi, M. A. Scarparo, J. G. Ramos, A. R. Vasconcellos, M. L. Barros, Z. Zhiayao, and A. Kiel, Informational statistical thermodynamics and thermal laser stereolithography, J. Non-Equilib. Thermodyn. **22**, 197 (1997).

[65] P. Bartolo and I. Gibson, *History of lithographic process* (Springer, Berlin, 2011).

[66] K. Grandfield, Bone, implants, and their interfaces, Phys. Today **68**(4), 40 (2015).

[67] J. G. Ramos, C. A. B. Silva, C. G. Rodrigues, and R. Luzzi, Criteria for contraction of description in higher-order generalized hydrodynamics (unpublished).

[68] C. G. Rodrigues, C. A. B. Silva, J. G. Ramos, and R. Luzzi, Maxwell times in higher-order generalized hydrodynamics: classical fluids, and carriers and phonons in semiconductors (unpublished).

[69] A. R. B. Castro, A. R. Vasconcellos, and R. Luzzi, Thermoelastic analysis of a silicon surface under X-ray free-electron-laser irradiation, Rev. Sci. Instrum. **81**, 073102 (2010); C. G. Rodrigues, A. R. Vasconcellos, and R. Luzzi, Mesoscopic hydro-thermodynamics of phonons in semiconductors: heat transport in III-nitrides, Eur. Phys. J. B **86**, 200 (2013); Thermal conductivity in higher-order generalized hydrodynamics: characterization of nanowires of silicon and gallium nitride, Physica E **60**, 50 (2014).

[70] C. G. Rodrigues, A. R. B. Castro, and R. Luzzi, Higher-order generalized hydrodynamics of carriers and phonons in semiconductors in the presence of electric fields: macro to nano, (unpublished); arXiv:1505.05015.

[71] C. G. Rodrigues, A. R. Vasconcellos, R. Luzzi, and V. N. Freire, Nonlinear transport properties of doped III-N. and GaAs polar semiconductors: a comparison, J. Appl. Phys. **98**, 043703 (2005).

[72] H. Spohn, Kinetic equations from Hamiltonian dynamics: Markovian limits, Rev. Mod. Phys. **52**, 569 (1980).

[73] C. Truesdell, *Rational Thermodynamics* (McGraw-Hill, New York, 1985), and 2nd enlarged edition (Springer, Berlin, 1988).

[74] D. Burnett, The distribution of velocities in a slightly non-uniform gas, Proc. London Math. Soc. **s2-39**, 385 (1935).