

## A nonequilibrium ensemble formalism: Criterion for truncation of description

J. Galvão Ramos, Áurea R. Vasconcellos, and Roberto Luzzi

Citation: *The Journal of Chemical Physics* **112**, 2692 (2000); doi: 10.1063/1.480843

View online: <http://dx.doi.org/10.1063/1.480843>

View Table of Contents: <http://scitation.aip.org/content/aip/journal/jcp/112/6?ver=pdfcov>

Published by the [AIP Publishing](#)

---

### Articles you may be interested in

[Elasticity of flexible and semiflexible polymers with extensible bonds in the Gibbs and Helmholtz ensembles](#)  
J. Chem. Phys. **136**, 154906 (2012); 10.1063/1.4704607

[Statistical mechanical theory for nonequilibrium systems. X. Nonequilibrium phase transitions](#)  
J. Chem. Phys. **131**, 184509 (2009); 10.1063/1.3259194

[Transient hydrodynamical behavior by dynamical nonequilibrium molecular dynamics: The formation of convective cells](#)  
J. Chem. Phys. **131**, 064106 (2009); 10.1063/1.3174392

[Unbiased sampling of lattice Hamilton path ensembles](#)  
J. Chem. Phys. **125**, 154103 (2006); 10.1063/1.2357935

[A nonequilibrium statistical grand-canonical ensemble: Description in terms of flux operators](#)  
J. Chem. Phys. **109**, 2099 (1998); 10.1063/1.476723

---



**2014 Special Topics**

PEROVSKITES

2D MATERIALS

MESOPOROUS MATERIALS

BIOMATERIALS/  
BIOELECTRONICS

METAL-ORGANIC  
FRAMEWORK  
MATERIALS

**AIP** | APL Materials

**Submit Today!**

# A nonequilibrium ensemble formalism: Criterion for truncation of description

J. Galvão Ramos, Áurea R. Vasconcellos, and Roberto Luzzi

*Instituto de Física “Gleb Wataghin,” Universidade Estadual de Campinas, Unicamp 13083-970 Campinas, São Paulo, Brazil*

(Received 30 November 1998; accepted 2 November 1999)

In the framework of a nonequilibrium statistical ensemble formalism, consisting of the so-called Nonequilibrium Statistical Operator Method, we discuss the question of the choice of the space of thermohydrodynamic states. We consider in particular the relevant question of the truncation of description (reduction of the dimension of the state space). A criterion for justifying the different levels of truncation is derived. It depends on the range of wavelengths and frequencies which are the relevant ones for the characterization, in terms of normal modes, of the thermohydrodynamic motion in a nonequilibrium open system. Applications to the cases of thermal-sensitive resins and of  $n$ -doped polar semiconductors are done, numerical results are presented, and experimental observation is discussed. © 2000 American Institute of Physics. [S0021-9606(00)50705-3]

## I. INTRODUCTION

The study of dissipative systems not so near to equilibrium conditions, that is, outside the so-called linear or Onsagerian regime, has received plenty of attention in recent decades. This is the result of the demands created by several recent important developments in science and technology. Accordingly, these facts have required the elaboration of appropriate theoretical studies implying, mainly, those able to provide satisfactory approaches in kinetic theory, irreversible thermodynamics and nonclassical hydrodynamics, as well as a response function theory, for systems arbitrarily away from equilibrium. All of them can be covered in a unified way resorting to a statistical mechanics for nonequilibrium processes. A quite promising one, as noticed by Zwanzig,<sup>1</sup> is a particular form of a nonequilibrium ensemble formalism, namely, the Nonequilibrium Statistical Operator Method. [The different approaches can be put under the unifying umbrella of a variational principle—maximization of the informational statistical entropy—and we shall refer to it as MaxEnt-NESOM (Ref. 2–7).]

MaxEnt-NESOM provides foundations for a statistical thermodynamics of irreversible processes (dubbed Informational Statistical Thermodynamics, IST for short),<sup>8–11</sup> and a nonclassical hydrodynamics.<sup>12</sup> A MaxEnt-NESOM-based response function theory is described in, for example, Refs. 2, 13–16, and some applications to the case of pump–probe experiments in the photoinjected plasma in semiconductors are reported in, for example, Refs. 17–20. Irreversible thermodynamics and hydrodynamics as field theories (describing the values and evolution of space and time dependent macrovariables) are based in MaxEnt-NESOM on a generalized nonequilibrium grand-canonical ensemble.<sup>21–23</sup> The latter is characterized by the density of particles and the density of energy, together with their fluxes to all orders, as required by the MaxEnt-NESOM-closure-like condition for the set of kinetics equations.<sup>2–7, 22, 23</sup> Hence, the MaxEnt-NESOM-kinetic theory introduces a double infinite set of coupled nonlinear

integrodifferential equations of evolution, to be solved for given (in the experiment under consideration) initial and boundary conditions.

Practical theoretical analyses of real physical situations require to introduce a truncation of description. *This truncation implies in retaining the information considered as relevant for the problem in hands, and to disregard nonrelevant information.*<sup>24, 25</sup> For carrying on this procedure a criterion needs be derived, which, in a sense, should be one playing an analog of what is done in the case of the solution of Boltzmann equation via the Hilbert–Chapman–Enskog method, where the Knudsen number provides a kind of control parameter.

Considering a system of two classic fluids in weak mutual interaction, we derive a criterion for truncation of description in MaxEnt-NESOM thermohydrodynamics. For better visualization we introduce first a simplifying treatment, consisting into decoupling the motions of matter and energy (i.e., thermostriiction effects are neglected). For the motion of mass we determine a criterion for the separation of the domains of validity of classical (or Onsagerian) and of two extended thermohydrodynamics. The connection with Bogoliobov’s principle of correlation weakening and hierarchy of relaxation times<sup>26–28</sup> is evidenced. Finally, applications to the cases of thermosensitive resins and of  $n$ -doped direct-gap polar semiconductors are done, numerical results are presented, and experimental observation is discussed.

## II. THERMOHYDRODYNAMICS OF A BROWNIAN-TYPE SYSTEM

We consider a fluid of  $N$  particles of mass  $m$  interacting with another fluid of  $N_B$  particles of mass  $M$ . The first is the system of interest to be analyzed, and the second, to be called a bath and with  $N_B \gg N$ , is assumed to be constantly kept at a fixed temperature  $T_0$  through a good thermal contact with

an ideal reservoir at this temperature. For simplicity, and to obtain a more clear picture of the question, we use a classical treatment. The Hamiltonian is

$$H = H_0 + H_{0B} + H', \quad (1)$$

where

$$H_0 = \int d^3r \int d^3p (p^2/2m) \hat{n}_1(\mathbf{r}, \mathbf{p} | \Gamma), \quad (2)$$

$$H_{0B} = \sum_{\mu=1}^{N_B} P_{\mu}^2/2M, \quad (3)$$

$$H' = \sum_{\mu=1}^{N_B} \int d^3r \int d^3p \mathcal{V}(|\mathbf{r} - \mathbf{R}_{\mu}|) \hat{n}_1(\mathbf{r}, \mathbf{p} | \Gamma). \quad (4)$$

In these equations  $H_0$  and  $H_{0B}$  are the Hamiltonians of the free system and bath, respectively, and  $H'$  stands for the interaction between system and bath via the central potential  $\mathcal{V}(|\mathbf{r}_j - \mathbf{R}_{\mu}|)$ , where  $\mathbf{r}_j$  ( $j=1, 2, \dots, N$ ) and  $\mathbf{R}_{\mu}$  ( $\mu=1, 2, \dots, N_B$ ) are the respective coordinates, and we call  $\mathbf{p}_j$  and  $\mathbf{P}_{\mu}$  the corresponding linear momenta. Moreover, we have introduced the single-particle dynamical density function

$$\hat{n}_1(\mathbf{r}, \mathbf{p} | \Gamma) = \sum_{j=1}^N \delta(\mathbf{r} - \mathbf{r}_j) \delta(\mathbf{p} - \mathbf{p}_j), \quad (5)$$

with  $\Gamma$  indicating a point in the phase space of classical mechanical states of the system.

We consider thermohydrodynamic characteristics of this system in the statistical approach provided by MaxEnt-NESOM. For that purpose we start with a nonequilibrium generalized grand-canonical ensemble.<sup>21-23</sup> The description of the nonequilibrium state of the system is done in terms of the density of particles and the density of energy, namely,

$$\hat{n}(\mathbf{r} | \Gamma) = \int d^3p \hat{n}_1(\mathbf{r}, \mathbf{p} | \Gamma) = \sum_{j=1}^N \delta(\mathbf{r} - \mathbf{r}_j), \quad (6)$$

$$\begin{aligned} \hat{h}(\mathbf{r} | \Gamma) &= \int d^3p (p^2/2m) \hat{n}_1(\mathbf{r}, \mathbf{p} | \Gamma) \\ &= \sum_{j=1}^N (p_j^2/2m) \delta(\mathbf{r} - \mathbf{r}_j), \end{aligned} \quad (7)$$

and their fluxes of all orders, which are

$$\hat{\mathbf{I}}_n(\mathbf{r} | \Gamma) = \int d^3p \mathbf{u}(\mathbf{p}) \hat{n}_1(\mathbf{r}, \mathbf{p} | \Gamma), \quad (8)$$

$$\hat{\mathbf{I}}_h(\mathbf{r} | \Gamma) = \int d^3p (p^2/2m) \mathbf{u}(\mathbf{p}) \hat{n}_1(\mathbf{r}, \mathbf{p} | \Gamma), \quad (9)$$

$$\hat{I}_n^{[r]}(\mathbf{r} | \Gamma) = \int d^3p u^{[r]}(\mathbf{p}) \hat{n}_1(\mathbf{r}, \mathbf{p} | \Gamma), \quad (10)$$

$$\hat{I}_h^{[r]}(\mathbf{r} | \Gamma) = \int d^3p (p^2/2m) u^{[r]}(\mathbf{p}) \hat{n}_1(\mathbf{r}, \mathbf{p} | \Gamma), \quad (11)$$

with  $r=2, 3, \dots$ , indicating the order of the flux and its corresponding tensorial rank, and where we have introduced  $\mathbf{u}(\mathbf{p}) = \mathbf{p}/m$  and the  $r$ -rank tensor,

$$u^{[r]}(\mathbf{p}) = \left[ \left( \frac{\mathbf{p}}{m} \right) \cdots (r\text{-times}) \cdots \left( \frac{\mathbf{p}}{m} \right) \right], \quad (12)$$

the brackets indicating tensorial product of  $r$ -times the generating velocity vector  $\mathbf{u}(\mathbf{p})$ .

Hence, Eqs. (6) and (7), and (8)–(11) define the set of basic dynamical variables for the description of the thermohydrodynamics of the system under consideration. The nonequilibrium statistical operator, which is a superoperator of these dynamical variables, is given and discussed in Ref. 21. Finally, the basic set of macrovariables, which are the nonequilibrium thermodynamic variables, is composed of the average values over the nonequilibrium ensemble of the dynamical variables of Eqs. (6)–(11). In this way, it is introduced the space of states of a statistical thermodynamics dubbed Informational Statistical Thermodynamics (IST for short).<sup>8-11</sup>

The equations of evolution are simply the average over the nonequilibrium ensemble of Hamilton equations of motion, that is,

$$\frac{\partial}{\partial t} I_j^{[r]}(\mathbf{r}, t) = \int d\Gamma \varrho_{\varepsilon}(\Gamma | t) \{ \hat{I}_j^{[r]}(\mathbf{r} | \Gamma), H \}, \quad (13)$$

where  $\{ , \}$  stands for Poisson's brackets and

$$I_j^{[r]}(\mathbf{r}, t) = \int d\Gamma \hat{I}_j^{[r]}(\mathbf{r} | \Gamma) \varrho_{\varepsilon}(\Gamma | t), \quad (14)$$

indicates the corresponding nonequilibrium thermodynamic macrovariable ( $j=h$  or  $n$ ;  $r=0, 1, 2, \dots$ ) with  $\varrho_{\varepsilon}(\Gamma | t)$  being the statistical operator taken in Zubarev's approach.<sup>3,4</sup> The right-hand side of Eq. (13) is extremely difficult to calculate. A way around is to introduce a kind of perturbation expansion of this term, in the form of an infinite series of collision operators, corresponding, roughly speaking, to two, three, etc. particle collisions, plus a contribution associated to an equation of conservation,<sup>2,29</sup> that is, in the present case these equations are<sup>21-23</sup>

$$\frac{\partial}{\partial t} I_j^{[r]}(\mathbf{r}, t) + \nabla \cdot I_j^{[r+1]}(\mathbf{r}, t) = J_j^{(2)[r]}(\mathbf{r}, t), \quad (15)$$

where  $\nabla \cdot$  stands for the divergence operator, and considering weak interactions, we have written the Markovian limit of the equations of evolution, retaining contributions only up to second order in the interaction strengths present in the collision operator  $J^{(2)}$  defined in Refs. 2–4, 29.

We can noticed that Eq. (15) represents a double set (for  $j=h$  and  $n$ ) of a very large number ( $r=0, 1, 2, \dots$ ) of coupled equations. They are, as a general rule, nonlinear integrodifferential equations, instantaneous in time because the Markovian approximation we have introduced, but are non-local in space (that is, space correlations are present).<sup>22</sup>

### III. THE TRUNCATION PROCEDURE

In order to discuss the introduction of a truncation procedure and its characterization—meaning a criterion for it—we further simplify the presentation in order to avoid cumbersome expressions that would obscure the physical interpretation. For that purpose we decouple the equations for

particle and for energy motion, what implies into neglecting thermostriktion effects, and in what follows we concentrate the attention on the movement of particles, characterized by  $n(\mathbf{r}, t)$  and its fluxes  $I_n^{[r]}(\mathbf{r}, t)$ ,  $r=1, 2, \dots$ . Further, both system and bath are taken as being in mutual thermal equilibrium at temperature  $T_0$ . We proceed by introducing a truncated description in which we take into account only the density of particles and its first two fluxes. Using Eq. (15) we obtain the equations of evolution for the basic variables, namely,

$$\frac{\partial}{\partial t} n(\mathbf{r}, t) + \nabla \cdot \mathbf{I}_n(\mathbf{r}, t) = 0, \quad (16)$$

$$\frac{\partial}{\partial t} \mathbf{I}_n(\mathbf{r}, t) + \nabla \cdot I_n^{[2]}(\mathbf{r}, t) = -\frac{\mathbf{I}_n(\mathbf{r}, t)}{\tau_{n1}(x)}, \quad (17)$$

$$\frac{\partial}{\partial t} I_n^{[2]}(\mathbf{r}, t) + \nabla \cdot I_n^{[3]}(\mathbf{r}, t) = \frac{n(\mathbf{r}, t) \mathbf{1}^{[2]}}{m\beta_0 \tau_{n2}(x)} - \frac{I_n^{[2]}(\mathbf{r}, t)}{\tau_{n2}(x)}, \quad (18)$$

where  $\mathbf{1}^{[2]}$  is the unit second order rank tensor, and we have defined the characteristic times,

$$\tau_{n1}^{-1}(x) = \Omega \left[ \frac{1}{\sqrt{x(x+1)}} \right], \quad (19a)$$

$$\tau_{n2}^{-1}(x) = \Omega \left[ \frac{1}{\sqrt{x(x+1)}} \right] \frac{2x}{x+1}, \quad (19b)$$

with  $x = m/M$ , and

$$\Omega = \frac{n_R \beta_0 \mathcal{F}(0)}{3} \sqrt{\frac{\pi \beta_0}{2M}}, \quad (20)$$

where  $\beta_0 = 1/k_B T_0$ ,  $n_R$  is the density of particles in the bath, and

$$\mathcal{F}(0) = \frac{1}{V} \sum_{\mathbf{q}} q \psi^2(q), \quad (21)$$

where  $\psi(q)$  is the Fourier transform of the central potential  $\mathcal{V}(|\mathbf{r} - \mathbf{R}_\mu|)$ ,  $V$  is the volume of the system, and  $q$  is the modulus of vector  $\mathbf{q}$ .

Evidently, Eq. (16) is the equation of conservation for the density of particles, Eqs. (17) and (18) are balance equations for the fluxes, where on the right-hand side is present a term of decay of each of both fluxes, with characteristics times  $\tau_{n1}$  and  $\tau_{n2}$  (they are the analogous of Maxwell's relaxation time in his study of viscous motion<sup>30</sup>).

To close the system of Eqs. (16)–(18), we need to obtain an expression for the third order flux  $I_n^{[3]}$  in terms of the chosen three basic variables. This is done resorting to Heims–Jaynes perturbation expansion for averages,<sup>31</sup> but in the limit of weak fluxes, what allows us to take a *linear approximation* in the fluxes, amounting to keep only the first term in Heims–Jaynes expansion. For the sake of simplicity we omit here the explicit expression for  $I_n^{[3]}(\mathbf{r}, t)$  but instead we present the result we need in the process of deriving Eq. (23) below, namely,

$$\nabla \cdot (\nabla \cdot I_n^{[3]}(\mathbf{r}, t)) = \frac{1}{m\beta_0} [\nabla^2 \mathbf{I}_n(\mathbf{r}, t) + 2\nabla \cdot (\nabla \cdot \mathbf{I}_n(\mathbf{r}, t))], \quad (22)$$

where, as usual,  $\nabla$  is the gradient operator (we recall that  $\nabla \cdot$  is the the divergence operator).

Using Eqs. (16)–(18) and Eq. (22), after some algebra we obtain that

$$\left[ \frac{\partial^3}{\partial t^3} + \frac{1}{\tau_{\text{eff}}(x)} \frac{\partial^2}{\partial t^2} + \frac{1}{\theta_{n(2)}^2(x)} \frac{\partial}{\partial t} - \frac{c_{n(2)}^2(x)}{\tau_{n2}(x)} \nabla^2 \right] n(\mathbf{r}, t) = -\frac{1}{m\beta_0} \nabla \cdot [\nabla^2 \mathbf{I}_n(\mathbf{r}, t) + 2\nabla \cdot (\nabla \cdot \mathbf{I}_n(\mathbf{r}, t))], \quad (23)$$

where

$$c_{n(2)}^2(x) = 1/m\beta_0 = k_B T_0 / m = v_{\text{th}}^2 / 3, \quad (24)$$

with  $v_{\text{th}}$  being the so-called thermal velocity defined by  $m v_{\text{th}}^2 / 2 = 3 k_B T_0 / 2$ , and we have introduced the characteristic times

$$\tau_{\text{eff}}^{-1}(x) = \tau_{n1}^{-1}(x) + \tau_{n2}^{-1}(x) = \tau_{n+}(x) / \theta_{n(2)}^2(x), \quad (25a)$$

$$\tau_{n+}(x) = \tau_{n1}(x) + \tau_{n2}(x), \quad (25b)$$

$$\theta_{n(2)}(x) = [\tau_{n1}(x) \tau_{n2}(x)]^{1/2}. \quad (25c)$$

Neglecting the right-hand side of Eq. (23), because its contribution is proportional to the third order in the wave number and we only maintain contributions up to the second order in the wave number (the limit of wavelengths larger than the interparticle separation), Eq. (23) becomes

$$\left[ \frac{\partial^3}{\partial t^3} + \frac{1}{\tau_{\text{eff}}(x)} \frac{\partial^2}{\partial t^2} + \frac{1}{\theta_{n(2)}^2(x)} \frac{\partial}{\partial t} - \frac{c_{n(2)}^2(x)}{\tau_{n2}(x)} \nabla^2 \right] n(\mathbf{r}, t) = 0. \quad (26)$$

Equation (26) is a differential equation of third order in time, which we proceed to analyze. First, we notice the fact that if in this Eq. (26) we neglect the third derivative in time (smooth variation in time), it goes over a telegraphistlike (parabolic-type) equation, namely,

$$\left[ \frac{1}{\tilde{c}_{n(2)}^2(x)} \frac{\partial^2}{\partial t^2} + \frac{1}{D_{n(2)}(x)} \frac{\partial}{\partial t} - \nabla^2 \right] n(\mathbf{r}, t) = 0, \quad (27)$$

where  $\tilde{c}_{n(2)}$  is the velocity of propagation,

$$\tilde{c}_{n(2)}^2(x) = \left[ \frac{\tau_{\text{eff}}(x)}{\tau_{n2}(x)} \right] c_{n(2)}(x) = \frac{1}{3} \left[ \frac{\tau_{\text{eff}}(x)}{\tau_{n2}(x)} \right] v_{\text{th}}^2, \quad (28)$$

and  $D_{n(2)}(x)$ , playing the role of a diffusion coefficient, is given by

$$D_{n(2)}(x) = \tilde{c}_{n(2)}^2(x) \tau_{n+}(x) = c_{n(2)}^2(x) \tau_{n1}(x) = \frac{1}{3} v_{\text{th}}^2 \tau_{n1}(x). \quad (29)$$

Moreover, if in Eq. (27) we take  $\tilde{c}_{n(2)}$  going to infinity, however keeping  $D_{n(2)}$  finite, we get a Fick-type diffusion equation. We proceed next to look for a criterion for justifying the use of different truncations of description. For that purpose, we first begin to introduce a notation to characterize the different possible domains of validity (implying in the conditions which justify the use of a truncated description) of IST. We call it Informational-Statistical Thermodynamics of

$r$ -rank, for short  $IST\{r\}$ , the one in which are retained the densities and their fluxes only up to order  $r$  in the basic set of nonequilibrium thermodynamic variables.

We begin by considering the domains of validity, in wave number and frequency space, of  $IST\{0\}$ ,  $IST\{1\}$ , and  $IST\{2\}$ .

### A. Frontier of the domain of $IST\{0\}$ with $IST\{1\}$

First, we look for the eigenvalues of Eq. (27),  $\alpha_{(2)}$ , which provide the frequency dispersion spectrum. The characteristic equation is

$$\left[ \frac{\alpha_{(2)}(x, \mathbf{Q})}{\tilde{c}_{n(2)}(x)} \right]^2 + \frac{\alpha_{(2)}(x, \mathbf{Q})}{D_{n(2)}(x)} - Q^2 = 0, \quad (30)$$

where  $\mathbf{Q}$  is the wave vector ( $Q$  the wave number) associated with each normal mode of propagation.

Solving Eq. (30) the eigenvalues are

$$\alpha_{(2)}(x, \mathbf{Q})_{\pm} = -\frac{1}{2\tau_{n+}(x)} \pm \left[ \left( \frac{\tilde{c}_{n(2)}^2(x)}{2D_{n(2)}(x)} \right)^2 - \tilde{c}_{n(2)}^2(x)Q^2 \right]^{1/2}, \quad (31)$$

or, after using Eqs. (28) and (29), they can be written as

$$\alpha_{(2)}(x, \mathbf{Q})_{\pm} = -[2\tau_{n+}(x)]^{-1} \pm i\{\tilde{c}_{n(2)}^2(x)Q^2 - [2\tau_{n+}(x)]^{-2}\}^{1/2}. \quad (32)$$

Inspection of Eq. (32) tells us that for

$$2\tilde{c}_{n(2)}(x)\tau_{n+}(x)Q > 1, \quad (33)$$

the motion consists of *damped undulatory motion*, propagating with velocity  $\tilde{c}_{n(2)}(x)$ , a frequency given by the square root in Eq. (32) (a renormalized soundlike dispersion relation), and a lifetime of the order of  $2\tau_{n+}(x)$ .

On the other hand, for values of  $Q$  sufficiently small (large wavelengths) such that the inequality

$$2\tilde{c}_{n(2)}(x)\tau_{n+}(x)Q < 1, \quad (34)$$

is satisfied,  $\alpha_{(2)}$  is a real number and the *motion is overdamped*, consisting of two contributions decaying with lifetimes,

$$-\alpha_{(2)}(x, \mathbf{Q})_+ \approx \tau_{n+}^{-1}(x), \quad (35)$$

$$-\alpha_{(2)}(x, \mathbf{Q})_- \approx D_{n(2)}(x)Q^2. \quad (36)$$

For very small wave numbers (very long wavelengths) such that  $[\tau_{n+}(x)]^{-1} \gg D_{n(2)}(x)Q^2$ , the contribution with the lifetime of Eq. (35) dies down more rapidly than the other, and this overdamped motion consist of a diffusive motion. In fact,  $\alpha_{(2)}$  of Eq. (36) is the eigenvalue of the equation of diffusion with a diffusion coefficient given by Eq. (29); this result is well known from textbook analyses of the telegraphist equation.<sup>32</sup> We call attention to the fact that the transition from damped wave motion to near diffusive motion, becomes evident in experiments related to the technological process of thermal-laser stereolithography<sup>33</sup> briefly described in next section.

We can now derive a boundary between  $IST\{0\}$  and  $IST\{1\}$ , which are, respectively, the equivalent at the mechanical-statistical level of description of Classical Irreversible Thermodynamics (e.g., Ref. 34) and earlier versions of Extended Irreversible Thermodynamics (e.g., Ref. 35). Such a boundary may be set at the wavelength

$$\begin{aligned} \lambda_{(01)}(x) &= Q_{(01)}^{-1}(x) = 2\tilde{c}_{n(2)}(x)\tau_{n+}(x) \\ &= \frac{2}{3}v_{th}\tau_{n1}(x) = 2D_{n(2)}(x)/\tilde{c}_{n(2)}(x), \end{aligned} \quad (37)$$

when the square root in Eq. (32) becomes null, passing from real to imaginary values. We recall that the characteristic times  $\tau_{n+}$  and  $\tau_{n1}$  are given in Eqs. (25b) and (19a), respectively, the relation between the renormalized velocity and the thermal velocity in Eq. (28), and the diffusion coefficient in Eq. (29).

We stress the point that then *overdamped motion is characteristic of movements involving wavelengths  $\lambda > \lambda_{(01)}$ , and nearly pure diffusive motion follows in the case of very long wavelengths or more precisely for  $\lambda \gg \lambda_{(01)}$ .*

Let us reconsider this last point in an alternative way. Equation (27) can be written as

$$\left[ \frac{\partial}{\partial t} - D_{n(2)}(x)\nabla^2 \right] n(\mathbf{r}, t) = -\frac{D_{n(2)}(x)}{\tilde{c}_{n(2)}^2(x)} \frac{\partial^2}{\partial t^2} n(\mathbf{r}, t), \quad (38)$$

the left-hand side being of the form of Fick's diffusion equation. To evaluate when the latter is a good approximation we consider when the right-hand side can be neglected in comparison with the left. We look for the eigenvalues  $\alpha_{(1)}$  of this equation, but introducing a kind of perturbation procedure, consisting of looking into the influence of the right-hand side when the movement is nearly diffusive. The exact eigenvalue equation is

$$\alpha_{(1)}(x, \mathbf{Q}) + D_{n(2)}(x)Q^2 = -\frac{D_{n(2)}(x)}{\tilde{c}_{n(2)}^2(x)} \alpha_{(1)}^2(x, \mathbf{Q}), \quad (39)$$

but introducing on the right, in place of  $\alpha_{(1)}$ , the eigenvalue  $\alpha_{(2)}$  of Eq. (36), Eq. (39) becomes

$$\alpha_{(1)}(x, \mathbf{Q}) = -D_{n(2)}(x)Q^2[1 - \tilde{\lambda}_D^2(x)Q^2], \quad (40)$$

where

$$\tilde{\lambda}_D(x) = \frac{D_{n(2)}(x)}{\tilde{c}_{n(2)}(x)} = \frac{1}{2}\lambda_{(01)}(x), \quad (41)$$

with  $\lambda_{(01)}$  is given by Eq. (37).

Therefore, we can expect that the purely diffusive motion is predominant when the last contribution in Eq. (40) is negligible as compared with the first, that is when

$$\tilde{\lambda}_D(x)Q \ll 1, \quad (42)$$

that is, for wavelengths much larger than  $\lambda_{(01)}$  as shown in the previous analysis.

Moreover, concluding this subsection we stress the fact that, because the dispersion relation relates frequency and wave number in the mode analysis of the motion, the above considered frontier also implies to low frequencies. In fact, using Eqs. (37) and (32), we have the boundary expressed now in terms of the frequency as

$$\omega_{(01)}(x) = \{\tilde{c}_{n(2)}^2(x)Q_{(01)}^2(x) - [2\tau_{n+}(x)]^{-2}\}^{1/2} = 0, \quad (43)$$

indicating a kind of “soft mode” transition, corresponding to a change from damped undulatory motion to an overdamped one, with diffusion at sufficiently long wavelengths.

**B. Frontier of the domain of IST{1} with IST{2}**

Let us consider now the transition from the regime of IST{1} to IST{2}. For that purpose we write Eq. (26) in the form,

$$\left[ \frac{1}{\tilde{c}_{n(2)}^2(x)} \frac{\partial^2}{\partial t^2} + \frac{1}{D_{n(2)}(x)} \frac{\partial}{\partial t} - \nabla^2 \right] n(\mathbf{r}, t) = - \frac{\tau_{\text{eff}}(x)}{\tilde{c}_{n(2)}^2(x)} \frac{\partial^3}{\partial t^3} n(\mathbf{r}, t), \quad (44)$$

the left-hand side being the telegraphistlike equation of Eq. (27). Next we proceed in a similar way as done in the last subsection. We look for the eigenvalues  $\alpha_{(3)}$  of Eq. (44), that is, the solution of the equation,

$$\alpha_{(3)}^2(x, \mathbf{Q}) + \frac{\tilde{c}_{n(2)}^2(x)}{D_{n(2)}(x)} \alpha_{(3)}(x, \mathbf{Q}) + \tilde{c}_{n(2)}^2(x)Q^2 = - \tau_{\text{eff}}(x)\alpha_{(3)}^3(x, \mathbf{Q}). \quad (45)$$

Next we approximate the right-hand side entering the modulus of the eigenvalue of the telegraphist equation,  $|\alpha_{(2)}(x, \mathbf{Q})_{\pm}|$ , of Eq. (31), in place of  $\alpha_{(3)}(x, \mathbf{Q})$ , and we reorganize the resulting approximated eigenvalue equation by dividing it by the fourth power of the velocity  $\tilde{c}_{n(2)}$  to obtain

$$\left[ \frac{\alpha_{(3)}(x, \mathbf{Q})}{\tilde{c}_{n(2)}(x)} \right]^2 + \frac{\alpha_{(3)}(x, \mathbf{Q})}{D_{n(2)}(x)} + Q^2 = \frac{\Delta \tilde{c}_{n(2)}^2(x, \mathbf{Q})}{\tilde{c}_{n(2)}^2(x)} Q^2, \quad (46)$$

where we have introduced the quantity,

$$\Delta \tilde{c}_{n(2)}^2(x, \mathbf{Q}) = \frac{1}{8} [\tau_{\text{eff}}(x)/\tau_{n+}^3(x)] \lambda_{(01)}^3(x) Q, \quad (47)$$

with  $D_{n(2)}$  given by Eq. (29).

Inspection of Eq. (46) tells us that we recover the approximate dispersion relation for the telegraphist equation, Eq. (32), i.e.,  $\alpha_{(3)} \approx \alpha_{(2)}$ , when it is verified that

$$\frac{\Delta \tilde{c}_{n(2)}^2(x, \mathbf{Q})}{\tilde{c}_{n(2)}^2(x)} \ll 1. \quad (48)$$

We can alternatively write this inequality in the form,

$$\lambda_{(12)}(x)Q \ll 1, \quad (49)$$

after introducing the characteristic wavelength,

$$\lambda_{(12)}(x) = \left[ \frac{\tau_{\text{eff}}(x)}{2\tau_{n+}(x)} \right] \lambda_{(01)}(x) = \left\{ \frac{\tau_{n1}(x)\tau_{n2}(x)}{2[\tau_{n1}(x) + \tau_{n2}(x)]^2} \right\} \lambda_{(01)}(x), \quad (50)$$

with  $\lambda_{(01)}(x)$  given by Eq. (37), or also as

$$\begin{aligned} \lambda_{(12)}(x) &= Q_{(12)}^{-1}(x) \\ &= \tilde{c}_{n(2)}(x)\tau_{\text{eff}}(x) \\ &= \frac{1}{\sqrt{3}} v_{\text{th}} \left[ \frac{\tau_{\text{eff}}(x)}{\tau_{n2}(x)} \right]^{1/2} \tau_{\text{eff}}(x) = \frac{D_{n(2)}(x)}{\tilde{c}_{n(2)}(x)} \left[ \frac{\tau_{\text{eff}}(x)}{\tau_{n2}(x)} \right]. \end{aligned} \quad (51)$$

Consequently, a description in the truncated IST{1} can be used when the motion, in its normal mode analysis, involves wavelengths verifying that

$$\lambda \gg Q_{(12)}^{-1}(x) = \lambda_{(12)}(x) = \tilde{c}_{n(2)}(x)\tau_{\text{eff}}(x). \quad (52)$$

Hence, *damped undulatory motion—governed by a telegraphistlike equation—is characteristic of movements involving wavelengths  $\lambda \gg \lambda_{(12)}$* . When this restriction is not met, that is,  $\lambda$  becomes of the order of  $\lambda_{(12)}$  we need to go over the domain of IST{3}. Moreover, from Eq. (50) we can see that always  $\lambda_{(12)}(x) < \lambda_{(01)}(x)$ .

**C. Characterization of the descriptions**

Summarizing, according to the results of the two previous subsections, we can characterize four regimes of thermohydrodynamic behavior in the given system. The use of each one depends, as we have seen, on the range of wavelengths (or, alternatively, through the dispersion relation, on the range of frequencies) that have a prevalence in the Fourier analysis of the motion of the density of particles in the given experimental conditions.

These four regimes are: (1) diffusive motion; (2) overdamped motion; (3) damped undulatory motion; (4) damped undulatory motion accompanied of an overdamped motion. These are the solutions, respectively, (1) of the diffusion equation; (2) and (3) of the telegraphist-like equation, Eq. (27); (4) of the third order equation, Eq. (26). Also, as noticed, this corresponds to descriptions in IST{0}, IST{1}, and IST{2}. Only the transition from undulatory damped to overdamped regimes is characterized by a clear cut frontier, namely,  $\lambda_{(01)} = 2\tilde{c}_{n(2)}\tau_{n+}$ . The others are characterized by the conditions of the motion to proceed in a regime of predominance of wavelengths much larger than  $\tilde{\lambda}_D = \tilde{c}_{n(2)}\tau_{n+}$  (almost purely diffusive), and  $\lambda_{(12)} = \tilde{c}_{n(2)}\tau_{\text{eff}}$  (almost purely undulatory damped).

We have determined, in the case of the Brownian-type model of Eq. (1) and in terms of the relation of masses  $x = m/M$ , the domains of validity of each of the regimes we have considered. In Fig. 1 are displayed the characteristic times  $\tau_{n1}$  and  $\tau_{n2}$ , in units of the quantity (with dimensions of time)  $\Omega^{-1}$  of Eq. (20). The boundary wavelengths, in the scaled form  $\tilde{\lambda} = (\Omega/v_{\text{th}})\lambda = \lambda/\Lambda$ , are shown in Fig. 2 in terms of  $x$ , thus providing the regions of validity of the truncations that lead to the different regimes.

**IV. SPECIFIC ILLUSTRATIONS AND EXPERIMENTAL OBSERVATION**

In this section we illustrate how it proceeds the change of regime between IST{1} and IST{2}, and its experimental observation. First, we can mention the quite interesting and illustrative example consisting in the study of the technological process of thermal laser stereolithography (better re-

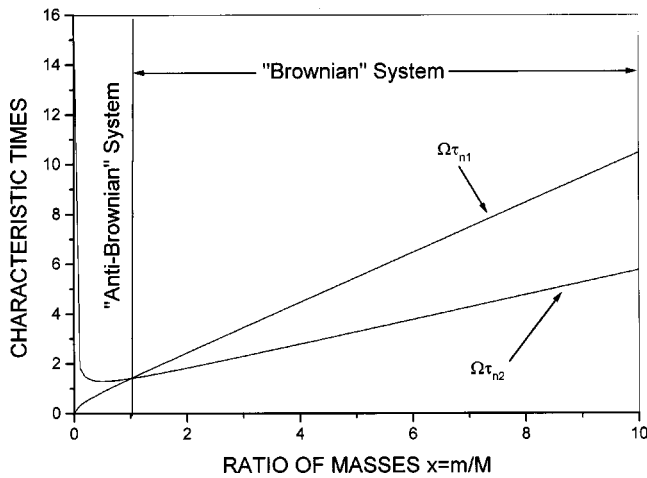


FIG. 1. Dependence on the ratio of masses of the characteristic times of Eq. (19), expressed in units of  $\Omega^{-1}$  of Eq. (20).

ferred to as rapid prototyping). The theoretical and experimental aspects are describe in detail in Ref. 33, to which we refer the reader, and here we only briefly summarize the results.

The process consists in sintering of a thermosensitive resin (by illumination with an infrared  $\text{CO}_2$ -laser) for creating prototypes for casting of parts for automotive, medical, etc. uses. Hence, it requires high definition in the production of the prototype, i.e., a rapid sintering well localized in the small region of laser beam focalization. As shown in Ref. 33 if the system is in the domain of  $\text{IST}\{2\}$ , there follows propagation of second sound (thermal) waves at long distances and the sample is ruined. This occurs when  $Q_{(01)} < r_0^{-1}$ , where  $r_0$  is the radius of the spot of laser-beam focalization on the resin ( $Q_{(01)}$  is referred to as  $k_M$  in Ref. 33). ‘‘Tampering’’ with the resin by adding aluminum powder (for example) modifies (decreases) the diffusivity  $D_{n(2)}$  and hence changes  $Q_{(01)}$  in such a way to have  $Q_{(01)} > r_0^{-1}$  [cf. Eq. (37)]. No wave propagation of heat occurs (regime of  $\text{IST}\{0\}$ ) and a

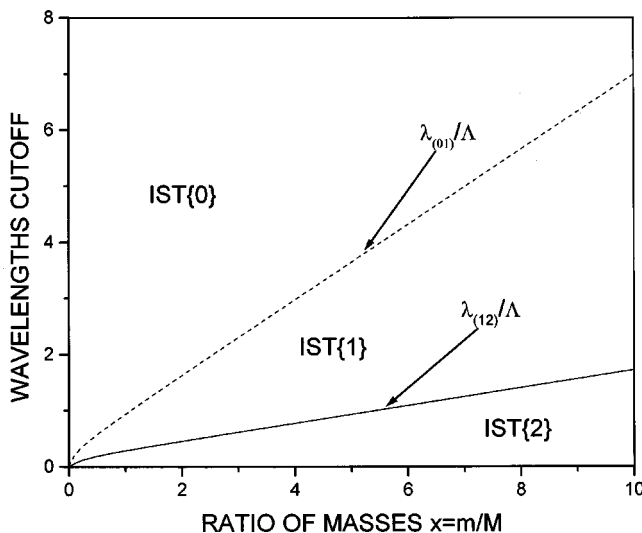


FIG. 2. The domain boundaries in scaled wavelengths as a function of the ratio of masses. Quantities  $\lambda_{(01)}$  and  $\lambda_{(12)}$  are given in terms of the scale  $\Lambda = v_{\text{th}}\Omega^{-1}$ .

well defined good prototype is produced. We may say that this change of regime can be ‘‘seen’’ in the photographs of Fig. 4 in Ref. 33, consisting in cylindrical models (rings) obtained using samples with varying values of  $Q_{(01)}$  ( $k_M$  in Ref. 33). This is in what relates to thermal perturbation (the one relevant to the technoindustrial process) but density perturbation is also present; in some cases it can be seen with the unaided eye (or using a simple magnifying lens) propagation of material waves in the pure resin but practically disappearing in the more and more doped resin. This indicates the transition of regime in the motion of the density as the one we are considering here. Figures 2 and 3 in Ref. 33 provide a description of the phenomenon, and numerical analyses are given in the text.

Another quite interesting illustration consists in the question of change of regime in the description of hydrodynamic properties now in the case of a system of mobile electrons in the conduction band of a  $n$ -doped direct-gap polar semiconductor. We can derive exact results for the characteristic times in terms of the physical parameters of the material and its thermodynamic state, and to obtain universal laws for the determination of the boundaries between the domains of the different truncation approaches. In this case we need to take a quantum mechanical approach, which, except for its particular algebra, is managed in the same way as the classical one of the previous section.

We further extend the considerations of the previous section—done for a classical fluid at room temperature—taking now the case when the electron system is driven out of equilibrium by the action of continuous laser illumination in phonon-assisted-free-carrier excitation. The nonequilibrium macroscopic (thermodynamic) state of the electron system is characterized by the concentration  $\bar{n}$  and the quasitemperature  $T_e^*$  it attains in the steady state (see, for example, Ref. 36). This quasitemperature is determined by the intensity of the pumping laser. This electron system interacts with the lattice vibrations, which are assumed to remain at the constant temperature  $T_0$  of a thermal reservoir. We keep only the largely predominant Fröhlich interaction between electrons and phonons in this polar materials.<sup>37</sup>

Moreover, we introduce besides the pair of global homogeneous quantities  $\bar{n}$  and  $T_e^*$  the local density and its two first fluxes. In reciprocal  $\mathbf{Q}$ -space they are

$$n(\mathbf{Q}, t) = \sum_{\mathbf{k}} n_{\mathbf{k}\mathbf{Q}}(t), \tag{53}$$

$$\mathbf{I}_n(\mathbf{Q}, t) = \sum_{\mathbf{k}} \frac{\hbar \mathbf{k}}{m^*} n_{\mathbf{k}\mathbf{Q}}(t), \tag{54}$$

$$I_n^{[2]}(\mathbf{Q}, t) = \frac{1}{3} \sum_{\mathbf{k}} \left| \frac{\hbar \mathbf{k}}{m^*} \right|^2 n_{\mathbf{k}\mathbf{Q}}(t) \hat{I}^{[2]}. \tag{55}$$

In these equations  $\epsilon_{\mathbf{k}} = \hbar^2 k^2 / 2m^*$  (in an effective mass approximation),  $\mathbf{k}$  and  $\mathbf{Q}$  run over the Brillouin zone;  $n_{\mathbf{k}\mathbf{Q}}(t) = \langle c_{\mathbf{k}+(1/2)\mathbf{Q}}^\dagger c_{\mathbf{k}-(1/2)\mathbf{Q}} | t \rangle$  is Dirac–Landau–Wigner single-particle density matrix, where  $c^\dagger(c)$  is the usual creation (annihilation operators) and we are omitting the spin index. The average value is over the auxiliary coarse-grained non-equilibrium statistical operator in MaxEnt–NESOM, that is,

$$n_{\mathbf{k}\mathbf{Q}}(t) = \text{Tr}\{c_{\mathbf{k}+(1/2)\mathbf{Q}}^\dagger c_{\mathbf{k}-(1/2)\mathbf{Q}} \bar{\mathcal{Q}}(t,0)\}, \quad (56)$$

as in Ref. 36 but augmented with the presence of the second order flux. Finally  $\hat{I}^{[2]}$  is the unit second rank tensor since because of isotropy  $I_n^{[2]}$  is diagonal with all components equal to one-third of its trace.

The equations of evolution are derived following the same kinetic theory<sup>22,23,29</sup> as in the previous section [cf. Eqs. (16)–(18)] which in the reciprocal space read as

$$\frac{\partial}{\partial t} n(\mathbf{Q},t) - i\mathbf{Q} \cdot \mathbf{I}_n(\mathbf{Q},t) = 0, \quad (57)$$

$$\frac{\partial}{\partial t} \mathbf{I}_n(\mathbf{Q},t) - i\mathbf{Q}\varphi_n(\mathbf{Q},t) = -\frac{\mathbf{I}_n(\mathbf{Q},t)}{\tau_{n1}(z)} + i\frac{\bar{n}}{m^*} \mathbf{Q}V(\mathcal{Q})n(\mathbf{Q},t), \quad (58)$$

$$\begin{aligned} \frac{\partial}{\partial t} \varphi_n(\mathbf{Q},t) - (10/3\beta m^*)i\mathbf{Q} \cdot \mathbf{I}_n(\mathbf{Q},t) \\ = \frac{n(\mathbf{Q},t)}{m^* \beta \tau_{n2}(z)} - \frac{\varphi_n(\mathbf{Q},t)}{\tau_{n2}(z)}. \end{aligned} \quad (59)$$

Equation (57) is the conservation equation for the density (matter), Eq. (58) is the balance equation for the density flux, and Eq. (59) the balance equation for one-third the trace of the second order flux. Moreover,  $\beta = 1/k_B T_e^*$  (reciprocal of the quasitemperature of the electrons);  $z = \hbar\omega_0/k_B T_e^* = T_E/T_e^*$ , with  $\omega_0$  the frequency of the LO phonons and  $k_B T_E = \hbar\omega_0$  introduces Einstein temperature for this phonons (it can be noticed that  $z$  plays here a similar role to  $x$  in Sec.III). We have taken into account only Fröhlich interaction of electrons with LO phonons since in this polar semiconductors it is much stronger than deformation potential and piezoelectric interactions. Moreover, we have introduced the reciprocal characteristic times,

$$\begin{aligned} \frac{1}{\tau_{n1}(z)} = \Omega_0 \frac{2}{3} z^{3/2} e^{-z/2} \left[ \left( 1 + 2\nu_0 + \frac{\nu_0}{\bar{\nu}} \right) K_1(z/2) \right. \\ \left. + \left( 1 - \frac{\nu_0}{\bar{\nu}} \right) K_0(z/2) \right], \end{aligned} \quad (60)$$

$$\frac{1}{\tau_{n2}(z)} = \Omega_0 \frac{4}{9} \left( \frac{k_B T_0}{\hbar\omega_0} \right) z^{3/2} \nu_0 e^{z/2} K_0(z/2), \quad (61)$$

where

$$\Omega_0 = \left( \frac{2\hbar\omega_0}{\pi m^*} \right)^{1/2} \left( \frac{eE_0}{\hbar\omega_0} \right), \quad (62)$$

$$\nu_0 = [\exp\{\hbar\omega_0/k_B T_0\} - 1]^{-1}, \quad (63)$$

$$\bar{\nu} = [e^z - 1]^{-1}, \quad (64)$$

and  $K_0$  and  $K_1$  are Bessel functions. In Eq. (60)  $\tau_{n1}$  is the electron momentum relaxation time<sup>38</sup> and Eq. (61) gives the electron density second flux Maxwell's characteristic time [the analogous of the one in Eq. (18)] which resembles that of energy.<sup>38</sup> Finally, in Eq. (58) the last term on the right-hand side accounts for the Coulomb interaction between electrons, dealt with in the random phase approximation,<sup>39,40</sup> where  $V(\mathcal{Q}) = 4\pi e^2/\epsilon_0 \mathcal{Q}^2$  is the Fourier transform of the

TABLE I. Scaling parameters and limiting wavelengths (at 300 K).

	$\Omega_0(s^{-1})$	$\Lambda_0(\text{cm})$	$\bar{\lambda}_{(01)}(\text{cm})$	$\bar{\lambda}_{(12)}(\text{cm})$
GaAs	$3.1 \times 10^{12}$	$1 \times 10^{-5}$	$3.4 \times 10^{-5}$	$0.25 \times 10^{-5}$
CdS	$4.5 \times 10^{13}$	$4.1 \times 10^{-7}$	$1.5 \times 10^{-7}$	$1.1 \times 10^{-7}$
GaN	$6.7 \times 10^{13}$	$4.3 \times 10^{-7}$	$5.9 \times 10^{-7}$	$2.5 \times 10^{-7}$

Coulomb potential ( $\epsilon_0$  is the static background dielectric constant) and  $\bar{n}$  is the concentration of the mobile electrons; this term gives rise to the plasma waves in the medium (result of the particles being charged) which is the equivalent of the sound waves in the system of Sec. III. To simplify matters we consider a low density, say  $\bar{n} \approx 10^{15} \text{ cm}^{-3}$ , in order to neglect this term and then to have equations quite similar to those of Sec. III. Finally,  $eE_0$  is the coupling strength in Fröhlich's electron-LO phonon interaction.<sup>38</sup>

Using Eqs. (57)–(59) we proceed with an analysis identical to the one used in Sec. III and, without going into details of the straightforward but lengthy algebra involved, we obtain the frontiers

$$\bar{Q}_{(01)}^{-1}(z) = \bar{\lambda}_{(01)}(z) \approx \{z/4\bar{\tau}_{n1}(z)[\bar{\tau}_{n1}(z) + \bar{\tau}_{n2}(z)]\}^{-1/2}, \quad (65)$$

$$\bar{Q}_{(12)}^{-1}(z) = \bar{\lambda}_{(12)}(z) \approx \left\{ z\bar{\tau}_{n2}(z) \left[ \frac{1}{\bar{\tau}_{n1}(z)} + \frac{1}{\bar{\tau}_{n2}(z)} \right]^3 \right\}^{-1/2}, \quad (66)$$

where  $\tau_{n1}(z) = \Omega_0 \bar{\tau}_{n1}(z)$ ;  $\tau_{n2}(z) = \Omega_0 \bar{\tau}_{n2}(z)$ ;  $\bar{\lambda}_{(01)} = \lambda_{(01)}/\Lambda_0$ ;  $\bar{\lambda}_{(12)} = \lambda_{(12)}/\Lambda_0$ , with  $\Lambda_0 = \Omega_0^{-1}(\hbar\omega_0/m^*)^{1/2}$ . Introducing in these Eqs. (65) and (66) the definitions of  $\Lambda_0$  and  $\Omega_0$  and Eqs. (25a) and (25b), we can rewrite Eqs. (65) and (66) in the form

$$\bar{\lambda}_{(01)}(z) = 2\bar{c}_{n(2)}(z)\bar{\tau}_+(z) = \frac{2}{\sqrt{3}} v_{\text{th}} \left[ \frac{\bar{\tau}_{\text{eff}}(z)}{\bar{\tau}_{n2}(z)} \right]^{1/2} \bar{\tau}_+(z), \quad (67)$$

$$\bar{\lambda}_{(12)}(z) = \bar{c}_{n(2)}(z)\bar{\tau}_{\text{eff}}(z) = \frac{1}{\sqrt{3}} v_{\text{th}} \left[ \frac{\bar{\tau}_{\text{eff}}(z)}{\bar{\tau}_{n2}(z)} \right]^{1/2} \bar{\tau}_{\text{eff}}(z), \quad (68)$$

which are of the same form of Eqs. (37) and (51).

Hence, for the classical-mechanical case of an ideal gas in interaction with a bath consisting of other ideal gas, and the quantum-mechanical case of an electron system (free Landau quasiparticles) in interaction with a bath consisting of the lattice vibrations (a gas of LO-phonons), and for low plasma frequency (low concentration of carriers), the frontiers  $\lambda_{(01)}$  and  $\lambda_{(12)}$  are formally identical [cf. Eqs. (37) and (51) with (67) and (68)].

We can see that written in reduced variables Eqs. (65) and (66) are universal for all direct-gap polar semiconductors, e.g., those of the type III-V, II-VI, III-nitrides, etc. In Table I we present numerical values of  $\Omega_0$  and  $\Lambda_0$  for three typical semiconductors, together with values of  $\bar{\lambda}_{(01)}$  and  $\bar{\lambda}_{(12)}$  corresponding to a quasitemperature of 300 K.

In Fig. 3 are displayed, as a function of the nonequilibrium steady state of the system characterized, for fixed  $\bar{n}$ , by a varying quasitemperature  $T_e^*$  (determined by the action of



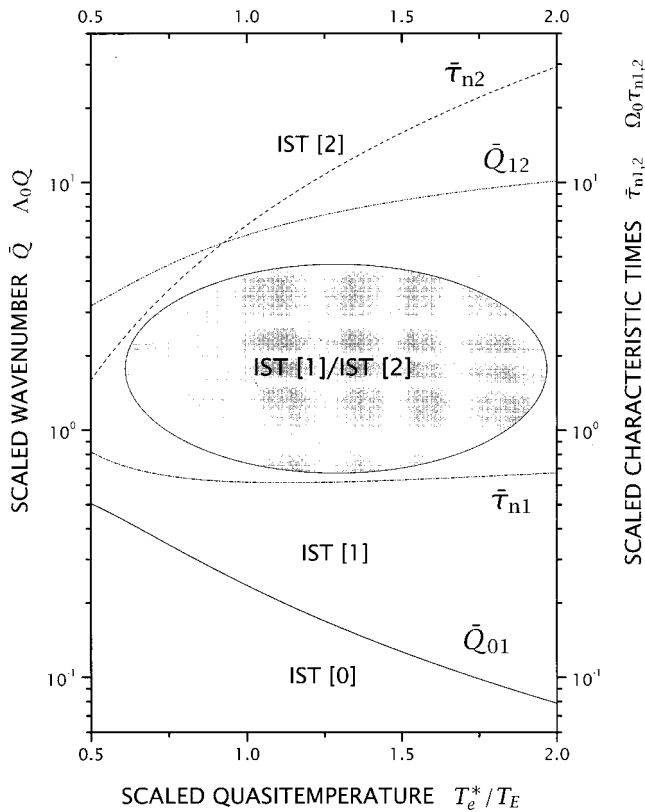


FIG. 3. The domain boundaries in scaled wavelengths versus carrier quasitemperature in the case of direct-gap polar semiconductors (full line and left ordinate), and the scaled characteristic times (dashed line and right ordinate). The shaded area corresponds to an intermediate interphase between descriptions IST{1} and IST{2}, that is, corrections to the IST{1} description begin to be relevant.

the constantly acting external pump, and given in units of Einstein temperature, i.e., as  $z^{-1} = T_e^*/T_E$ , the two main characteristic times (right ordinate and dashed lines) and the frontiers in wave number  $Q_{(01)}$  and  $Q_{(12)}$  (left ordinate and full lines). If we consider GaAs ( $T_E \approx 430$  K and  $\Lambda_0 \approx 10^3$  Å), the frontier wave numbers at  $T_c^* \approx 300$  K are  $Q_{(01)} \approx 3 \times 10^4$  cm<sup>-1</sup> and  $Q_{(12)} \approx 4 \times 10^5$  cm<sup>-1</sup>.

Experimental observation of the change from one domain of hydrodynamic modes to another, e.g., from damped undulatory mode to a diffusive mode, can be done using light scattering. The values of  $Q$  which can be analyzed are determined by the experimental geometry, going from zero in backward scattering to twice the photon wave number in forward scattering (hence, typically from near zero to roughly  $10^4 - 10^5$  cm<sup>-1</sup>). One can then follow the values of  $Q$  in this interval and what should be observed is that the so-called Brillouin doublet (Stokes and anti-Stokes bands of damped plasma waves) with bandwidths of the order of  $\tau_{n1}^{-1}$  collapse, on decreasing values of  $Q$ , in a shiftless so-called Rayleigh band with a width of the order of  $D_{n(2)}Q^2$ , where  $D$  is the diffusion coefficient. This is clear in the case of liquids,<sup>41</sup> but is not possible to see in the plasma in semiconductors since at low plasma frequencies the doublet of plasma wave bands becomes embedded in the Raman-Doppler band of scattering by single-particle excitations (e.g., Ref. 42).

## V. CONCLUDING REMARKS

We have considered a statistical ensemble formalism which provides microscopic (mechanical-statistical) foundations to the thermohydrodynamics of fluids or fluidlike systems like the plasma in semiconductors. This is, as noticed, the so-called Nonequilibrium Statistical Operator Method, and we have resorted to Zubarev's approach.

Here we have addressed a particular aspect of MaxEnt-NESOM, which arises when dealing with thermodynamic and thermohydrodynamic problems; it is the question of using truncation procedures, that is, an imposed restriction on the chosen set of basic macrovariables to be used for the description of the evolution of the macrostate of the system. Here we have considered a simple system (kind of a Brownian system of particles interacting with a thermal bath of a much larger number of other particles). Moreover, attempting to provide a better visualization of the results, we have resorted to a description at a classical-mechanical level. Of course these results can be extended to the case of fluids described at a quantum-mechanical level. Some specific results on this question, in the case of the thermohydrodynamics of the fluid of carriers in the photoinjected plasma in semiconductors, are reported in Refs. 20 and 43, and here we have presented, in a brief form, the case of polar semiconductors in Sec IV.

In Sec. III we have shown that a truncation criterion can be derived, which rests on the characteristics of the hydrodynamic motion that develops under the given experimental procedure.

First, in a qualitative manner, we can say that, as a general "thumb rule," the criterion indicates that a more and more restricted truncation can be used when larger and larger are the prevalent wavelengths in the motion. 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 space of basic macrovariables to be used for the description of the nonequilibrium thermodynamic state of the system.

This is connected with Bogoliubov's principle of correlation weakening and hierarchy of relaxation times, as our quantitative analysis have shown. However we have considered here only three cases involving a quite small number of basic variables (corresponding to IST{0}, IST{1}, and IST{2}), the results we derived point to a conjecture for a general truncation criterion, namely, a truncation 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,  $\lambda_{(r,r+1)} = \tilde{c}_{n(r)} \tau_{\text{eff}(r,r+1)}$ . In this expression  $\tilde{c}_{n(r)}$  is the velocity of propagation of the motion and  $\tau_{\text{eff}(r,r+1)}$  is a characteristic time involving the different characteristic times which appear in the equations of evolution (or 1867-Maxwell-type relaxation times for fluxes<sup>30</sup>). We notice that in our calculations  $\lambda_{(01)} = \tilde{c}_{n(2)} \tau_{(01)}$  and  $\lambda_{(12)} = \tilde{c}_{n(2)} \tau_{(12)}$ , where  $\tau_{(01)} = 2\tau_+$  and  $\tau_{(12)} = \tau_{\text{eff}}$ . These expressions, we recall, are identical for both types of systems we have considered, the classical one and the quantum one, with the quantities involved depending on the type of interaction between system

and bath (surroundings). In the classical case also on the ratio of masses,  $x$ , and in the quantum one on the ratio of the carrier temperature and the Einstein temperature of the polar phonons,  $z$ .

From the results of previous sections, the dependence on  $x$  of the two main characteristic times, namely  $\tau_{n1}$  and  $\tau_{n2}$ , are given by Eqs. (19a) and (19b), respectively. Figure 1 tells us that  $\tau_{n1}$  is larger than  $\tau_{n2}$  for  $x > 1$ , the crossover corresponding to  $x = 1$ . For  $x > 1$  we can consider the system as a Brownian one, and for  $x < 1$  as a, say, anti-Brownian one. As we have already noticed  $\lambda_{(01)}$  is always larger than  $\lambda_{(12)}$ , what is clearly evidenced in Fig. 2, and we reinforce the fact already stressed in the previous section that there is a clear cut frontier between the domains of IST{0} and IST{1}, but not in the following frontier, which is characterized by an inequality [cf. Eq. (49)]. Moreover, the predominance of a purely diffusive regime in the domain of IST{0} is also defined by an inequality, the one of Eq. (42).

In Sec. IV we considered two illustrative examples, allowing for experimental observations of the transition of domain. One is the study of the process of sintering of thermosensitive resins in laser-thermal stereolithography. The experimental results validate (in the case for thermal motion) the criteria we have developed here (complete details in Ref. 33). Another is the case of the fluid of electrons in  $n$ -doped direct-gap polar semiconductors. We have been able to derive general results for this family of materials, with numerical values to be obtained by simply specifying the two scaling quantities,  $\Omega_0$  and  $\Lambda_0$ , for each kind of material. The transition of domain between IST{0} and IST{1} can be evidenced via experiments of Raman scattering.

## ACKNOWLEDGMENTS

We acknowledge financial support provided to our group, on different occasions, by the State of São Paulo Research Agency (FAPESP), the National Research Council (CNPq), the Ministry of Planning (Finep), Unicamp Foundation (FAEP), IBM Brasil, USA-National Science Foundation (USA-Latinamerica Cooperation Project, NSF, Washington); the John Simon Guggenheim Memorial Foundation (New York, USA).

<sup>1</sup>R. Zwanzig, in *Perspectives in Statistical Physics*, edited by H. J. Raveché (North-Holland, Amsterdam, 1981).

<sup>2</sup>R. Luzzi and A. R. Vasconcellos, *Fortschr. Phys.* **38**, 887 (1990).

<sup>3</sup>D. N. Zubarev, *Nonequilibrium Statistical Thermodynamics* (Consultants Bureau, New York, 1974) [Neravnovesnaia Statisticheskaiia Termodinamika (Izd. Nauka, Moscow, 1971)].

<sup>4</sup>D. N. Zubarev, V. N. Morozov, and G. Röpke, *Statistical Mechanics of Nonequilibrium Processes* (Akademie Verlag, Berlin, 1996 and 1997, respectively), Vols. 1 and 2.

<sup>5</sup>D. N. Zubarev and V. P. Kalashnikov, *Teor. Mat. Fiz.* **1**, 137 (1969); [*Theor. Math. Phys.* **1**, 108 (1970)].

<sup>6</sup>J. G. Ramos, A. R. Vasconcellos, and R. Luzzi, *Fortschr. Phys.* **43**, 265 (1995).

<sup>7</sup>R. Luzzi, A. R. Vasconcellos, and J. G. Ramos, in *Foundations of a Nonequilibrium Ensemble Formalism*, in *Fundamental Theories of Physics Series*, edited by A. Van der Merwe (Kluwer Academic, Dordrecht, in press).

<sup>8</sup>L. S. Garcia-Colin, A. R. Vasconcellos, and R. Luzzi, *J. Non-Equilib. Thermodyn.* **19**, 24 (1994).

<sup>9</sup>A. R. Vasconcellos, R. Luzzi, and L. S. Garcia-Colin, *Phys. Rev. A* **43**, 6622 (1991).

<sup>10</sup>M. A. Tenan, A. R. Vasconcellos, and R. Luzzi, *Fortschr. Phys.* **47**, 1 (1997).

<sup>11</sup>R. Luzzi, A. R. Vasconcellos, and J. G. Ramos, *Fortschr. Phys.* **47**, 401 (1999); *Statistical Foundations of Irreversible Thermodynamics* in *Texte zur Physik Series*, edited by W. Ebeling (Teubner, Stuttgart-Leipzig, in press).

<sup>12</sup>J. G. Ramos, A. R. Vasconcellos, and L. S. Garcia-Colin, *Braz. J. Phys.* **27**, 585 (1997).

<sup>13</sup>V. P. Kalashnikov, *Teor. Mat. Fiz.* **9**, 94 (1971); [*Theor. Math. Phys.* **9**, 1003 (1971)].

<sup>14</sup>V. P. Kalashnikov, *Sov. Phys. Usp.* **9**, 94 (1971).

<sup>15</sup>R. Luzzi and A. R. Vasconcellos, *J. Stat. Phys.* **23**, 539 (1980).

<sup>16</sup>A. R. Vasconcellos, R. Luzzi, and L. S. Garcia-Colin, *Physica A* **221**, 478 (1995).

<sup>17</sup>A. C. Algarte, A. R. Vasconcellos, and R. Luzzi, *Phys. Rev. B* **54**, 11311 (1996).

<sup>18</sup>R. Luzzi, A. R. Vasconcellos, D. Jou, and J. Casas-Vázquez, *J. Chem. Phys.* **107**, 7383 (1997).

<sup>19</sup>A. R. Vasconcellos, R. Luzzi, and A. S. Esperidião, *Phys. Rev. B* **52**, 5021 (1995).

<sup>20</sup>R. Luzzi, A. R. Vasconcellos, J. Casas-Vázquez, and D. Jou, *Physica A* **248**, 111 (1998).

<sup>21</sup>J. Madureira, A. Vasconcellos, and R. Luzzi, *J. Chem. Phys.* **109**, 2099 (1998).

<sup>22</sup>J. R. Madureira, A. R. Vasconcellos, R. Luzzi, J. Cases-Vázquez, and D. Jou, *J. Chem. Phys.* **108**, 7568 (1998).

<sup>23</sup>J. R. Madureira, A. R. Vasconcellos, R. Luzzi, J. Cases-Vázquez, and D. Jou, *J. Chem. Phys.* **108**, 7580 (1998).

<sup>24</sup>R. Balian, Y. Alhassid, and H. Reinhardt, *Phys. Rep.* **131**, 1 (1986).

<sup>25</sup>R. Balian, <http://xxx.lanl.gov> (1 July 1999), cond-mat/9907015.

<sup>26</sup>N. N. Bogoliubov, in *Studies in Statistical Mechanics I*, edited by J. de Boer and G. E. Uhlenbeck (North-Holland, Amsterdam, 1962).

<sup>27</sup>N. N. Bogoliubov, *Lectures in Quantum Statistics* (Gordon and Breach, New York, 1967 and 1970, respectively), Vols. 1 and 2.

<sup>28</sup>A. R. Vasconcellos, A. C. Algarte, and R. Luzzi, *Physica A* **166**, 517 (1990).

<sup>29</sup>L. Lauck, A. R. Vasconcellos, and R. Luzzi, *Physica A* **168**, 789 (1990).

<sup>30</sup>J. C. Maxwell, *Philos. Trans. R. Soc. London* **157**, 49 (1867).

<sup>31</sup>S. P. Heims and E. T. Jaynes, *Rev. Mod. Phys.* **34**, 143 (1962), subsection b, pp. 148–150, and Appendix B, p. 164. [It should be noticed a misprint in the third line of their Eq. (B1) which must end in  $x^{n-1}$ .]

<sup>32</sup>P. M. Morse and H. Feschbach, *Methods of Theoretical Physics* (McGraw-Hill, New York, 1953).

<sup>33</sup>R. Luzzi, M. A. Scarparo, J. G. Ramos, A. R. Vasconcellos, M. L. Barros, Z. Zhiyao, and A. Kiel, *J. Non-Equilib. Thermodyn.* **22**, 197 (1997).

<sup>34</sup>S. de Groot and P. Mazur, *Nonequilibrium Thermodynamics* (North-Holland, Amsterdam, 1962).

<sup>35</sup>D. Jou, J. Casas-Vázquez, and G. Lebon, *Extended Irreversible Thermodynamics* (Springer, Berlin, 1993 and 1996), first and second enlarged editions respectively.

<sup>36</sup>A. C. Algarte, A. R. Vasconcellos, and R. Luzzi, *Phys. Status Solidi B* **173**, 487 (1992); T. Tome, A. R. Vasconcellos, and R. Luzzi, *Physica B* **144**, 376 (1987).

<sup>37</sup>J. M. Ziman, *Electrons and Phonons* (Clarendon, Oxford, 1960).

<sup>38</sup>E. Conwell, *High Field Transport in Semiconductors*, in *Solid State Physics*, edited by F. Seitz, D. Turnbull, and H. Ehrenreich (Academic, New York, 1967), Suppl. 9.

<sup>39</sup>D. Pines, *The Many-Body Systems* (Benjamin, Reading, 1962).

<sup>40</sup>D. Pines and P. Nozières, *The Theory of Quantum Liquids* (Benjamin, New York, 1966).

<sup>41</sup>See, for example, J. P. Hansen and I. R. McDonald, *Theory of Simple Liquids* (Academic, London, 1976).

<sup>42</sup>A. Mooradian and A. L. MacWhorter, in *Light Scattering Spectra of Solids*, edited by G. B. Wright (Springer, New York, 1969).

<sup>43</sup>A. R. Vasconcellos, R. Luzzi, and L. S. Garcia-Colin, *Physica A* **221**, 495 (1995).