Heat transport in a boson system: An information-theoretical approach

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(Received 2 October 1995; revised manuscript received 17 June 1996)

Resorting to what is termed informational statistical thermodynamics, namely, the microscopic foundations of irreversible thermodynamics in terms of the nonequilibrium informational ensemble, the problem of heat transport in a system of bosons is considered. In a truncated description of the macroscopic state of the system we derive the equations of evolution appropriate for an extended hydrodynamiclike approach. We particularize the analysis to those macrovariables corresponding to energy density and energy flux whose equations of evolution are nonlinear generalizations of Mori-Langevin equations. We arrive at an equation of propagation of thermal waves with damping. The thermal excitations are of the type of second sound. The different transport coefficients (like velocity of propagation, thermal diffusivity, relaxation times, etc.) receive an interpretation at the microscopic mechano-statistical level. We derive the limiting conditions to be imposed to recover Fourier's theory as an approximation. [S1063-651X(96)07311-4]

PACS number(s): 05.70.Ln, 82.20.Db, 82.20.Mj

I. INTRODUCTION

The analysis of heat propagation is one of the central motivations in irreversible thermodynamics. A thorough and deep description of results in this area, is due to Joseph and Preziosi [1]. In classical irreversible thermodynamics (CIT) [2], based on the local equilibrium assumption, the theory of heat propagation resorts to Fourier's constitutive equation which leads to a parabolic equation of diffusion. This implies that the thermal signals propagate at infinite speed at large frequencies, and further there is no agreement with experimental evidence in the short wavelength and/or high frequency domains as well as for large Mach numbers. To overcome these difficulties there exist several attempts to go beyond CIT in terms of phenomenological thermodynamic theories like extended irreversible thermodynamics (EIT) [3,4]. In EIT, Fourier's diffusion equation is generally replaced by a hyperbolic equation, of the telegraphist type, corresponding to wave propagation with damping. In a different approach, based on Boltzmann's equation for the pure phonon field, Guyer and Krumhansl [5] considered heat transport in dielectric crystals at low temperature and arrive at the conclusion that second sound may appear in some temperature range. The phenomenon of second sound was considered in the early works of Tisza [6] and Landau [7] in the case of helium II, and experimentally verified by Peschkov [8]. But second sound can be sustained in phononlike fluids in general [9], as well as in a system of electron carriers [10].

A rederivation of the Guyer-Krumhansl equation for heat transport in dielectrics in the framework of EIT, along with a variational formulation, is given in Ref. [11]. In the present paper, we consider the general case of energy and temperature propagation in a system of bosons in terms of a mechano-statistical formalism, namely, the nonequilibrium statistical operator method which is based on the information-theoretical approach of maximization of informational entropy (MaxEnt-NESOM for short) [12,13], and Zubarev's approach [14]. The MaxEnt-NESOM provides a nonlinear quantum transport theory of a large scope [15]—a far-reaching generalization of Mori's approach. In this theory, the transport coefficients, which are open parameters in phenomenological thermodynamic theories, are interpreted at the microscopic level. That is, they are given in terms of the underlying dynamical theory averaged with an appropriate MaxEnt-NESOM statistical distribution that characterizes the nonequilibrium macroscopic state of the system, and allows to incorporate spatial correlations (nonlocality in space) and time correlations (memory effects).

II. THE SYSTEM AND THE CHOICE OF THE BASIC VARIABLES

Consider a system consisting of a fluid of bosons, for example, the different branches of phonons in a solid state sample. The fluid is assumed to be in interaction with a thermal bath which is taken to be at a constant temperature T_0. The system of bosons is taken to be initially in an homogeneous state of reference and subsequently subjected to the presence of gradients of the different quantities that characterize its macroscopic state. Let $\omega_{\vec{q}}$ be the frequency dispersion relation of these bosons, with wave vector $\vec{q}$ running over an appropriate zone in reciprocal space (The Brillouin zone in the case of crystals). We write for the total Hamiltonian

$$\hat{H}=\hat{H}_0+\hat{H}', \tag{1}$$

where

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$$\hat{H}_0 = \sum_{\vec{q}} \hbar\omega_{\vec{q}}(b_{\vec{q}}^{\dagger}b_{\vec{q}} + \tfrac{1}{2}) + \hat{H}_B \equiv \hat{H}_b + \hat{H}_B, \tag{2a}$$

$$H' = \sum_{\vec{q}} (\lambda_{\vec{q}}\varphi_{\vec{q}}b_{\vec{q}}^{\dagger} + \lambda_{\vec{q}}^{*}\varphi_{\vec{q}}^{\dagger}b_{\vec{q}}) + \hat{H}_1. \tag{2b}$$

In Eq. (2a) the first term is the Hamiltonian of the free bosons, and H_B that of the thermal bath. Equation (2b) represents the interaction between both subsystems, and H_1 is the contribution to the Hamiltonian associated to interactions with external pumping sources. In these equations $b(b^{\dagger})$ are annihilation (creation) operators of bosons in the system considered, $\varphi(\varphi^{\dagger})$ are annihilation (creation) operators of excitations associated to the thermal bath, and λ is the coupling strength with the upper asterisk denoting complex conjugate. It is worth noticing that the separation of the Hamiltonian as given by Eq. (1) is an important prerequisite in MaxEnt-NESOM. The method proceeds as follows, a first step is to provide a characterization of the macroscopic state of the system in terms of an appropriate set of macrovariables. This is based on the closure condition provided by the so-called Zubarev-Peletminskii symmetry property [12–14,16]. This is done in a step by step procedure. First, the total Hamiltonian is separated into two parts—as done in Eq. (1)—where H_0 (called the relevant or secular part) is composed of the kinetic energies of the subsystems and, eventually, some of the interactions, namely those strong enough to have associated very short relaxation times (meaning those much smaller than the characteristic time scale in the experiment). The other H' contains the interactions related to the long-time relaxation mechanisms. Zubarev-Peletminskii closure condition (which at the mechano-statistical level is the counterpart of the principle of equipresence in phenomenological thermodynamics [17]), states that, given H_0 and the set of basic variables, say P_j, the commutator of P_j and H must verify that

$$[\hat{P}_j, \hat{H}_0] = \sum_k \alpha_{jk}\hat{P}_k, \tag{3}$$

where, in an appropriate representation, the α's are c numbers determined by H_0.

In the present description we select as an initial set of variables the density and energy density of the boson system, together with the energy of the thermal bath. More precisely, for convenience in the calculations we take their Fourier amplitudes of wave vector $\vec{Q}$, namely, $\{N(t), E(t), n(\vec{Q},t), h(\vec{Q},t), E_B\}$, where N and E are the homogeneous values ($\vec{Q}=\vec{0}$), n and ε the inhomogeneous ($\vec{Q} \neq \vec{0}$) contributions, and E_B is the energy of the thermal bath. These are the macrovariables; the corresponding dynamical quantities are indicated by $\hat{N}, \hat{H}_b, \hat{n}(\vec{Q}), \hat{\epsilon}(\vec{Q}), \hat{H}_B$, with $\hat{H}_B$ and $\hat{H}_b$, defined in Eq. (2a). Application of the closure condition of Eq. (3) requires the introduction as basic variables of the vectorial fluxes of particles $\hat{\vec{p}}(\vec{Q})$, and of energy, denoted by $\hat{\vec{I}}(\vec{Q})$, as well as all the higher order (tensorial) fluxes of particles and energy. According to the procedure all these quantities are viewed as basic variables. A truncation procedure is required, and we take the basic set of dynamical variables composed of

$$\{\hat{N}; \hat{H}_b; \hat{\vec{P}}; \hat{\vec{I}}; \hat{n}(\vec{Q}); \hat{h}(\vec{Q}); \hat{\vec{p}}(\vec{Q}); \hat{\vec{I}}(\vec{Q}); \hat{H}_B\}, \tag{4a}$$

quantities given by

$$\hat{n}(\vec{Q}) = \sum_{\vec{q}} \hat{\nu}_{\vec{q}\vec{Q}};$$

$$\hat{\varepsilon}(\vec{Q}) = \sum_{\vec{q}} \frac{\hbar}{2}(\omega_{\vec{q}+\vec{Q}} + \omega_{\vec{q}})\hat{\nu}_{\vec{q}\vec{Q}};$$

$$\hat{\vec{p}}(\vec{Q}) = \sum_{\vec{q}} \frac{1}{2}\vec{\nabla}_{\vec{q}}(\omega_{\vec{q}+\vec{Q}} - \omega_{\vec{q}})\hat{\nu}_{\vec{q}\vec{Q}};$$

$$\vec{I}(\vec{Q}) = \sum_{\vec{q}} \frac{\hbar}{4}(\omega_{\vec{q}+\vec{Q}} + \omega_{\vec{q}})\vec{\nabla}_{\vec{q}}(\omega_{\vec{q}+\vec{Q}} - \omega_{\vec{q}})\hat{\nu}_{\vec{q}\vec{Q}};$$

with

$$\hat{\nu}_{\vec{q}\vec{Q}} = b_{\vec{q}+\vec{Q}}^{\dagger}b_{\vec{q}},$$

and the quantities $\hat{N}$, $\hat{H}_b$, $\hat{\vec{P}}$, and $\hat{\vec{I}}$ correspond to set $Q=0$ in the equations above. Moreover, the accompanying set of thermodynamic macrovariables is indicated by

$$\{N(t); E(t); \vec{P}(t); \vec{I}(t); n(\vec{Q},t); h(\vec{Q},t); \vec{p}(\vec{Q},t); \vec{I}(\vec{Q},t); E_B\}, \tag{4b}$$

where, we recall, $\vec{Q} \neq 0$ and the truncation process is discussed in Sec. V. The set of Eqs. (4) is a combination of homogeneous and inhomogeneous quantities. All these quantities are expressed per unit volume.

With the choice of Eqs. (4) the auxiliary coarse-grained MaxEnt-NESOM statistical operator [12] is given by

$$\overline{\rho(t,0)} = \exp\Big\{ -\phi(t) - F_1(t)\hat{N} - F_2(t)\hat{H}_b - \vec{F}_3(t)\cdot\hat{\vec{P}} - \vec{F}_4(t)\cdot\hat{\vec{I}}_0 - \sum_{\vec{Q}\neq 0} [f_1(\vec{Q},t)\hat{n}(\vec{Q}) + f_2(\vec{Q},t)\hat{h}(\vec{Q}) + \vec{f}_3(\vec{Q},t)\cdot\hat{\vec{p}}(\vec{Q}) + \vec{f}_4(\vec{Q},t)\cdot\hat{\vec{I}}(\vec{Q})] - \beta_0\hat{H}_B \Big\}, \tag{5}$$

where ϕ ensures the normalization of $\overline{\rho}$ (it plays the role of the logarithm of a nonequilibrium partition function), the eight F_j and f_j are MaxEnt-Lagrange multipliers (related to the intensive variables of nonequilibrium thermodynamics), and $\beta_0 = 1/k_B T_0$. The MaxEnt-NESOM fine-grained statistical operator is a functional of the coarse-grained one of Eq. (5), which in the case of Zubarev's approach is given by [14]

$$\rho_\varepsilon(t) = \exp\Big\{ \ln \overline{\rho(t,0)} - \int_{-\infty}^{t} dt' e^{\varepsilon(t'-t)} \frac{d}{dt'} \ln \overline{\rho(t',t'-t)} \Big\}, \tag{6}$$

where the infinitesimal positive ϵ, which ensures the irreversible evolution of the system, goes to zero after the calculation of averages has been performed. Furthermore, the first variable in the argument of $\overline{\rho}$ refers to the time dependence of the Lagrange multipliers, while the second corresponds to the time dependence of the dynamical variables in Heisenberg representation.

Having defined the macroscopic state of the system we next look for its evolution under the action of thermal perturbations resulting from an inhomogeneous state of initial preparation.

III. THE EQUATIONS OF EVOLUTION

Here we derive the equations of evolution for the basic variables resorting to the MaxEnt-NESOM generalized nonlinear quantum transport theory [15]. According to this theory, the Liouville equation for the statistical operator can be transformed into an integral equation, which admits an iterative solution. A detailed description can be found in [16]. For the present purposes it suffices to mention that the evolution equations for the basic variables can be written in terms of an infinite series of contributions to the collision operator. If we call Q_j and $\hat{P}_j$ the basic variables and associated dynamical quantities, respectively, we have that [15]

$$\frac{d}{dt}Q_j(t)=\sum_{m=0}^{\infty}\Omega_j^{(m)}(t), \tag{7}$$

where the right-hand side is composed of an infinite series of partial collision operators, as described in Appendix A.

In what follows we stop the iterative process at the second order (that is we take $m=0$; 1; and 2 which implies two-particle collisions but includes nonlocality in space and memory effects) to find, first for the homogeneous variables, that

$$\frac{d}{dt}N(t)=\frac{2\pi}{\hbar^2}\sum_{\vec{q}}|\lambda_{\vec{q}}|^2\mathcal{A}(\vec{q};t), \tag{8a}$$

$$\frac{d}{dt}E(t)=\frac{2\pi}{\hbar^2}\sum_{\vec{q}}|\lambda_{\vec{q}}|^2\hbar\omega_{\vec{q}}\mathcal{A}(\vec{q},t)+S_E(t), \tag{8b}$$

$$\frac{d}{dt}\vec{P}(t)=\frac{2\pi}{\hbar^2}\sum_{\vec{q}}|\lambda_{\vec{q}}|^2\vec{\nabla}_{\vec{q}}\omega_{\vec{q}}\mathcal{A}(\vec{q},t)+S_P(t), \tag{8c}$$

$$\frac{d}{dt}\vec{I}(t)=\frac{2\pi}{\hbar^2}\sum_{\vec{q}}|\lambda_{\vec{q}}|^2\hbar\omega_{\vec{q}}\vec{\nabla}_{\vec{q}}\omega_{\vec{q}}\mathcal{A}(\vec{q},t), \tag{8d}$$

where

$$\mathcal{A}(\vec{q},t)=\int_{-\infty}^{\infty}\frac{d\omega}{\pi}\int_{-\infty}^{t}dt'\ \exp\{[\varepsilon+i(\omega_{\vec{q}}-\omega)](t'-t)\}\times[\mathcal{J}_{\vec{q}}(\omega)[\nu_{\vec{q}}(t')+1]-\mathcal{K}_{\vec{q}}(\omega)\nu_{\vec{q}}(t')], \tag{9a}$$

with, we recall, ε going to zero, and

$$\nu_{\vec{q}}(t)=\mathrm{Tr}\{b_{\vec{q}}^{\dagger}b_{\vec{q}}\overline{\rho(t,0)}\}, \tag{9b}$$

We have also introduced the spectral representations $\mathcal{J}$ and $\mathcal{K}$ for the average values of the excitations of the thermal bath, namely,

$$\langle\varphi_{\vec{q}}^{\dagger}(\tau)\varphi_{\vec{q}}\rangle=\int_{-\infty}^{\infty}\frac{d\omega}{\pi}\mathcal{J}_{\vec{q}}(\omega)e^{i\omega\tau}, \tag{9c}$$

$$\langle\varphi_{\vec{q}}(\tau)\varphi_{\vec{q}}^{\dagger}\rangle=\int_{-\infty}^{\infty}\frac{d\omega}{\pi}\mathcal{K}_{\vec{q}}(\omega)e^{i\omega\tau}. \tag{9d}$$

Finally, $S_E(t)$ and $S_P(t)$ in Eqs. (8b) and (8c) stand for the contributions due to the pumping source, whose origin is in the interaction energy operator H_1 of Eq. (2b). For simplicity, we assume that the pumping source couples to the system in such a way to increase the homogeneous part of the energy and momentum, but does not affect the flux of energy and the inhomogeneous variables. A continuous constant pumping would produce a stationary homogeneous state after a transient time has elapsed; this condition will be used later on.

The equations of evolution for the inhomogeneous ($Q\neq 0$) variables are

$$\frac{\partial}{dt}n(\vec{Q},t)=i\vec{Q}\cdot\vec{p}(\vec{Q},t)+\sum_{\vec{q}}J(\vec{q},\vec{Q};t), \tag{10a}$$

$$\frac{\partial}{\partial t}h(\vec{Q},t)=i\vec{Q}\cdot\vec{I}(\vec{Q},t)+\sum_{\vec{q}}\frac{\hbar}{2}(\omega_{\vec{q}+\vec{Q}}+\omega_{\vec{q}})J(\vec{q},\vec{Q},t), \tag{10b}$$

$$\frac{\partial}{\partial t}\vec{p}(\vec{Q},t)=i\vec{Q}\cdot\varphi(\vec{Q},t)+\sum_{\vec{q}}\vec{v}(\vec{q},\vec{Q})(J\vec{q},\vec{Q};t), \tag{10c}$$

$$\frac{\partial}{\partial t}\vec{I}(\vec{Q},t)=i\vec{Q}\cdot\psi(\vec{Q},t)+\sum_{\vec{q}}\frac{\hbar}{2}(\omega_{\vec{q}+\vec{Q}}+\omega_{\vec{q}})\times\vec{v}(\vec{q},\vec{Q})J(\vec{q},\vec{Q};t), \tag{10d}$$

where

$$J(\vec{q},\vec{Q};t)=\frac{\pi}{\hbar^2}\left\{\int_{-\infty}^{t}dt'e^{\varepsilon(t'-t)}|\lambda_{\vec{q}}|^2[\mathcal{J}_{\vec{q}}(\omega)-\mathcal{K}_{\vec{q}}(\omega)]\exp\{i(\omega_{\vec{q}}-\omega)(t'-t)\}+\text{same with exchange }\vec{q}\to\vec{q}+\vec{Q}\right\}\nu_{\vec{q}\vec{Q}}(t'), \tag{11a}$$

φ and ψ are the flux of the flux of matter and of energy,

$$\nu_{\vec{q}\vec{Q}}(t)=\mathrm{Tr}\{b_{\vec{q}+\vec{Q}}^{\dagger}b_{\vec{q}}\overline{\rho(t,0)}\}, \tag{11b}$$

and

$$\vec{v}(\vec{q},\vec{Q})=\vec{\nabla}_{\vec{q}}\omega_{\vec{q}}+\frac{1}{2}\vec{Q}\nabla_{\vec{q}}^2\omega_{\vec{q}}+\cdots \tag{11c}$$

an expression that arises from $\vec{Q}\cdot\vec{v}=(\omega_{\vec{q}+\vec{Q}}-\omega_{\vec{q}})/2$, when expanded in increasing powers of $\vec{Q}$.

We recall that we have assumed that the external sources act only on the homogeneous variables, not being a supplier to the inhomogeneous variables. Hence, the terms involving J in Eqs. (10) are exclusively of the kind of relaxation-dissipative contributions as a result of the coupling with the thermal bath.

At this point we clearly see that, as a consequence of the truncation procedure in the choice of the basic variables, the equations of evolution do not constitute a closed set. Hence, the next step is to express the variables corresponding to the higher order fluxes φ and ψ in terms of the basic variables. Taking into account the expressions for these higher order fluxes and also the expressions for the collision operators [cf. Eq. (10a)] appearing in the right-hand side of Eqs. (10), we need to express $\nu_{\vec{q}\vec{Q}}(t)$ of Eq. (11b) in terms of the basic variables. For that purpose we first separate the homogeneous and inhomogeneous contributions in the auxiliary statistical operator of Eq. (5), namely,

$$\overline{\rho(t,0)}=\exp\{A+B\}/\mathrm{Tr}\{\exp[A+B]\}, \tag{12}$$

where B refers to the inhomogeneous contribution, that is,

$$B=-\sum_{\vec{Q}\neq 0}\{f_1(\vec{Q},t)\hat{n}(\vec{Q})+f_2(\vec{Q},t)\hat{h}(\vec{Q})+\vec{f}_3(\vec{Q},t)\cdot\hat{\vec{p}}(\vec{Q}) +\vec{f}_4(\vec{Q},t)\cdot\hat{\vec{I}}(\vec{Q})\}, \tag{13}$$

while A contains the homogeneous contributions. We introduce also the statistical operator for the homogeneous state, defined by

$$\overline{\rho_h}(t,0)=\exp\{-\phi_h(t)-F_1(t)\hat{N}-F_2(t)\hat{H}_p-\vec{F}_3(t)\cdot\hat{\vec{p}} -\vec{F}_4(t)\cdot\hat{\vec{I}}-\beta_0\hat{H}_B\}, \tag{14}$$

with ϕ_h ensuring its normalization.

Resorting to Heims-Jaynes perturbation expansion for averages [18], we find at first order (linear approximation) in the inhomogeneities contained in operator B, that

$$\nu_{\vec{q}\vec{Q}}(t)=a_1(\vec{q},\vec{Q};t)f_1(\vec{Q},t)+a_2(\vec{q},\vec{Q};t)f_2(\vec{Q},t) +\vec{a}_3(\vec{q},\vec{Q};t)\cdot\vec{f}_3(\vec{Q},t)+\vec{a}_4(\vec{q},\vec{Q};t)\cdot\vec{f}_4(\vec{Q},t), \tag{15}$$

where the coefficients $a_j(\vec{q},\vec{Q};t)$ are listed in Appendix B.

After replacing $\nu_{\vec{q}\vec{Q}}$ given by Eq. (15) in the expressions for φ, ψ, and J of Eqs. (10), the right-hand sides in Eqs. (10) become dependent on the four Lagrangian multipliers f_1, f_2, $\vec{f}_3$, and $\vec{f}_4$. But to close the system of equations, we can relate these Lagrange multipliers to the basic variables since the latter, are linear combinations of $\nu_{\vec{q}\vec{Q}}$. We are then left with a system of equations that can be written in the matricial form

$$\begin{bmatrix} n(\vec{Q},t)\\ h(\vec{Q},t)\\ \vec{p}(\vec{Q},t)\\ \vec{I}(\vec{Q},\vec{t})\end{bmatrix}=-\hat{M}(\vec{Q},t)\begin{bmatrix} f_1(\vec{Q},t)\\ f_2(\vec{Q},t)\\ \vec{f}_3(\vec{Q},t)\\ \vec{f}_4(\vec{Q},t)\end{bmatrix}. \tag{16}$$

For simplicity we take the limit of small Q's, and this assumption allows us to neglect Q in all the kinetic coefficients a_j and M: this is equivalent to take in Eqs. (10), which are nonlocal in space and memory dependent, a local in space approximation, meaning that spatial correlations are neglected. In this limit matrix M simplifies considerably and its elements are listed in Appendix C.

After inversion of matrix M we can, from Eq. (16), obtain the Lagrange multipliers f in terms of the inhomogeneous variables, and next replacing in Eq. (15) these expressions for the f_j yields $\nu_{\vec{q}\vec{Q}}$ in terms of the basic variables. We omit the lengthy and cumbersome resulting expressions and limit our present analysis to specific calculations for a simplified situation in Sec. IV. The relevant point to be kept in mind here is that we have derived a closed set of equations of evolution for the selected basic variables of Eq. (4b), with the kinetic coefficients given at the microscopic level, that is in terms of the dynamics of the constituent particles.

The set of equations of evolution describe transport of matter and of energy and, as we have seen, both phenomena are coupled together through cross-kinetic terms. In what follows we concentrate our attention on the thermal motion alone, decoupling it from the material motion, that is we neglect cross-kinetic terms. As a consequence we have only to consider the equations for the energy density and its flux.

IV. SECOND SOUND IN IST

Within the above assumptions, namely, decoupling of material and heat motion, and omission of spatial correlations, but keeping memory effects contained in the collision operator $\Omega^{(2)}$ (all other higher order collision operators are neglected) we are left with relatively simple equations for the energy density and its flux. First we note that under the conditions just stated it follows that

$$\nu_{\vec{q}\vec{Q}}(t)=M_{22}^{-1}(t)a_2(\vec{q};t)h(\vec{Q},t)+M_{44}^{-1}(t)\vec{a}_4(\vec{q};t)\cdot\vec{I}(\vec{Q},t), \tag{17}$$

where $a_2(\vec{q};t)$ and $\vec{a}_4(\vec{q};t)$ stand for a_2 and $\vec{a}_4$ of Appendix B with $\vec{Q}=0$. If in addition we assume isotropy the tensor $\underset{\sim}{M}_{44}$ becomes a scalar times the unit $\underset{\sim}{1}$ tensor, given by

$$M_{44}(t)=\frac{1}{3}\sum_{\vec{q}}(\hbar\omega_{\vec{q}})^2|\vec{\nabla}_{\vec{q}}\omega_{\vec{q}}|^2\eta(\vec{q},t)\underset{\sim}{1}, \tag{18}$$

with η defined in Eq. (C1.g) and since $\omega_{\vec{q}}$ is an even function of $\vec{q}$ it follows that $\vec{M}_{24}=\vec{M}_{42}=0$.

Replacing Eq. (17) into Eqs. (10b) and (10d) we find that

$$\frac{\partial}{\partial t}h(\vec{Q},t)=i\vec{Q}\cdot\vec{I}(\vec{Q},t)-\Theta_{\varepsilon}^{-1}(t)*h(\vec{Q},t), \tag{19a}$$

$$\frac{\partial}{\partial t}\vec{I}(\vec{Q},t)=\lambda_\varepsilon(t)i\vec{Q}h(\vec{Q},t)-\Theta_I^{-1}(t)*\vec{I}(\vec{Q},t)$$
$$-\Lambda(t)*(Q^2+[\vec{Q}\vec{Q}])\vec{I}(\vec{Q},t), \qquad (19b)$$

where $*$ stands for the convolutionlike product defined by

$$\Theta_\varepsilon^{-1}(t)*h(\vec{Q},t)=\int_{-\infty}^{\infty}dt'\,\Theta_\varepsilon^{-1}(t-t';t')h(\vec{Q},t'), \quad (20)$$

and so on; the presence of such terms clearly shows that memory effects are incorporated in the theory. Furthermore, in Eqs. (19) the time dependent kinetic coefficients, namely, λ_ε, Λ, Θ_ε, and Θ_I are given in Appendix D.

Furthermore, if we introduce the quantity $\beta(\vec{Q},t)$ such that $\beta(0,t)=F_2(t)$ and $\beta(\vec{Q},t)=f_2(\vec{Q},t)$, for $\vec{Q}\neq 0$, and $\hat{\varepsilon}(\vec{Q})$ such that $\hat{\varepsilon}(0)=H_b$ and $\hat{h}(\vec{Q})=\hat{\varepsilon}(\vec{Q})$, for $\vec{Q}\neq 0$, we can write in the exponent of the statistical operator of Eq. (5) that

$$F_2(t)\hat{H}_b+\sum_{\vec{Q}\neq 0}f_2(\vec{Q},t)\hat{h}(\vec{Q})=\sum_{\vec{Q}}\beta(\vec{Q},t)\hat{\varepsilon}(\vec{Q}). \qquad (21a)$$

Similarly, introducing $\vec{\alpha}(\vec{Q},t)$ such that $\vec{\alpha}(\vec{Q},t)=\vec{f}_4(\vec{Q},t)$ for $\vec{Q}\neq 0$, and $\hat{\vec{\mathcal{J}}}(Q)$ such that $\hat{\vec{\mathcal{J}}}(0)=\hat{\vec{I}}$ and $\hat{\vec{\mathcal{J}}}(\vec{Q})=\vec{I}(\vec{Q})$ for $\vec{Q}\neq\vec{0}$, we can write

$$\vec{F}_4(t)\hat{\vec{I}}+\sum_{\vec{Q}\neq O}\vec{f}_4(\vec{Q},t)\hat{\vec{I}}(\vec{Q})=\sum_{\vec{Q}}\vec{\alpha}(\vec{Q},t)\hat{\vec{\mathcal{J}}}(\vec{Q},t). \qquad (21b)$$

In the context of informational statistical thermodynamics the Lagrange multiplier $\beta(\vec{Q},t)$ can be interpreted as the Fourier transform of the reciprocal of a local nonequilibrium temperature (to be referred to as a quasitemperature), namely, $\beta(\vec{r},t)\equiv 1/k_BT(\vec{r},t)$ [19]. We can also write $T^*(\vec{r},t)=T^*(t)+\Delta T^*(\vec{r},t)$, where T^* is the average homogeneous nonequilibrium temperature and ΔT^* its local deviation; in the linearized (local) theory one has that $\Delta T^*\ll T^*$. On the other hand,

$$h(\vec{Q},t)=-M_{22}(t)f_2(\vec{Q},t), \qquad (22a)$$

$$\vec{I}(\vec{Q},t)=-M_{44}(t)\vec{f}_4(\vec{Q},t), \qquad (22b)$$

for $\vec{Q}\neq 0$, as a result of Eq. (16) and isotropy, and making use of the fact that $\Delta T^*\ll T^*$, we can write

$$\vec{\nabla}\varepsilon(\vec{r},t)=-M_{22}(t)\vec{\nabla}\beta(\vec{r},t)\simeq\frac{M_{22}(t)}{k_BT^{*2}_{(t)}}\vec{\nabla}T(\vec{r},t). \quad (23)$$

We are now in condition to transform back the equations of evolution, Eqs. (8b), (8d), (10b), and (10c), to obtain them in direct space, where they read as

$$\frac{\partial}{\partial t}\varepsilon(\vec{r},t)=-\mathrm{div}\,\vec{\mathcal{J}}(\vec{r},t)-\Theta_\varepsilon^{-1}(t)*\varepsilon(\vec{r},t)+\xi_\varepsilon(t), \qquad (24a)$$

$$\frac{\partial}{\partial t}\vec{\mathcal{J}}(\vec{r},t)=-\lambda_\varepsilon(t)\vec{\nabla}\varepsilon(\vec{r},t)-\Theta_I^{-1}(t)*\vec{\mathcal{J}}(\vec{r},t)$$
$$-\Lambda(t)*(\vec{\nabla}^2+[\vec{\nabla}\vec{\nabla}])\vec{\mathcal{J}}(\vec{r},t)+\xi_I(t), \qquad (24b)$$

where $\varepsilon(\vec{r},t)$ and $\vec{\mathcal{J}}(\vec{r},t)$ (which are the averages of $\hat{\epsilon}$ and $\hat{\vec{\mathcal{J}}}$) have the Fourier transforms $\varepsilon(\vec{Q},t)$ and $\vec{\mathcal{J}}(\vec{Q},t)$, while ξ_ε and ξ_I account for the action of the external pumping source.

Equations (24) are local in space as a result of the approximation we introduced consisting in neglecting the dependence on $\vec{Q}$ of the kinetic coefficients $a_j(\vec{Q},t)$ and $M(\vec{Q},t)$. Moreover, Eqs. (24) are, within the approximations we have introduced, of the type of Mori's equations [20]: the first term on the right-hand side is in Mori's terminology a precession term, while the second (encompassing retroeffects or memory) is a relaxation term where Θ_ε and Θ_I play the role of relaxation times which, we recall, depend on the time evolution of the homogeneous state of reference.

Let us return to Eq. (19b), wherein the last term is neglected ($\Lambda=0$) and take a quasistationary flux, namely, $\partial\vec{\mathcal{J}}/\partial t\simeq 0$. Assuming that the convolution product is invertible, Eq. (24b) becomes, once Eq. (23) is taken into account, a Fourier-like constitutive equation, with memory effects included, namely,

$$\mathcal{J}(\vec{r},t)=-\kappa(t)*\vec{\nabla}T^*(\vec{r},t)$$
$$=-\int_{-\infty}^{\infty}dt'\,\kappa(t-t';t')\vec{\nabla}T^*(r,t'), \qquad (25)$$

where κ plays the role of a thermal conductivity given by

$$\kappa(t-t';t')=\Theta_I(t-t';t')\lambda_\varepsilon(t')\frac{M_{22}(t')}{k_BT^2(t')}. \qquad (26)$$

Thus, in this limiting case, one recovers the results of CIT. Going back to Eq. (19b), after using Eqs. (24a) and (23), we can write

$$\frac{\partial}{\partial t}\varepsilon(\vec{r},t)=\kappa(t)*\vec{\nabla}^2T^*(\vec{r},t)-\Theta_\varepsilon^{-1}(t)*\varepsilon(\vec{r},t)+\sigma_\varepsilon(t), \qquad (27)$$

where the last two term are the contributions accounting for the exchange of energy with the thermal bath and energy pumping by the external source. Furthermore, taking the homogeneous state as stationary, so that all the kinetic coefficients are constant in time, it follows from Eq. (22b) and the definition of $\beta(\vec{r},t)$ that

$$\frac{\partial}{\partial t}\varepsilon(\vec{r},t)\simeq(M_{22}/k_BT^2)\frac{\partial}{\partial t}T^*(\vec{r},t), \qquad (28)$$

After substitution of Eq. (28) into Eq. (27), taking into account that in the stationary state $\xi_\varepsilon=0$ and neglecting the dissipative term $\Theta_\varepsilon^{-1}*\varepsilon$, Fourier's classical heat diffusion equation, namely,

$$\left[\frac{\partial}{\partial t} - D\vec{\nabla}^2\right] T^*(\vec{r},t) = 0, \tag{29}$$

is retrieved, where the heat diffusivity coefficient D is given by

$$D = (k_B T/M_{22})\kappa = \lambda_\varepsilon M_{44}/M_{22}, \tag{30}$$

with

$$\kappa = M_{22}\Theta_2/k_B T^{*2}, \tag{31}$$

being the thermal conductivity. It needs to be stressed that these two kinetic coefficients have a complicate dependence on the quasitemperature T^*, arising out of the presence of T^* in the distribution functions ν of Eq. (B1f) in Appendix B (we recall that $F_2 = 1/k_B T^*$).

Hence, as noticed, we have recovered the results contained in CIT; let us extend them beyond its domain of validity. Differentiating Eq. (24a) with respect to time we find that

$$\frac{\partial^2}{\partial t^2}\varepsilon(\vec{r},t) = -\operatorname{div}\frac{\partial}{\partial t}\vec{\mathcal{J}}(\vec{r},t) - \frac{\partial}{\partial t}[\Theta_\varepsilon^{-1}(t) * \varepsilon(\vec{r},t)] + \frac{d}{dt}\xi_\varepsilon(t), \tag{32}$$

and using Eq. (24b) for the time derivative of the flux, we obtain an equation of evolution for the variable $\varepsilon(\vec{r},t)$, namely,

$$\left[\frac{\partial^2}{\partial t^2} + \Theta^{-1}(t) * \frac{\partial}{\partial t} - \lambda_\varepsilon(t)\vec{\nabla}^2\right]\varepsilon(\vec{r},t) = -\operatorname{div}[\Theta_I^{-1}\Lambda(t) * (\vec{\nabla}^2 + [\vec{\nabla}\vec{\nabla}])]\vec{\mathcal{J}}(\vec{r},t) + \frac{d}{dt}\xi_\varepsilon(t). \tag{33}$$

Equation (32) is a kind of a generalization of the telegraphist equation with sources, which is of the hyperbolic type instead of the parabolic type obtained in CIT. In Eq. (33) we have introduced the compound relaxation time

$$\Theta^{-1}(t) = \Theta_\varepsilon^{-1}(t) + \Theta_I^{-1}(t). \tag{34}$$

Let us next consider, as before, the case of a stationary homogeneous state, and so since all kinetic coefficients are defined as averages over this state, they become constant in time. Under this condition Eq. (33) becomes

$$\left[\frac{\partial^2}{\partial t^2} + \Theta^{-1}\frac{\partial}{\partial t} - \lambda_\varepsilon\vec{\nabla}^2\right]\varepsilon(\vec{r},t) = \operatorname{div}[\kappa^{-1} - \Lambda(\vec{\nabla}^2 + [\vec{\nabla}\vec{\nabla}])]\vec{\mathcal{J}}(\vec{r},t). \tag{35}$$

It should be noticed that by writing Eq. (35) care was taken of the fact that $d\xi_\varepsilon/dt = 0$ in the background stationary homogeneous state of reference. Taking into account the relation between the energy density and the nonequilibrium temperature as expressed by Eqs. (23), we obtain an equation of evolution for the temperature, namely,

$$\left[\frac{1}{c_T^2}\frac{\partial^2}{\partial t^2} + \frac{1}{D_T}\frac{\partial}{\partial t} - \vec{\nabla}^2\right] T^*(\vec{r},t) = -\operatorname{div}[\kappa^{-1} - l^2(\vec{\nabla}^2 + [\vec{\nabla}\vec{\nabla}])]\vec{\mathcal{J}}(\vec{r},t), \tag{36}$$

where

$$D_T = \lambda_\varepsilon\Theta = c_T^2\Theta; \quad c_T^2 = \lambda_\varepsilon; \quad l^2 = (kT^2/\lambda_\varepsilon M_{22})\Lambda. \tag{37}$$

Equation (36) is an inhomogeneous differential equation of the telegraphist type, describing damped wave propagation with velocity c_T. The inhomogeneous term, i.e., the one on the right-hand side, is a term involving sinks or sources, depending on the rate of change in space of the energy flux. Equation (36) is similar to the one derived by Guyer and Krumhansl [5], implying the propagation of second sound. It is also of the form of the equations derived within the context of phenomenological EIT [11]. However, it ought to be noticed that the last term in Eq. (35) (containing the Laplacian and the tensorial product of gradients) has here a different origin from the one in Ref. [5, 11]. While in the latter it is a consequence of including the second order flux of the energy as a basic variable, here it arises out of residual nonlocal corrections to the energy flux relaxation time. Hence, we have shown that the results of CIT and EIT, at least concerning the problem of heat propagation, are contained as particular limiting cases of IST. In Sec. V, we summarize and discuss some consequences arising from Eq. (35).

V. CONCLUDING REMARKS

We have considered the problem of heat transport in matter in the context of statistical thermodynamics based on MaxEnt-NESOM. It has been shown that an exact description in its domain of application would require the use of a set of infinite moments of the one-particle distribution function. In the spirit of extended irreversible thermodynamics a truncation of this set was performed by keeping the density and energy density and their respective fluxes as relevant variables. The equations of evolution for these variables are obtained in terms of the MaxEnt-NESOM generalized nonlinear quantum theory. The resulting transport equations are nonlinear and nonlocal in space and noninstantaneous in time as they contain space correlations and memory, but, because of the truncation procedure, this set of equations is not closed. To close the system one needs to express the one-particle distribution in terms of the set of basic variables, what has been done in Sec. III resorting to a linearized approximation in Heims-Jaynes perturbation expansion for averages. For simplicity, we have decoupled the movement of energy from that of matter, that is, we have neglected the cross-kinetic terms that relate both. Furthermore, taking a local in space approximation—meaning neglecting spacial correlations—we have derived the equations of evolution for the energy density and the energy flux. They are of the type of Mori's transport equations, involving terms in the form of an equation of continuity plus dissipative contributions with memory. Two time dependent (i.e., depending on the evolving nonequilibrium state of the system) relaxation times are introduced: the first, Θ_ε, is associated to energy density and the second Θ_I to energy flux. A space and time dependent nonequilibrium quasitemperature is also defined within the scope of the theory.

From the coupled set of equations of evolution for the energy density and the energy flux, we were able to show that, in the long wavelength limit and for an energy flux weakly varying in time, the equations of CIT namely, Fourier's constitutive and diffusion equations, are retrieved [both containing memory effects]. If such restrictions are removed, one recovers Guyer-Krumhansl-like equation for the energy density and for the quasitemperature. Within the limit of small gradients, the hyperbolic telegrapher's equation is recovered. Therefore, it is proved that, within this restricted treatment of the general method of the MaxEnt-NESOM, the system may sustain damped wave propagation of energy (or equivalently temperature), which is of the type of second sound.

Let us next consider the question of the truncation procedure. As already noticed in the paragraph following Eq. (3), the closure condition requires, in principle, a description that needs to incorporate the densities (of matter and of energy) and their fluxes to all orders. A truncation at a certain order is necessary, together with a criterion to assert that the information retained is the relevant one, and the neglected one is irrelevant. It is known from phenomenological theories that a more and more extended set of basic variables needs be introduced when the characteristic lengths become shorter and shorter. In other words, a more and more reduced set of basic variables is required as more and more homogeneous the motion becomes. This can be demonstrated in the case of the statistical thermodynamics founded on the MaxEnt-NESOM, to be called information statistical thermodynamics (IST for short) [21]: If we call IST(r), or rth level of description of IST, meaning that are kept as basic variables the densities and their fluxes up to order r (r is also the tensorial rank of the flux, with $r=1$ being the usual vectorial ones), one can define the range of wavelengths going from infinite ($Q=0$) to a cutoff one ($\lambda_{\rm co}^{(r)}=2\pi/Q_{\rm co}^{(r)}$), for which such a description becomes a good one to determine thermodynamic and hydrodynamic properties of the system under the given conditions. For $r>2$ it is, in general, not an easy task to determine $\lambda_{\rm co}$. A particular analysis has been done for the case of propagation of plasma waves in the carrier system of the photoinjected plasma in semiconductors [22]. In that paper the dispersion relation of plasmons obtained in several levels of IST was compared with the exact result; it was shown that a group velocity correct up to second power in wave number Q follows in IST(4). Moreover, the cutoff wavelength is shown to be $\lambda_{\rm co}^{[4]}=2\pi/Q_{\rm co}=2\pi\overline{c}\,\overline{\tau}_{\rm pl}$, where $\overline{c}$ is the average velocity of propagation of the charge density excitation and $\tau_{\rm pl}$ the plasma-wave period. It appears that, as a general rule, the cutoff frequency is given by an average velocity of propagation of the excitation multiplied by a characteristic time [21]. This is shown in the case of the second sound propagation in the boson systems described in the preceding section, however restricted to the study of the boundary between IST(0) and IST(1), that is to say, at the phenomenological level between CIT and the original form of EIT. Let us proceed to define the domain of validity of CIT (in particular, of Fourier's diffusion equation) with respect to EIT (hyperbolic equation for propagation of heat waves). If in Eq. (35) we neglect the right-hand side (i.e., assuming a weak spacial rate of change of the energy flux), we can easily derive the frequency dispersion relation for the second sound, i.e., the one arising from the secular equation

$$\frac{\omega^2}{c_T^2}+(i/D_T)\,\omega-Q^2=0, \tag{38}$$

where $c_T(=\lambda_\varepsilon^{1/2})$ may be viewed as the phase velocity. Solving Eq. (38) with respect to ω and recalling that $\Theta=D_T^2/c_T^2$ [see Eqs. (37)], it is found that

$$\omega(Q)=-\frac{i}{2\Theta}\pm\left(c_T^2Q^2-\frac{1}{4\Theta^2}\right)^{1/2}, \tag{39}$$

which corresponds to wave propagation (second sound) under the condition $c_TQ>(2\Theta)^{-1}$. Evidently for a given c_T and Θ this inequality is satisfied for sufficiently large values of Q, i.e., not too long wave numbers. Consider now very low frequencies while the thermal diffusivity D_T is kept finite. In this case, it follows from Eq. (38) that the frequency ω is equal to iD_TQ^2, which is the result expected by considering directly Fourier's diffusion equation of CIT. This indicates that CIT may be considered as a good approximation in the limit of very short frequencies. Furthermore, we see that the result $\omega=iD_TQ^2$ is valid at very long wavelengths. It is then shown that the system goes from the wave propagation regime of EIT (second sound) to the Fourier's diffusive regime of CIT, when passing from condition $2c_TQ\Theta>1$ to $2c_TQ\Theta<1$, that is, when going from the damped to the overdamped regime in the propagation of the thermal excitation. It is thus clear that CIT is contained in EIT, and becomes a good approximation for describing overdamped regimes of the second sound propagation. As stressed earlier, this corresponds to phenomena with predominance of very long wavelengths and very low frequencies. Therefore, the cutoff frequency is, in this case, given by

$$\lambda_{\rm co}^{[1]}=2\pi/Q_{\rm co}^{[1]}=4\pi c_T\Theta, \tag{40}$$

where the velocity of propagation c_T and the characteristic time Θ depend on the nonequilibrium macroscopic state of the system, with $c_T^2=\lambda_\varepsilon$ given by Eq. (D 1a) and Θ by Eq. (34), and the two relaxation times are given by Eqs. (D 1c and D1d). As an illustration let us consider the behavior of longitudinal optical phonons in the case of the photoinjected plasma in polar semiconductors. The thermal bath consists then of the fluid of carriers (electrons and holes), and the interaction between LO phonons and carriers is via the Fröhlich potential [23], and the numerical calculations are performed using parameters characteristic of GaAs. The evaluation of the velocity of propagation [via λ_ε of Eq. (D1a)] is easy to perform once we take into account that the LO-phonon dispersion relation has a small width. It is found that c_T^2 is nearly the average of the square of the LO-phonon group velocity, in the case of GaAs we find that, roughly, $c_T\sim1.6\times10^5$ cm/sec. The characteristic time Θ becomes practically the energy relaxation time, since for GaAs $\Theta_1\gg\Theta_\varepsilon$, and Θ_ε can be calculated to be approximated by $\Theta_\varepsilon\approx\Theta_\varepsilon^{(c)}/nv_{\rm cell}$, where $\Theta_\varepsilon^{(c)}$ is the energy-relaxation time of carriers resulting from collisions with the LO phonons, given in Ref. [24], n is the carrier concentration, and $v_{\rm cell}$ the volume of the unit cell. In this case the velocity of propagation

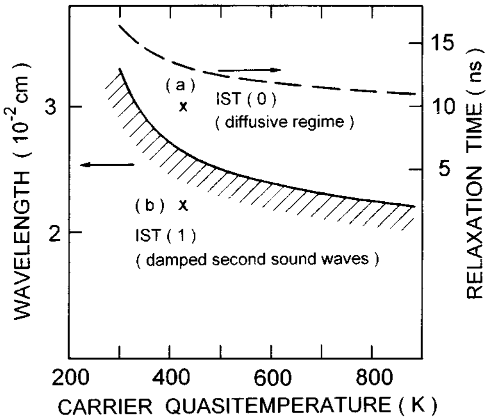

FIG. 1. The energy-relaxation time (right ordinate) and the line separating the domains of damped wave propagation and overdamped regime with diffusive motion for different values of wavelength (left ordinate).

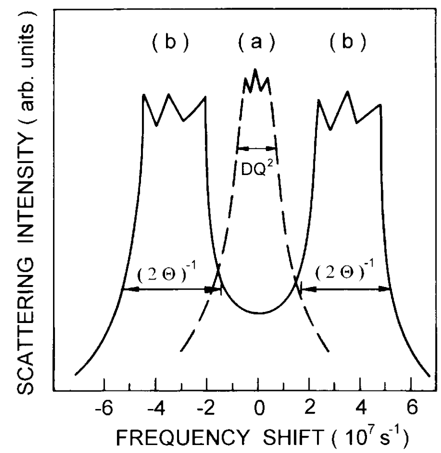

FIG. 2. Contributions to the Raman spectrum by the thermal excitation in two different cases: (a) a single central (shiftless) Rayleigh-like band (dashed line) and (b) a Brillouin-like doublet (full line), which correspond to the situations indicated by cross points labeled correspondingly (a) and (b) in Fig. 1.

is nearly a constant, independent of the macroscopic state of the system, but this is not true for the energy-relaxation time. As an illustration, let us consider that the LO phonons remain near equilibrium (say at $T_b \cong 300$ K), and that the photoexcited carriers, with given density $n = 1.4\times10^{17}$ cm^{-3}, may have quasitemperatures ranging from 300 to 800 K. Using these results we have represented in Fig. 1 the energy-relaxation time (right ordinate) in terms of the carrier quasitemperature. We have drawn the line that corresponds to the cutoff wave number $Q_{co}^{[1]} = 2\pi/\lambda_{co}^{[1]}$, which separates the domain of validity of IST(0) (or CIT) and IST(1) (or EIT). It is seen that the cutoff value of wavelength is roughly in the small range 4×10^{-2} cm$\leqslant \lambda_{co}^{[1]} \leqslant 2\times10^{-2}$ cm. To determine the next cutoff wavelength $\lambda_{co}^{[2]}$, an additional and more elaborate analysis is required. Moreover, it is noticed that there is a minimum cutoff, and therefore a limiting truncation, since there is no physical meaning for movements with wavelengths smaller than the dimension of the unit cell, that is $2\pi/\lambda_{min} = Q_{min} = 2Q_B$, where Q_B is the radius of the Brillouin zone, which, in GaAs is 5.6×10^7 cm^{-1}, so that $\lambda_{min} \simeq 5.6\times10^{-8}$ cm.

The change of regime—from damped to overdamped—is well evidenced in Raman scattering experiments: damped second sound propagation gives rise to a Brillouin-like doublet at frequency shifts $\pm[c_T^2 Q^2 - (2\Theta)^{-2}]^{1/2}$ and linewidth $(2\Theta)^{-1}$, while in the overdamped regime one should observe a single Rayleigh band with linewidth $D_T Q^2$ and no frequency shift. This is illustrated in Fig. 2.

Summarizing, MaxEnt-NESOM, which provides a very powerful formalism for the construction of statistical thermodynamic and hydrodynamic theories, is here applied to the study of a system of bosons in interaction with a second system acting as a thermal bath. The highly nonlinear, nonlocal in space and memory-dependent equations of evolution for the densities and their fluxes, when under the linear approximation in the deviations from the homogeneous state have a structure reminiscent of generalized Mori-Newton-Langevin equations (however, in a quantum representation). By assuming that the reference homogeneous state is time independent (the simplest case is equilibrium, or, in general, a nonequilibrium situation but arising out of the application of a constant source of excitation) we have the full equivalent of Mori's approach. Neglecting space correlations we obtain a hyperbolic-type equation of evolution of the telegraphist type, akin to Maxwell-Cattaneo-Vernotte equations of EIT) which admits two kinds of motion: a predominant propagating one, namely, a damped wave propagation of second sound, which, at long wavelengths and low frequencies, goes over to a predominant diffusive movement. The situation considered here corresponds to the two lowest orders of truncation in the description of the macroscopic nonequilibrium state of the system. Higher and higher levels of description (by increasing the number of basic variables) are necessary when motions involve steeper space and time variations, thus requiring a Fourier analysis involving shorter wavelengths and higher frequencies).

ACKNOWLEDGMENTS

Two of the authors (A.R.V., R.L.) acknowledge financial support from the São Paulo State Research Agency (FAPESP) and the Brazilian National Research Council (CNPq). One of the authors (G.L.) thanks the European Community for support under Contract ERB-CHRX-CT92-0007, and the Belgian Interuniversity Poles of Attraction (Grants PAI 21 and 29) iniciated by the Belgian State Science Policy Programing.

APPENDIX A: THE COLLISION OPERATORS IN EQ. (7)

The first collision operators in Eq. (7) are

$$\Omega_j^{(0)} = \mathrm{Tr}\{[\hat{P}_j, \hat{H}_0]\overline{\rho(t,0)}\}, \quad \text{(A1a)}$$

$$\Omega_j^{(1)} = \mathrm{Tr}\{[\hat{P}_j, \hat{H}']\overline{\rho(t,0)}\}, \quad \text{(A1b)}$$

$$\Omega_j^{(2)}=\left(\frac{1}{i\hbar}\right)^2\int_{-\infty}^{t}dt'e^{\varepsilon(t'-t)}\mathrm{Tr}\{[\hat{H}'(t'-t)_0,(\hat{H}',\hat{P}_j)]\times\overline{\rho(t',t'-t)_0}\}+\frac{1}{i\hbar}\sum_k\int_{-\infty}^{t}dt'e^{\varepsilon(t'-t)}\Omega_k^{(1)}\times\frac{\delta}{\delta Q_k(t')}\mathrm{Tr}\{[\hat{H}',\hat{P}_j]\overline{\rho(t',t'-t)_0}\}, \quad \text{(A1c)}$$

etc. Subindex naught indicates evolution of operators in Heisenberg representation with H_0, and δ stands for functional derivative; the higher order terms are of ever increasing complexity.

APPENDIX B: COMPLEMENT TO EQ. (15)

The coefficients a_j in Eq. (15) are

$$a_1(\vec{q},\vec{Q};t)=[[1-\exp\{\Delta(\vec{q},\vec{Q};t)]/\Delta(\vec{q},\vec{Q};t)]\nu_{\vec{q}}^{h}(1+\nu_{\vec{q}+\vec{Q}}^{h}), \quad \text{(B1a)}$$

$$\Delta(\vec{q},\vec{Q};t)=F_2(t)\hbar(\omega_{\vec{q}+\vec{Q}}-\omega_{\vec{q}})+\vec{F}_3(t)\cdot\vec{\nabla}_{\vec{q}}(\omega_{\vec{q}+\vec{Q}}-\omega_{\vec{q}})+\vec{F}_4(t)\cdot[\hbar\omega_{\vec{q}+\vec{Q}}\vec{\nabla}_{\vec{q}}\omega_{\vec{q}+\vec{Q}}-\hbar\omega_{\vec{q}}\vec{\nabla}_{\vec{q}}\omega_{\vec{q}}], \quad \text{(B1b)}$$

$$a_2(\vec{q},\vec{Q};t)=\frac{\hbar}{2}(\omega_{\vec{q}+\vec{Q}}+\omega_{\vec{q}})a_1(\vec{q},\vec{Q};t), \quad \text{(B1c)}$$

$$\vec{a}_3(\vec{q},\vec{Q};t)=\vec{v}(\vec{q},\vec{Q})a_1(\vec{q},\vec{Q};t), \quad \text{(B1d)}$$

$$\vec{a}_4(\vec{q},\vec{Q};t)=\frac{\hbar}{2}(\omega_{\vec{q}+\vec{Q}}+\omega_{\vec{q}})\vec{v}(\vec{q},\vec{Q})a_1(\vec{q},\vec{Q};t), \quad \text{(B1e)}$$

where $\vec{v}$ is defined in Eq. (11c), and

$$\nu_{\vec{q}}^{h}=\mathrm{Tr}\{b_{\vec{q}}^{\dagger}b_{\vec{q}}\rho_h(t,0)\}=[e^{y_{\vec{q}}}-1]^{-1}, \quad \text{(B1f)}$$

with

$$y_{\vec{q}}=F_1+F_2\hbar\omega_{\vec{q}}+\vec{\nabla}_{\vec{q}}\omega_{\vec{q}}(\vec{F}_3+\hbar\omega_{\vec{q}}\vec{F}_4). \quad \text{(B1g)}$$

APPENDIX C: COMPONENTS OF MATRIX $\hat{M}$ IN EQ. (16)

The elements of matrix $\hat{M}$ in Eq. (16) in the limit of small Q are

$$M_{11}(t)=\sum_{\vec{q}}\eta(\vec{q},t);\quad M_{12}(t)=M_{21}(t)=\sum_{\vec{q}}\hbar\omega_{\vec{q}}\eta(\vec{q},t); \quad \text{(C1a)}$$

$$\vec{M}_{13}(t)=\vec{M}_{31}(t)=\sum_{\vec{q}}\vec{\nabla}_{\vec{q}}\omega_{\vec{q}}\eta(\vec{q},t);$$

$$\vec{M}_{14}(t)=\vec{M}_{41}(t)=\sum_{\vec{q}}\hbar\omega_{\vec{q}}\vec{\nabla}_{\vec{q}}\omega_{\vec{q}}\eta(\vec{q},t); \quad \text{(C1b)}$$

$$M_{22}(t)=\sum_{\vec{q}}(\hbar\omega_{\vec{q}})^2\eta(\vec{q},t);$$

$$\vec{M}_{23}(t)=\vec{M}_{32}(t)=\vec{M}_{14}(t)=\vec{M}_{41}(t); \quad \text{(C1c)}$$

$$\underset{\sim}{M}_{33}(t)=\sum_{\vec{q}}[\vec{\nabla}_{\vec{q}}\omega_{\vec{q}}\vec{\nabla}_{\vec{q}}\omega_{\vec{q}}]\eta(\vec{q},t);$$

$$\vec{M}_{24}(t)=\vec{M}_{42}(t)=\sum_{\vec{q}}(\hbar\omega_{\vec{q}})\vec{\nabla}_{\vec{q}}\omega_{\vec{q}}\eta(\vec{q},t); \quad \text{(C1d)}$$

$$\underset{\sim}{M}_{34}(t)=\vec{M}_{43}(t)=\sum_{\vec{q}}\hbar\omega_{\vec{q}}[\vec{\nabla}_{\vec{q}}\omega_{\vec{q}}\vec{\nabla}_{\vec{q}}\omega_{\vec{q}}]\eta(\vec{q},t); \quad \text{(C1e)}$$

$$\underset{\sim}{M}_{44}(t)=\sum_{\vec{q}}(\hbar\omega_{\vec{q}})^2[\vec{\nabla}_{\vec{q}}\omega_{\vec{q}}\vec{\nabla}_{\vec{q}}\omega_{\vec{q}}]\eta(\vec{q},t); \quad \text{(C1f)}$$

and where

$$\eta(\vec{q})=\nu_{\vec{q}}^{h}(t)[1+\nu_{\vec{q}}^{h}(t)]. \quad \text{(C1g)}$$

APPENDIX D: THE KINETIC COEFFICIENTS IN EQS. (19)

The kinetic coefficients in Eqs. (19) are

$$\lambda_\varepsilon(t)=\frac{1}{3}\sum_{\vec{q}}\hbar\omega_{\vec{q}}(\vec{\nabla}_{\vec{q}}\omega_{\vec{q}})^2a_2(\vec{q};t)M_{22}^{-1}(t), \quad \text{(D1a)}$$

$$\Lambda(t'-t;t')=H(t-t')e^{\varepsilon(t'-t)}\frac{2\pi}{\hbar}\times\sum_{\vec{q}}|\lambda_{\vec{q}}|^2M_{44}^{-1}(t')\times\frac{1}{12}\vec{\nabla}_{\vec{q}}\omega_{\vec{q}}\cdot\vec{a}_4(\vec{q};t)G_{\vec{q}}(t'-t), \quad \text{(D1b)}$$

$$\Theta_\varepsilon^{-1}(t'-t;t')=H(t-t')e^{\varepsilon(t'-t)}\frac{2\pi}{\hbar^2}\times\sum_{\vec{q}}|\lambda_{\vec{q}}|^2M_{22}^{-1}(t')a_2(\vec{q};t)G_{\vec{q}}(t'-t), \quad \text{(D1c)}$$

$$\Theta_I^{-1}(t'-t;t')=H(t-t')e^{\varepsilon(t-t')}\frac{2\pi}{\hbar^2}\times\sum_{\vec{q}}|\lambda_{\vec{q}}|^2M_{44}^{-1}(t')\hbar\omega_{\vec{q}}\times\frac{1}{3}\vec{\nabla}_{\vec{q}}\omega_{\vec{q}}\cdot\vec{a}_4(\vec{q};t')G_{\vec{q}}(t'-t), \quad \text{(D1d)}$$

where

$$G_{\vec{q}}(t'-t)=\int_{-\infty}^{\infty}\frac{d\omega}{\pi}\,[\mathcal{K}_{\vec{q}}(\omega)-\mathcal{J}_{\vec{q}}(\omega)]\times\exp[i(\omega_{\vec{q}}-\omega)(t'-t)], \tag{D1e}$$

and $H(t-t')$ is Heaviside's step function. We recall that Eqs. (19) correspond to $\vec{Q}\neq 0$. The equations for the homogeneous state ($Q=0$) are Eqs. (8a) and (8b) where populations $\nu_{\vec{q}}$ are given by Eq. (9b), since the linear contributions in the inhomogeneous variables—which are obtained using the linearized Heims-Jaynes expansion—vanish.

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