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Maxwell times in higher-order generalized hydrodynamics: Classical fluids, and carriers and phonons in semiconductors

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A family of what can be so-called Maxwell times which arises in the context of higher-order generalized hydrodynamics (HOGH; also called mesoscopic hydrothermodynamics) is evidenced. This is done in the framework of a HOGH built within a statistical formalism in terms of a nonequilibrium statistical ensemble formalism. It consists in a description in terms of the densities of particles and energy and their fluxes of all orders, with the motion described by a set of coupled nonlinear integro-differential equations involving them. These Maxwell times have a fundamental role in determining the type of hydrodynamic motion that the system would display in the given conditions and constraints. They determine a Maxwell viscous force not present in the usual hydrodynamic equations, for example, in Navier-Stokes equation.

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I. INTRODUCTION

We present what can be dubbed as a generalization of Maxwell time [1], which can also be referred to as generalized Maxwellian relaxation time [2], a family of which is present in the evolution equations of higher-order hydrodynamics, also dubbed as mesoscopic hydrothermodynamics (MHT) [3–6]. Such generalized Maxwell times are associated with the dampening of densities of particles (molecules in a classical fluid) or quasiparticles (Bloch-band electrons, harmonic phonons, magnons, polaritons, etc., in solid-state matter, in semiconductors for example), and of their energy density, together with the fluxes of all orders of both.

The origin of Maxwell time goes back to the fundamental article by Maxwell in 1867 on the dynamical theory of gases [1], in the section related to viscoelasticity, and which is being expressed as the quotient of the dynamical viscosity coefficient with the modulus of rigidity. According to Maxwell, it may be called the "time of relaxation" of the elastic force. It has been noticed [2] that, given a fluid subjected to some variable external forces, which vary periodically in time with frequency ω, when the period $1/\omega$ is large compared with Maxwell time θ, i.e., $\omega\theta \ll 1$, the fluid under consideration will behave as an ordinary viscous fluid. If, however, the frequency ω is sufficiently large (so that $\omega\theta \gg 1$, the fluid will behave as an amorphous solid.

We present a detailed study of the family of generalized Maxwell times that arise in a mesoscopic hydrothermodynamics, built upon a nonequilibrium statistical ensemble formalism (NESEF for short) [7–10], at the classical and quantum-mechanical levels of higher-order generalized hydrodynamics (HOGH) described in Refs. [5,6,11,12].

They are evidenced in the equations of evolution of the densities of particles and energy and their fluxes of all orders that are at the fundamentals of MHT. We recall that the dynamical equations for these basic variables are in NESEF, the classical (Hamilton) or quantum (Heisenberg) equations for the corresponding mechanical quantities averaged over the nonequilibrium statistical state. Therefore, the densities and each of the fluxes have associated these generalized Maxwell times, which depend on the microscopic characteristics of the system (interaction potential, mass, etc.) and on the temperature (in equilibrium or out of it).

As it has been stated in the Abstract, these generalized Maxwell times have a fundamental role in determining the type of hydrodynamic motion that the system would display in the conditions and constraints that are present, thus determining the contracted description in MHT to be used, that is, the one in terms of a reduced number of fluxes up to a certain order [4]. It may be noticed that a particular generalized Maxwell time is present in a viscous force that arises in a generalized Navier-Stokes equation in the framework of MHT.

In Sec. II Maxwell times are evidenced in the case of a classical MHT of a fluid of particles embedded in a thermal bath, while in Sec. III it is done in the case of a MHT at the quantum level of a system of phonons in semiconductors, and in Sec. IV it is done in the case of a MHT at the quantum level of a system of electrons in doped semiconductors.

II. MAXWELL TIMES IN THE MHT OF A CLASSICAL FLUID

Construction of HOGH in the framework of a NESEF is reported in Ref. [5], which provides an approach enabling for the coupling and simultaneous treatment of the kinetic and hydrodynamic levels of description. It is based on a complete thermostatistical approach in terms of the densities of matter and energy and their fluxes of all orders, as well as on their direct and cross correlations, covering systems arbitrarily far removed from equilibrium. The resulting set of coupled nonlinear integro-differential hydrodynamic equations are the evolution equations of a Grad-type approach involving the moments of all orders of the single-particle distribution

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$f_1(\mathbf{r},\mathbf{p};t)$, derived from a generalized kinetic equation built in the framework of a NESEF [13].

The moments of the single-particle distribution function, in momentum space $\mathbf{p}$, are the hydrodynamic variables

$$n(\mathbf{r},t) = \int d^3p f_1(\mathbf{r},\mathbf{p};t), \tag{1}$$

which represents the densities of particles, the first flux or current of particles,

$$\mathbf{I}_n(\mathbf{r},t) = \int d^3p\, \mathbf{u}(\mathbf{p}) f_1(\mathbf{r},\mathbf{p};t), \tag{2}$$

where

$$\mathbf{u}(\mathbf{p}) = \frac{\mathbf{p}}{m}. \tag{3}$$

$\mathbf{I}_n$ is multiplied by the mass is the momentum density. Moreover, the second-order flux is

$$I_n^{[2]}(\mathbf{r},t) = \int d^3p\, \mathbf{u}^{[2]}(\mathbf{p}) f_1(\mathbf{r},\mathbf{p};t), \tag{4}$$

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

$$I_n^{[\ell]}(\mathbf{r},t) = \int d^3p\, \mathbf{u}^{[\ell]}(\mathbf{p}) f_1(\mathbf{r},\mathbf{p};t) \tag{5}$$

are the higher-order fluxes of order $\ell \geqslant 3$ [the previous three of Eqs. (1), (2) and (4), are those for $\ell = 0,1$ and 2 respectively], where $\mathbf{u}^{[\ell]}$ is the ℓ-rank tensor consisting of the inner tensorial product of ℓ vectors $\mathbf{u}$ of Eq. (3); that is,

$$\mathbf{u}^{[\ell]}(\mathbf{p}) = \left[\frac{\mathbf{p}}{m}\frac{\mathbf{p}}{m}\cdots(\ell \text{ times})\cdots\frac{\mathbf{p}}{m}\right]. \tag{6}$$

This is what can be called the *family of hydrodynamical variables describing the material motion*, i.e., the set

$$\left\{n(\mathbf{r},t);\ \mathbf{I}_n(\mathbf{r},t);\ \left\{I_n^{[\ell]}(\mathbf{r},t)\right\}\right\}, \tag{7}$$

with $\ell = 2,3,\ldots$, which we call the n-MHT family.

On the other hand, present is the *family of hydrodynamical variables describing the thermal motion*, which we call the h-MHT family, consisting of

$$h(\mathbf{r},t) = \int d^3p\, \frac{p^2}{2m} f_1(\mathbf{r},\mathbf{p};t), \tag{8}$$

$$\mathbf{I}_h(\mathbf{r},t) = \int d^3p\, \frac{p^2}{2m}\frac{\mathbf{p}}{m} f_1(\mathbf{r},\mathbf{p};t), \tag{9}$$

$$I_h^{[\ell]}(\mathbf{r},t) = \int d^3p\, \frac{p^2}{2m}\mathbf{u}^{[\ell]}(\mathbf{p}) f_1(\mathbf{r},\mathbf{p};t), \tag{10}$$

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

$$\left\{h(\mathbf{r},t);\ \mathbf{I}_h(\mathbf{r},t);\ \left\{I_h^{[\ell]}(\mathbf{r},t)\right\}\right\}, \tag{11}$$

which are, respectively, the density of energy, its first vectorial flux (heat current), and the higher-order tensorial fluxes. It can be noticed that in this case of a parabolic type energy-momentum dispersion relation, $E(p) = p^2/2m$, the set of Eq. (11) is encompassed in the previous one: In fact,

$$h(\mathbf{r},t) = \frac{m}{2}\mathrm{Tr}\left\{I_n^{[2]}(\mathbf{r},t)\right\}, \tag{12}$$

$$\mathbf{I}_h(\mathbf{r},t) = \frac{m}{2}\mathrm{Tr}_2\left\{I_n^{[3]}(\mathbf{r},t)\right\}, \tag{13}$$

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

$$I_h^{[\ell]}(\mathbf{r},t) = \frac{m}{2}\mathrm{Tr}_2\left\{I_n^{[\ell+2]}(\mathbf{r},t)\right\}, \tag{14}$$

for all the other higher-order fluxes of energy; that is, any flux of energy of order ℓ is contained in the flux of matter of order $\ell + 2$.

Let us consider the equations of evolutions for the basic macrovariables of the n-MHT family (particle motion), which for the general flux of order ℓ ($\ell = 0,1,2,\ldots$) is

$$\frac{\partial}{\partial t} I_n^{[\ell]}(\mathbf{r},t) = \int d^3p\, \mathbf{u}^{[\ell]}(\mathbf{p})\frac{\partial}{\partial t} f_1(\mathbf{r},\mathbf{p};t). \tag{15}$$

Using in Eq. (15) the evolution equations for $f_1(\mathbf{r},\mathbf{p};t)$ of Ref. [13] it follows the general set of coupled equations for the density, $\ell = 0$, the current, $\ell = 1$, and all the other higher-order fluxes, $\ell \geqslant 2$, a cumbersome set of coupled integro-differential equations reported in Ref. [5]. In those equations the second term on the right in the one describing, the evolution of the flux of order ℓ, is the one that contains the Maxwell time $\theta_{n\ell}$ associated with such flux, namely,

$$\theta_{n\ell}^{-1} = \ell|a_{\tau 0}| + \ell(\ell-1)|b_{\tau 1}|, \tag{16}$$

with the coefficients $a_{\tau 0}$ and $b_{\tau 1}$ given by

$$a_{\tau 0} = \frac{\mathcal{V}}{(2\pi)^3}\frac{4\pi}{3}\int dQ\, Q^4 f_{\tau 0}(Q), \tag{17}$$

with

$$f_{\tau 0}(Q) = -\frac{n_R M \beta_0^{3/2}\pi}{\mathcal{V}\sqrt{2\pi}m^2}\frac{|\psi(Q)|^2}{Q}\left(\frac{m}{M}+1\right), \tag{18}$$

where $\psi(Q)$ is the Fourier transform of the potential energy $w(|\mathbf{r}_j - \mathbf{R}_\mu|)$, between the jth particle at position $\mathbf{r}$ and the one in the thermal bath at position $\mathbf{R}_\mu$, n_R is the density of particles in the thermal bath, $\mathcal{V}$ is the volume, and $\beta_0^{-1} = k_B T_0$, with T_0 being the temperature of the thermal bath, and

$$b_{\tau 1} = -\frac{a_{\tau 0}}{5}\left(\frac{m}{M}+1\right)^{-1}, \tag{19}$$

where m and M are the mass of the particles and of the particles in the thermal bath, respectively. According to Eqs. (16) and (19), we can write

$$\theta_{n\ell}^{-1} = -\ell|a_{\tau 0}|\left[1 + \frac{1}{5}(\ell-1)\left(\frac{M}{m+M}\right)\right], \tag{20}$$

and it can be noticed that $|a_{\tau 0}|$ is the reciprocal of the Maxwell time of the first flux, which is the reciprocal of the relaxation time of the linear momentum $\mathbf{p}(\mathbf{r},t)$, once $\mathbf{p}(\mathbf{r},t) = m\mathbf{I}_n(\mathbf{r},t)$.

Maxwell times of Eq. (16) have their origin from the collision integral $J_\tau^{(2)}(\mathbf{r},\mathbf{p};t)$ in the kinetic equation for the single-particle distribution present in Eq. (A.11) in Appendix A in Ref. [13]. It arises out of the interaction with the thermal bath in the contributions called effective friction force and diffusion in momentum space.

It follows from Eq. (16) that we can write

$$\theta_{n\ell}^{-1} = \ell\left[1 + \frac{M}{5(m+M)}(\ell-1)\right]\theta_{n1}^{-1}, \tag{21}$$

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

$$\frac{\theta_{n_{\ell+1}}}{\theta_{n_\ell}} = \frac{\ell}{\ell+1}\,\frac{5(1+x)+\ell-1}{5(1+x)+\ell}, \tag{22}$$

for $\ell = 1,2,3,\ldots$ and where $x = m/M$, then the ordered sequence

$$\theta_{n_1} > \theta_{n_2} > \theta_{n_3} \cdots > \theta_{n_\ell} > \theta_{n_{\ell+1}} > \cdots \tag{23}$$

is verified, and it can be seen that $\theta_{n_\ell} \to 0$ as $\ell \to \infty$. Moreover, according to Eq. (21) it follows that

$$\theta_{n_\ell} = \frac{5(1+x)}{\ell[5(1+x)+\ell-1]}\theta_{n_1}. \tag{24}$$

Comparing with the second flux ($\ell = 2$), which is the one related to the pressure tensor, it follows that for Brownian particles ($x \gg 1$) $\theta_{n_2} \simeq \theta_{n_1}/2$ and for Lorentz particles ($x \ll 1$) $\theta_{n_2} \simeq 5\theta_{n_1}/12$. A comparison with the third flux leads to the results that $\theta_{n_3} \simeq \theta_{n_1}/3$ and $\theta_{n_3} \simeq 5\theta_{n_1}/21$ for the Brownian and Lorentz particles, respectively. For any ℓ we do have, approximately,

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

$$\theta_{n_\ell} \simeq \frac{\theta_{n_1}}{\ell}, \tag{25}$$

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

$$\theta_{n_\ell} \simeq \frac{5}{(4+\ell)\ell}\theta_{n_1}, \tag{26}$$

or $\theta_{n_\ell} \simeq 5\theta_{n_1}/\ell^2$ for large ℓ.

According to Eq. (22), as the order of the flux largely increases, its Maxwell characteristic time approaches zero, and $\theta_{n_{\ell+1}}/\theta_{n_\ell} \simeq 1$, with both practically null. Figure 1 displays the ratio of some Maxwell-characteristic times with the one of the linear momentum in terms of the ratio m/M.

We emphasized that the hierarchy shown in Eq. (23) evidences the important fact of the ever-decreasing value of the Maxwell times with the increasing order of the fluxes. This is quite relevant for the question of how to introduce a contracted description (i.e., keeping a reduced number of fluxes) for characterizing the particular type of hydrodynamic motion (diffusion, damped waves, etc.) that the system displays, as shown later on.

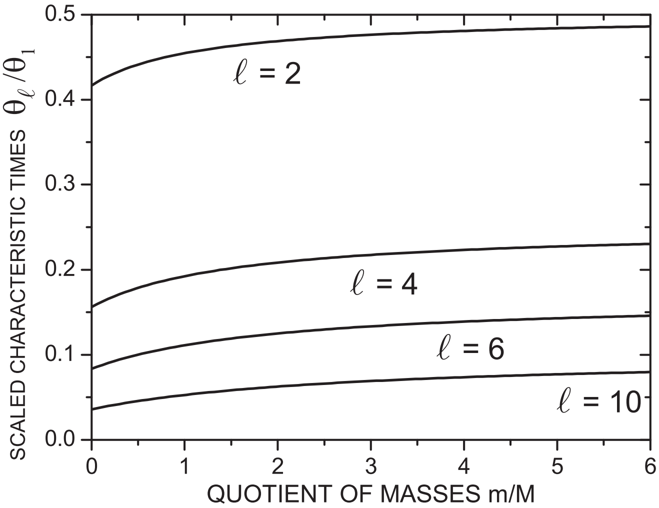

FIG. 1. The quotient between Maxwell-characteristic times and the one of the first flux as a function of $x = m/M$.

III. MAXWELL TIMES IN THERMAL TRANSPORT

In this section we concentrate attention on the evolution of the thermal quantities

$$\left\{h(\mathbf{r},t);\ \mathbf{I}_h(\mathbf{r},t);\ \left\{I_h^{[\ell]}(\mathbf{r},t)\right\}\right\}, \tag{27}$$

with $\ell = 2,3,\ldots$, that is, the density of energy and its fluxes of all orders given in Eqs. (8) to (10). Their evolution equations are

$$\frac{\partial}{\partial t}I_h^{[\ell]}(\mathbf{r},t) = \int d^3p\,\frac{p^2}{2m}\mathbf{u}^{[\ell]}(\mathbf{p})\frac{\partial}{\partial t}f_1(\mathbf{r},\mathbf{p};t), \tag{28}$$

in which we need to introduce the kinetic equation for the single particle $f_1(\mathbf{r},\mathbf{p};t)$, which is given in Ref. [13]. Performing the lengthy calculations involved, we finally arrive at the general evolution equations ($\ell = 0,1,2,\ldots$) reported in Ref. [5], in which

$$\begin{aligned}\frac{\partial}{\partial t}I_h^{[\ell]}(\mathbf{r},t) + \nabla\cdot I_h^{[\ell+1]}(\mathbf{r},t)\\ = \mathcal{F}(\mathbf{r},t)I_n^{[\ell+1]}(\mathbf{r},t) - \sum_{s=1}^{\ell}\sigma(1,s)\big[\mathcal{F}(\mathbf{r},t)I_h^{[\ell-1]}(\mathbf{r},t)\big]\\ + \theta_{h_\ell}^{-1}I_h^{[\ell]}(\mathbf{r},t) + a_{L0}\sum_{s=1}^{\ell}\sigma(1,s)\big[\nabla I_h^{[\ell-1]}(\mathbf{r},t)\big]\\ + 2(\ell+3)a_{L1}\nabla\cdot I_h^{[\ell+1]}(\mathbf{r},t) + S_h^{[\ell]}(\mathbf{r},t),\end{aligned} \tag{29}$$

and present is the reciprocal of the Maxwell time θ_{h_ℓ} associated with the ℓth-order flux of energy given by

$$\theta_{h_\ell}^{-1} = (\ell+2)|a_{\tau 0}| + [\ell^2 + 5(\ell+1)]|b_{\tau 1}|. \tag{30}$$

Taking into account that

$$|b_{\tau 1}| = \frac{1}{5(1+x)}|a_{\tau 0}|, \tag{31}$$

it follows that Maxwell times have the property that

$$\frac{\theta_{h_{\ell+1}}}{\theta_{h_\ell}} = \frac{5(\ell+2)(1+x)+\ell^2+5(\ell+1)}{5(\ell+3)(1+x)+(\ell+1)^2+5(\ell+2)} < 1, \tag{32}$$

for $\ell = 0,1,2,3,\ldots,$ and where $x = m/M$. The ordered sequence

$$\theta_{h_0} > \theta_{h_1} > \theta_{h_2} > \theta_{h_3} > \cdots > \theta_{h_\ell} > \theta_{h_{\ell+1}} > \cdots \tag{33}$$

is verified in an analogous condition on the Maxwell times associated to the particle motion. It may be noticed that for large ℓ,θ_ℓ goes as ℓ^{-2}, i.e., going to zero as $\ell \to \infty$.

For the Brownian particle ($x \gg 1$) the ratio in Eq. (32) tends asymptotically to $(\ell+2)/(\ell+3)$, while for Lorentz particles ($x \ll 1$) the ratio tends to $[\ell^2+5(2\ell+3)]/[(\ell+1)^2+5(2\ell+5)]$. Considering that the Maxwell time of the first flux of matter, θ_{n_1}, is $|a_{\tau 0}|^{-1}$ [cf. Eq. (20)], we can establish the relation between it and the Maxwell time for the energy

$$\theta_{h_0} = \frac{1+x}{2x+3}\theta_{n_1}, \tag{34}$$

which tells us that $\theta_{h_0} < \theta_{n_1}$. For a Brownian particle $\theta_{h_0} = \theta_{n_1}/2$, and for a Lorentz particle $\theta_{h_0} = \theta_{n_1}/3$. Moreover, for general ℓ we have that

$$\theta_{h_\ell} = \frac{5(1+x)}{5(\ell+2)(1+x)+\ell^2+5(\ell+1)}\theta_{n_1}. \tag{35}$$

Therefore, recalling that the first flux of matter multiplied by the particle mass is the linear momentum density, as a general rule we can state that the energy relaxation time is smaller than momentum relaxation time. As already noticed at the end of the previous section, the hierarchy shown in Eq. (33) is quite relevant for choosing the contracted description to be used.

We proceed next to consider the case of a MHT at a quantum-mechanical level for the cases of phonons and electrons in semiconductors.

IV. MAXWELL TIMES IN MHT OF PHONONS IN SEMICONDUCTORS

We consider a system of longitudinal acoustic LA phonons in a semiconductor in anharmonic interaction with the accompanying transverse acoustic TA phonons. The sample is in contact with a thermostat at temperature T_0. An external pumping source drives the LA-phonon system out of equilibrium. The system is characterized at the microscopic level by the Hamiltonian

$$\hat{H} = \hat{H}_{0S} + \hat{H}_{0B} + \hat{H}_{SB} + \hat{H}_{SP}, \tag{36}$$

which consists of the Hamiltonian of the free LA phonons

$$\hat{H}_{0S} = \sum_{\mathbf{q}} \hbar\omega_{\mathbf{q}}(a^\dagger_{\mathbf{q}}a_{\mathbf{q}} + 1/2), \tag{37}$$

where $\omega_{\mathbf{q}}$ is the frequency dispersion relation and the sum on $\mathbf{q}$ runs over the Brillouin zone, and the one of the TA phonons, which we call the thermal bath in which the LA phonons are embedded, given by

$$\hat{H}_{0B} = \sum_{\mathbf{q}} \hbar\Omega_{\mathbf{q}}(b^\dagger_{\mathbf{q}}b_{\mathbf{q}} + 1/2), \tag{38}$$

where $\Omega_{\mathbf{q}}$ is the frequency dispersion relation; $a^\dagger_{\mathbf{q}}$ ($a_{\mathbf{q}}$) and $b^\dagger_{\mathbf{q}}$ ($b_{\mathbf{q}}$) are the corresponding creation (annihilation) operators in mode $\mathbf{q}$.

Moreover, the interaction of the LA phonons with the thermal bath is given by

$$\hat{H}_{SB} = \sum_{\mathbf{k},\mathbf{q}} M_{\mathbf{k},\mathbf{q}} a_{\mathbf{q}} b^\dagger_{\mathbf{k}+\mathbf{q}} b^\dagger_{-\mathbf{k}} + \text{H.c.}, \tag{39}$$

where we have retained the only process that contributes to the kinetic equations (LA $\leftrightarrows$ TA + TA) and we have neglected nonlinear contributions; $M_{\mathbf{k},\mathbf{q}}$ accounts for the coupling strengths. Finally, $\hat{H}_{SP}$ is the interaction energy operator for the phonons and an external pumping source, to be specified in each case.

At the macroscopic level (the nonequilibrium thermodynamic state) NESEF requires first to specify the basic variables that are to be used to characterize the nonequilibrium ensemble [7–10]. *A priori*, when the system is initially driven away from equilibrium, it is necessary to include all the observables of the system that is attained introducing many-particle dynamical operators [14,15]; in the present case it suffices to take only the single-phonon dynamical operators $\hat{\nu}_{\mathbf{q},\mathbf{Q}} = a^\dagger_{\mathbf{q}+\mathbf{Q}/2}a_{\mathbf{q}-\mathbf{Q}/2}$ in the second-quantization representation in reciprocal space. The two-phonon dynamical operator and higher-order ones can be ignored because of Bogoliubov's principle of correlation weakening [15]. Moreover, it would be necessary to also include the amplitudes $a^\dagger_{\mathbf{q}}$ and $a_{\mathbf{q}}$ because their eigenstates are the coherent states [16] and the phonon pairs [17]: Both are disregarded because they are of no practical relevance for the problem considered here. Another basic microdynamical variable that needs to be incorporated is the energy of the bath, and then the NESEF-basic set is composed of

$$\{\hat{\nu}_{\mathbf{q}},\, \hat{\nu}_{\mathbf{q},\mathbf{Q}},\, \hat{H}_{0B}\}, \tag{40}$$

where we have separated out the so-called populations, $\hat{\nu}_{\mathbf{q}} = a^\dagger_{\mathbf{q}}a_{\mathbf{q}}$, from those with $\mathbf{Q} \neq 0$, which are related to the change in space of the populations (they are also called coherences [18]).

Therefore, for the present case the nonequilibrium statistical operator is

$$\varrho_\epsilon(t) = \exp\left\{-\hat{S}(t,0) + \int_{-\infty}^{t} dt' e^{\epsilon(t'-t)} \frac{d}{dt'}\hat{S}(t',t'-t)\right\}, \tag{41}$$

where

$$\begin{aligned} \hat{S}(t,0) &= -\ln \bar{\varrho}(t,0) \\ &= \phi(t) + \sum_{\mathbf{q}} F_{\mathbf{q}}(t) a^\dagger_q a_q \\ &\quad + \sum_{\mathbf{q}\mathbf{Q}\neq 0} F_{\mathbf{q}\mathbf{Q}}(t) a^\dagger_{q+Q/2} a_{q-Q/2} + \beta_0 \hat{H}_{0B}, \end{aligned} \tag{42}$$

$$\hat{S}(t',t'-t) = e^{-(t'-t)\hat{H}/i\hbar}\hat{S}(t',0)e^{(t'-t)\hat{H}/i\hbar}, \tag{43}$$

$\hat{H}_{0B}$ is given in Eq. (38), $\phi(t)$, which ensures the normalization of $\bar{\varrho}$ and ϱ_ϵ, plays the role of a logarithm of a nonequilibrium partition function $\bar{Z}(t)$, and $\beta_0 = 1/(k_B T_0)$.

The average values of the microdynamical variables in set (40) over the nonequilibrium ensemble provide the variables that characterize the nonequilibrium macroscopic state of the system, which we indicate by

$$\{\nu_{\mathbf{q}}(t),\, \nu_{\mathbf{q}\mathbf{Q}}(t),\, E_B\}, \tag{44}$$

and the nonequilibrium thermodynamic variables conjugated to them are

$$\{F_{\mathbf{q}}(t),\, F_{\mathbf{qQ}}(t),\, \beta_0\}. \tag{45}$$

Going over to direct space (antitransforming Fourier in variable $\mathbf{Q}$), we obtain the space and crystalline momentum-dependent distribution function $\nu_{\mathbf{q}}(\mathbf{r},t)$, in terms of which is built the phonon higher-order generalized hydrothermodynamics, which consists of two families of hydrodynamical variables, namely, the one associated with the quasiparticles (the phonons) motion (we call it the n family),

$$\big\{n(\mathbf{r},t),\, \mathbf{I}_n(\mathbf{r},t),\, \big\{I_n^{[\ell]}(\mathbf{r},t)\big\}\big\}, \tag{46}$$

where $\ell = 2,3,\ldots$, and $n(\mathbf{r},t)$ stands for the number of phonons at time t in position $\mathbf{r}$, namely,

$$n(\mathbf{r},t) = \sum_{\mathbf{q}} \nu_{\mathbf{q}}(\mathbf{r},t), \tag{47}$$

the first flux of this quantity

$$\mathbf{I}_n(\mathbf{r},t) = \sum_{\mathbf{q}} \nabla_{\mathbf{q}}\omega_{\mathbf{q}}\, \nu_{\mathbf{q}}(\mathbf{r},t), \tag{48}$$

and the higher-order fluxes

$$I_n^{[\ell]}(\mathbf{r},t) = \sum_{\mathbf{q}} u^{[\ell]}(\mathbf{q})\, \nu_{\mathbf{q}}(\mathbf{r},t), \tag{49}$$

with $\ell = 2,3,\ldots$, defining the ℓ-order flux (ℓ-rank tensor), where

$$u^{[\ell]}(\mathbf{q}) = [\nabla_{\mathbf{q}}\omega_{\mathbf{q}} \cdots \ell \text{ times} \cdots \nabla_{\mathbf{q}}\omega_{\mathbf{q}}] \tag{50}$$

is a ℓ-rank tensor consisting of the tensorial inner product of ℓ times the group velocity of the $\mathbf{q}$-mode phonon, $\nabla_{\mathbf{q}}\omega_{\mathbf{q}}$.

On the other hand, we do have the family associated with the energy motion (heat transport, and we call it the h family)

$$\big\{h(\mathbf{r},t),\, \mathbf{I}_h(\mathbf{r},t),\, \big\{I_h^{[\ell]}(\mathbf{r},t)\big\}\big\}, \tag{51}$$

where

$$h(\mathbf{r},t) = \sum_{\mathbf{q}} \hbar\omega_{\mathbf{q}}\nu_{\mathbf{q}}(\mathbf{r},t), \tag{52}$$

$$\mathbf{I}_h(\mathbf{r},t) = \sum_{\mathbf{q}} \hbar\omega_{\mathbf{q}}\nabla_{\mathbf{q}}\omega_{\mathbf{q}}\, \nu_{\mathbf{q}}(\mathbf{r},t), \tag{53}$$

$$I_h^{[\ell]}(\mathbf{r},t) = \sum_{\mathbf{q}} \hbar\omega_{\mathbf{q}} u^{[\ell]}(\mathbf{q})\, \nu_{\mathbf{q}}(\mathbf{r},t), \tag{54}$$

which are, respectively, the energy density, its first (vectorial) flux, and the higher-order ($\ell = 2,3,\ldots$) tensorial fluxes at time t in position $\mathbf{r}$.

Consequently, the hydrodynamic equations of motion (evolution equations for the quantities above) are

$$\frac{\partial}{\partial t} I_p^{[\ell]}(\mathbf{r},t) = \sum_{\mathbf{q}} K_p^{[\ell]}(\mathbf{q}) \frac{\partial}{\partial t}\nu_{\mathbf{q}}(\mathbf{r},t), \tag{55}$$

where, for $p \equiv n$, $K_n^{[\ell]}(\mathbf{q}) = u^{[\ell]}(\mathbf{q})$ and for $p \equiv h$, $K_h^{[\ell]}(\mathbf{q}) = \hbar\omega_{\mathbf{q}} u^{[\ell]}(\mathbf{q})$, recalling that $\ell = 0$ corresponds to the densities, $\ell = 1$ to the vectorial fluxes, and $\ell \geqslant 2$ to the higher-order fluxes.

Evidently, all the evolution equations in Eq. (55) are determined by the unique equation of motion for the single-phonon distribution function $\nu_{\mathbf{q}}(\mathbf{r},t)$. It follows from the evolution equation, which results in taking the average over the nonequilibrium ensemble of the quantum-mechanical Heisenberg equation of motion for the microdynamical variable $\hat{\nu}_{\mathbf{qQ}} = a^{\dagger}_{\mathbf{q}+\mathbf{Q}/2}a_{\mathbf{q}-\mathbf{Q}/2}$ (for practical convenience it is calculated in reciprocal space); that is,

$$\frac{\partial}{\partial t}\nu_{\mathbf{q},\mathbf{Q}}(t) = \mathrm{Tr}\left\{\frac{1}{i\hbar}[\hat{\nu}_{\mathbf{qQ}},\hat{H}]\varrho_{\epsilon}(t) \times \varrho_B\right\}, \tag{56}$$

where $\varrho_{\epsilon}(t)$ is the nonequilibrium statistical operator of Eq. (41) and ϱ_B is the canonical statistical distribution of the thermal bath (the TA phonons) at the temperature T_0. Performing such average is extremely difficult and then it is necessary to resort to the introduction of a practical nonlinear quantum kinetic theory [7–10,19,20], which, for the present case, can be used in the approximation consisting in retaining in the collision integral contributions up to second order in the interaction strength (Markovian approximation [9,19,21]). In that approximation it follows, after going over to direct space, a generalization of the so-called Peierls-Boltzmann equation given by [22–24]

$$\frac{\partial}{\partial t}\nu_{\mathbf{q}}(\mathbf{r},t) = -\nabla\cdot\nabla_{\mathbf{q}}\tilde{\omega}_{\mathbf{q}}\nu_{\mathbf{q}}(\mathbf{r},t) - \Gamma_{\mathbf{q}}\left[\nu_{\mathbf{q}}(\mathbf{r},t) - \nu^0_{\mathbf{q}}\right] + J_{\mathbf{q}S}(\mathbf{r},t), \tag{57}$$

where $J_{\mathbf{q}S}$ contains the effect of the presence of external sources, to be specified in each particular case, and

$$\nu^0_{\mathbf{q}} = \frac{1}{e^{\beta_0\hbar\omega_{\mathbf{q}}} - 1}$$

is the distribution in equilibrium,

$$\tilde{\omega}_{\mathbf{q}} = \omega_{\mathbf{q}} + P_{\mathbf{q}}, \tag{58}$$

with

$$P_{\mathbf{q}} = \frac{\pi}{\hbar^2}\sum_{\mathbf{k}} |M_{\mathbf{kq}}|^2 \frac{1 + \nu^{TA}_{\mathbf{k}} + \nu^{TA}_{\mathbf{k}+\mathbf{q}}}{\Omega_{\mathbf{k}+\mathbf{q}} + \Omega_{\mathbf{k}} - \omega_{\mathbf{q}}}, \tag{59}$$

which is the so-called self-energy correction, and

$$\Gamma_{\mathbf{q}} = \frac{\pi}{\hbar^2}\sum_{\mathbf{k}} |M_{\mathbf{kq}}|^2\big(1 + \nu^{\mathrm{TA}}_{\mathbf{k}} + \nu^{\mathrm{TA}}_{\mathbf{k}+\mathbf{q}}\big) \times \delta(\Omega_{\mathbf{k}+\mathbf{q}} + \Omega_{\mathbf{k}} - \omega_{\mathbf{q}}) + \overline{\Gamma}_{\mathbf{q}} \tag{60}$$

plays the role of the reciprocal of a relaxation time per mode, say $\tau^{-1}_{\mathbf{q}}$ (towards the equilibrium distribution), where

$$\nu^{TA}_{\mathbf{k}} = \frac{1}{e^{\beta_0\hbar\Omega_{\mathbf{k}}} - 1} \tag{61}$$

is the distribution in equilibrium at temperature T_0 of the TA phonons. In Eq. (60) we have written explicitly the known contribution due to the anharmonic interaction, and in a Mathiessen rule [25] also indicated in $\overline{\Gamma}_{\mathbf{q}}$ is the sum of the inverse of the relaxation times due to the presence of impurities, imperfections, boundary conditions, etc.

Using Eq. (57) in Eq. (55), we obtain for the set of evolution equations that

$$\frac{\partial}{\partial t} I_p^{[\ell]}(\mathbf{r},t) = \sum_{\mathbf{q}} \{ K_p^{[\ell]}(\mathbf{q})[-\nabla \cdot \nabla_{\mathbf{q}} \tilde{\omega}_{\mathbf{q}}] \nu_{\mathbf{q}}(\mathbf{r},t) - \Gamma_{\mathbf{q}} [\nu_{\mathbf{q}}(\mathbf{r},t) - \nu_{\mathbf{q}}^0] \} + J_{pS}^{[\ell]}(\mathbf{r},t) \tag{62}$$

for both families of sets (46) and (51), $p \equiv n$ and $p \equiv h$, respectively. A closure for the set of these equations must be introduced, that is, to express $\nu_{\mathbf{q}}(\mathbf{r},t)$, which appears on the right-hand side in terms of the hydrodynamic variables in the sets of Eqs. (46) and (51). First, it can be noticed that Eq. (62) involves an enormous set of coupled nonlinear integro-differential equations; i.e., both densities together with their fluxes of all orders are coupled through all these equations. To proceed further it is necessary to introduce a *contraction of description*, that is to say, to reduce the number of variables to be used, as described elsewhere [9,10,26]. Moreover, the two families in the sets of Eqs. (46) and (51) are coupled by cross terms that account for thermostriction effects. In cases where these effects are not particularly relevant they can be disregarded and we obtain two independent sets of evolution equations, one for the n family and the other for the h family.

Admitting that the just-mentioned conditions are well satisfied, we introduce a contracted description of first order and proceed to analyze the evolution equations for the energy density and its first flux. The resulting equations are [24]

$$\frac{\partial}{\partial t} h(\mathbf{r},t) + \nabla \cdot \mathbf{I}_h(\mathbf{r},t) = a_L(t) \nabla \cdot \mathbf{I}_h(\mathbf{r},t) - \theta_h^{-1}(t) h(\mathbf{r},t) + J_{hS}(\mathbf{r},t), \tag{63}$$

$$\frac{\partial}{\partial t} \mathbf{I}_h(\mathbf{r},t) + \nabla \cdot I_h^{[2]}(\mathbf{r},t) = b_L^{[2]}(t) \cdot \nabla h(\mathbf{r},t) - \theta_I^{-1}(t) \mathbf{I}_h(\mathbf{r},t) + \mathbf{J}_{IS}(\mathbf{r},t), \tag{64}$$

where

$$a_L(t) = \sum_{\mathbf{q}} \hbar\omega_{\mathbf{q}} \mathbf{a}_I(\mathbf{q},t) \cdot \nabla_{\mathbf{q}} P_{\mathbf{q}}, \tag{65}$$

$$b_L^{[2]}(t) = \sum_{\mathbf{q}} \hbar\omega_{\mathbf{q}} a_h(\mathbf{q},t) [\nabla_{\mathbf{q}} P_{\mathbf{q}} : \nabla_{\mathbf{q}} \omega_{\mathbf{q}}], \tag{66}$$

$$a_h(\mathbf{q},t) = \hbar\omega_{\mathbf{q}} \nu_{\mathbf{q}}(t)[1+\nu_{\mathbf{q}}(t)] \times \left\{ \sum_{\mathbf{q}} (\hbar\omega_{\mathbf{q}})^2 \nu_{\mathbf{q}}(t)[1+\nu_{\mathbf{q}}(t)] \right\}^{-1}, \tag{67}$$

$$\mathbf{a}_I(\mathbf{q},t) = \hbar\omega_{\mathbf{q}} \nu_{\mathbf{q}}(t)[1+\nu_{\mathbf{q}}(t)] \left\{ \sum_{\mathbf{q}} (\hbar\omega_{\mathbf{q}})^2 \nu_{\mathbf{q}}(t) \times [1+\nu_{\mathbf{q}}(t)][\nabla_{\mathbf{q}}\omega_{\mathbf{q}} \cdot \nabla_{\mathbf{q}}\omega_{\mathbf{q}}] \right\}^{-1} \nabla_{\mathbf{q}}\omega_{\mathbf{q}}, \tag{68}$$

where $P_{\mathbf{q}}$ and $\Gamma_{\mathbf{q}}$ are given in Eqs. (59) and (60), and

$$\nu_{\mathbf{q}}(t) = \frac{1}{e^{F_{\mathbf{q}}(t)} - 1}, \tag{69}$$

with $F_{\mathbf{q}}$ of Eq. (45); we recall that

$$I_h^{[2]}(\mathbf{Q},t) = \sum_{\mathbf{q}} \hbar\omega_{\mathbf{q}} [\nabla_{\mathbf{q}}\omega_{\mathbf{q}} \nabla_{\mathbf{q}}\omega_{\mathbf{q}}] \nu_{\mathbf{q}\mathbf{Q}}(t), \tag{70}$$

and J_{hS} and $\mathbf{J}_{IS}$ are the contributions due to the coupling with the external sources that are present, which are to be specified in each case being considered.

Finally,

$$\theta_h^{-1}(t) = \sum_{\mathbf{q}} w_h(\mathbf{q},t) \Gamma_{\mathbf{q}}, \tag{71}$$

and

$$\theta_I^{-1}(t) = \sum_{\mathbf{q}} w_I(\mathbf{q},t) \Gamma_{\mathbf{q}}, \tag{72}$$

with

$$w_h(\mathbf{q},t) = \frac{(\hbar\omega_{\mathbf{q}})^2 \nu_{\mathbf{q}}(1+\nu_{\mathbf{q}})}{\sum_{\mathbf{q}'} (\hbar\omega_{\mathbf{q}'})^2 \nu_{\mathbf{q}'}(1+\nu_{\mathbf{q}'})}, \tag{73}$$

$$w_I(\mathbf{q},t) = \frac{(\hbar\omega_{\mathbf{q}})^2 \nu_{\mathbf{q}}(1+\nu_{\mathbf{q}})}{\sum_{\mathbf{q}'} (\hbar\omega_{\mathbf{q}'})^2 \nu_{\mathbf{q}'}(1+\nu_{\mathbf{q}'})} \frac{|\nabla_{\mathbf{q}}\omega_{\mathbf{q}}|^2}{|\nabla_{\mathbf{q}'}\omega_{\mathbf{q}'}|^2}, \tag{74}$$

which have the property of normalization; that is, it is verified that

$$\sum_{\mathbf{q}} w_h(\mathbf{q},t) = 1, \tag{75}$$

and

$$\sum_{\mathbf{q}} w_I(\mathbf{q},t) = 1. \tag{76}$$

Equations (71) and (72) define the reciprocal of Maxwell times associated with energy and its first flux, respectively, in this MHT of order 1. We can see that each Maxwell time follows a kind of Mathiessen rule: Its inverse is a superposition of the reciprocal of the relaxation times of each mode $\tau_{\mathbf{q}}^{-1} = \Gamma_{\mathbf{q}}$, multiplied by a weighting function $w(\mathbf{q},t)$. Because of the normalization condition [Eqs. (75) and (76)], each $w(\mathbf{q},t)$ can be considered as the probability at each time t of the contribution of the mode-relaxation time $\tau_{\mathbf{q}}$.

In a Debye model ($\omega_{\mathbf{q}} = sq$, where s is the sound velocity) both Maxwell times are equal, i.e.,

$$\theta_h^{-1}(t) = \theta_I^{-1}(t) = \frac{\sum_{\mathbf{q}} (sq)^2 \nu_{\mathbf{q}}(1+\nu_{\mathbf{q}}) \Gamma_{\mathbf{q}}}{\sum_{\mathbf{q}} (sq)^2 \nu_{\mathbf{q}}(1+\nu_{\mathbf{q}})}, \tag{77}$$

and we recall that $q \leqslant q_{\text{Debye}}$.

Taking into account that $|\nabla_{\mathbf{q}}\omega_{\mathbf{q}}| \simeq s$ for small values of q and that $|\nabla_{\mathbf{q}}\omega_{\mathbf{q}}| < s$ for intermediate to large values of q, we can estimate that, in general, $\theta_h > \theta_I$. It is conjectured that we would do have a hierarchy,

$$\theta_h > \theta_I > \theta_{I_2} > \cdots,$$

quite similar to the case of the classical fluid of previous sections.

V. MAXWELL TIMES IN MHT OF ELECTRONS IN SEMICONDUCTORS

We consider the case of a n-doped polar semiconductor, e.g., n-GaAs or n-GaN, whose Hamiltonian quantum-mechanical operator is

$$\hat{H} = \hat{H}_{0e} + \hat{H}_{\text{eph}} + \hat{H}_{0\text{ph}} + \hat{H}_{e\varphi}, \tag{78}$$

where $\hat{H}_{0e}$ is the Hamiltonian of the carriers (a concentration n_0 of electrons in conduction band) taken in the effective mass approximation, with energy dispersion relation $\epsilon_{\mathbf{k}} = \hbar^2k^2/2m^*$. $\hat{H}_{\text{eph}}$ is the Hamiltonian of the interactions of carriers and optical and acoustical phonons: We consider in this case of polar semiconductors only the polar (Fröhlich) interaction with LO phonons, which is by far the predominant process of relaxation of the carriers to the lattice. $\hat{H}_{0\text{ph}}$ is the Hamiltonian of the free LO phonons. $\hat{H}_{e\varphi}$ accounts for the interaction of the carriers with external pumping sources. We assume that the LO phonons remain in equilibrium with an external thermal reservoir at temperature T_0. The polarization effects (due the Coulomb interaction) modifying the mean-field potential of the band states is not included; that is, we disregard the contribution from the plasmon states.

Indicating by $c_{\mathbf{k}}(c_{\mathbf{k}}^\dagger)$ the creation and annihilation operators in band states $\mathbf{k}$ (we omit the spin index), as in the case of phonons in the previous section we introduce as basic microdynamical variables for the corresponding NESEF the quantities

$$\{\hat{n}_{\mathbf{kQ}} = c_{\mathbf{k+Q}/2}^\dagger c_{\mathbf{k-Q}/2};\ \hat{H}_{0\text{ph}}\}. \tag{79}$$

For $Q = 0$, $\hat{n}_{\mathbf{k}} = c_{\mathbf{k}}^\dagger c_{\mathbf{k}}$ is the operator occupation number in state $\mathbf{k}$, and the others with $\mathbf{Q} \neq 0$ account for variations in space. For the LO phonons we have taken $\hat{H}_{0\text{ph}}$ once, as said; we consider them in constant equilibrium at temperature T_0 and therefore described by a canonical distribution. Hence, the statistical operator in NESEF of the electrons is

$$\varrho_\epsilon(t) = \exp\left\{-\hat{S}(t,0) + \int_{-\infty}^{t} dt' e^{\epsilon(t'-t)} \hat{S}(t',t'-t)\right\}, \tag{80}$$

where

$$\begin{aligned}\hat{S}(t_1,t_2) &= -\ln\bar{\varrho}(t_1,t_2)\\ &= \phi(t_1) + \sum_{\mathbf{k}}\left[F_{\mathbf{k}}(t_1)\hat{n}_{\mathbf{k}}(t_2) + \sum_{\mathbf{Q}\neq 0} F_{\mathbf{kQ}}(t_1)\hat{n}_{\mathbf{kQ}}(t_2)\right],\end{aligned} \tag{81}$$

where we recall that ϕ ensures the normalization of both $\bar{\varrho}$ and ϱ_ϵ, and $F_{\mathbf{k}}$ and $F_{\mathbf{kQ}}$ are the nonequilibrium thermodynamic variables conjugated to the basic ones, $\hat{n}_{\mathbf{k}}$ and $\hat{n}_{\mathbf{kQ}}$ ($\mathbf{Q} \neq 0$). In Eq. (81) t_1 refers to the evolution in time of the nonequilibrium thermodynamic variables and t_2 to the evolution in time of the dynamical variables (Heisenberg representation).

Following the formalism we proceed to the derivation of the kinetic equation for the variable

$$n_{\mathbf{kQ}}(t) = \text{Tr}\{\hat{n}_{\mathbf{kQ}}\varrho_\epsilon(t)\}. \tag{82}$$

In the Markovian approximation, after a calculation in reciprocal space and next going over to direct space, it follows for

$$f_{\mathbf{k}}(\mathbf{r},t) = \sum_{\mathbf{Q}} n_{\mathbf{kQ}}(t)e^{i\mathbf{Q}\cdot\mathbf{r}} \tag{83}$$

that

$$\begin{aligned}&\frac{\partial}{\partial t} f_{\mathbf{k}}(\mathbf{r},t) + \frac{i}{\hbar}\nabla_{\mathbf{k}}\epsilon_{\mathbf{k}}\cdot\nabla_{\mathbf{r}} f_{\mathbf{k}}(\mathbf{r},t)\\ &\quad= \frac{2\pi}{\hbar}\sum_{\mathbf{q}} |\mathcal{C}_{\mathbf{q}}|^2\{[\nu_{\mathbf{q}}(t)+1] f_{\mathbf{k+q}}(\mathbf{r},t)[1 - f_{\mathbf{k}}(\mathbf{r},t)]\\ &\qquad - \nu_{\mathbf{q}}(t) f_{\mathbf{k}}(\mathbf{r},t)[1 - f_{\mathbf{k+q}}(\mathbf{r},t)]\}\delta(\epsilon_{\mathbf{k+q}} - \epsilon_{\mathbf{k}} - \hbar\omega_{\mathbf{q}})\\ &\qquad - \frac{2\pi}{\hbar}\sum_{\mathbf{q}} |\mathcal{C}_{\mathbf{q}}|^2\{[\nu_{\mathbf{q}}(t)+1] f_{\mathbf{k}}(\mathbf{r},t)[1 - f_{\mathbf{k-q}}(\mathbf{r},t)]\\ &\qquad - \nu_{\mathbf{q}}(t) f_{\mathbf{k-q}}(\mathbf{r},t)[1 - f_{\mathbf{k}}(\mathbf{r},t)]\}\delta(\epsilon_{\mathbf{k-q}} - \epsilon_{\mathbf{k}} + \hbar\omega_{\mathbf{q}})\}\\ &\qquad + J_{S\mathbf{k}}(\mathbf{r},t),\end{aligned} \tag{84}$$

where $\mathcal{C}_{\mathbf{q}}$ is the matrix element of the Fröhlich electron-LO-phonon interaction, $\omega_{\mathbf{q}}$ the frequency dispersion relation of the LO phonons (we recall that $\epsilon_{\mathbf{k}} = \hbar^2k^2/2m^*$), $J_{S\mathbf{k}}$ the interaction with external sources to be specified in each case, and $\nu_{\mathbf{q}}$ is the population of the LO phonons in equilibrium at temperature T_0.

As in previous sections, we introduce the hydrothermodynamic variables

$$I_p^{[\ell]}(\mathbf{r},t) = \sum_{\mathbf{k}} K_p^{[\ell]}(\mathbf{k}) f_{\mathbf{k}}(\mathbf{r},t), \tag{85}$$

$$K_n^{[\ell]}(\mathbf{k}) = \left[\frac{\hbar\mathbf{k}}{m^*}\cdots\ell\text{ times}\cdots\frac{\hbar\mathbf{k}}{m^*}\right], \tag{86}$$

$$K_h^{[\ell]}(\mathbf{k}) = \frac{\hbar^2k^2}{2m^*}K_n^{[\ell]}(\mathbf{k}), \tag{87}$$

corresponding to the families of particle motion ($p \equiv n$) and energy motion ($p \equiv h$). The evolution equations are evidently given by

$$\frac{\partial}{\partial t} I_p^{[\ell]}(\mathbf{r},t) = \sum_{\mathbf{k}} K_p^{[\ell]}(\mathbf{k})\frac{\partial}{\partial t} f_{\mathbf{k}}(\mathbf{r},t). \tag{88}$$

In what follows, for better visualization, we restrict the analysis to a description of order 2 of the heat transport, introducing the reduced set of basic variables consisting of

$$\{h(\mathbf{r},t);\ I_h(\mathbf{r},t);\ I_{h2}(\mathbf{r},t)\}, \tag{89}$$

where

$$h(\mathbf{r},t) = \sum_{\mathbf{k}} \frac{\hbar^2k^2}{2m^*} f_{\mathbf{k}}(\mathbf{r},t), \tag{90}$$

$$\mathbf{I}_h(\mathbf{r},t) = \sum_{\mathbf{k}} \frac{\hbar\mathbf{k}}{m^*} f_{\mathbf{k}}(\mathbf{r},t), \tag{91}$$

and we separate the second-order flux $I_h^{[2]}(\mathbf{r},t)$ in the trace part and the remaining traceless part, which is neglected. The trace of $I^{[2]}$ is

$$I_{h2}(\mathbf{r},t) = \sum_{\mathbf{k}}\left(\frac{\hbar k}{m^*}\right)^2 f_{\mathbf{k}}(\mathbf{r},t). \tag{92}$$

The auxiliary statistical operator is then given by

$$\bar{\varrho}(t,0) = \exp\left\{-\phi(t,0) - \sum_{\mathbf{Q}}[F_h(\mathbf{Q},t)\hat{h}(\mathbf{Q}) + \boldsymbol{\varphi}_h(\mathbf{Q},t)\cdot\mathbf{I}_h(\mathbf{Q},t) + F_{h2}(\mathbf{Q},t)I_{h2}(\mathbf{Q})]\right\}, \tag{93}$$

which follows from Eq. (81) after taking, to be consistent with the contraction introduced, that

$$F_{\mathbf{kQ}}(t) = \frac{\hbar^2k^2}{2m^*}F_h(\mathbf{Q},t) + \frac{\hbar^2k^2}{2m^*}\hbar\mathbf{k}\cdot\boldsymbol{\varphi}_h(\mathbf{Q},t) + \left(\frac{\hbar k}{m^*}\right)^2 F_{h2}(\mathbf{Q},t). \tag{94}$$

The equations of evolution for these hydrothermodynamic variables in the absence of external sources are

$$\frac{\partial}{\partial t}h(\mathbf{r},t) = -\nabla\cdot\mathbf{I}_h(\mathbf{r},t) - \theta_h^{-1}h(\mathbf{r},t) - a_0I_{h2}(\mathbf{r},t), \tag{95}$$

$$\frac{\partial}{\partial t}\mathbf{I}_h(\mathbf{r},t) = -\nabla I_{h2}(\mathbf{r},t) - \theta_{I_h}^{-1}\mathbf{I}_h(\mathbf{r},t), \tag{96}$$

$$\frac{\partial}{\partial t}I_{h2}(\mathbf{r},t) = -\frac{q}{m^*\beta}\nabla\cdot\mathbf{I}_h(\mathbf{r},t) - a_2h(\mathbf{r},t) - \theta_{I_{h2}}^{-1}I_{h2}(\mathbf{r},t). \tag{97}$$

The expression for the trace of the divergence of the third-order flux in terms of the basic macrovariables, namely,

$$\mathrm{Tr}\{\nabla\cdot I_h^{[3]}(\mathbf{r},t)\} = \frac{q}{m^*\beta}\nabla\cdot\mathbf{I}_h(\mathbf{r},t) + a_2h(\mathbf{r},t), \tag{98}$$

was obtained resorting to Heims-Jaynes perturbation expansion for averages [27] around the homogeneous state, where

$$a_2 = \frac{1}{m^*\beta\theta_{I_2}}, \tag{99}$$

and it has been used that

$$f_{\mathbf{k}}(t) = 4n_0[\pi\hbar^2\beta(t)/2m^*]^{3/2}\times e^{-\hbar^2k^2\beta(t)/2m^*}, \tag{100}$$

meaning that we have considered the carriers' system as being in a nondegenerate statistical state, i.e., in which it is verified that $n_0\Lambda_{\mathrm{BT}}^3 \ll 1$, where Λ_{BT} is de Broglie thermal wavelength in nonequilibrium, namely, $\Lambda_{\mathrm{BT}}(t) = \sqrt{\hbar^2\beta(t)/m^*}$, n_0 is the density of carriers, and

$$\beta(t) = \frac{1}{k_BT^*(t)}, \tag{101}$$

with T^* being the nonequilibrium temperature (quasitemperature) of the electrons, and in Eq. (81), making the identification

$$F_{\mathbf{k}}(t) \equiv \frac{\hbar^2k^2}{2m^*}\beta(t), \tag{102}$$

and it has been used that $n_0 = 10^{18}$ cm^{-3} and $T_0 = 300$ K.

In Eqs. (95) to (97) are present the Maxwell times θ_h, θ_{I_h}, and $\theta_{I_{h2}}$, associated with the energy, its vectorial (first) flux (current of heat), and the second flux, respectively. They are given by

$$\theta_h^{-1} = \frac{14}{5}\xi\tau_0^{-1}, \tag{103}$$

$$\theta_{I_h}^{-1} = \frac{2}{25}\xi\theta_h^{-1} = \frac{2}{25}\frac{14}{5}\xi^2\tau_0^{-1}, \tag{104}$$

$$\theta_{I_{h2}}^{-1} = \frac{1}{28}\xi^2\theta_h^{-1} = \frac{1}{28}\frac{14}{5}\xi^3\tau_0^{-1}, \tag{105}$$

where

$$\xi = \beta\hbar\omega_0 = \frac{\hbar\omega_0}{k_BT^*} \tag{106}$$

is the ratio of the LO phonons quantum of energy (in the dispersionless Einstein model) to the nonequilibrium kinetic energy of the electrons, and

$$\frac{1}{\tau_0} = \sqrt{\frac{8\hbar\omega_0z^3e^z}{9\pi m_e^*}}(eE_0)\beta\nu_{LO}k_0(z), \tag{107}$$

is the inverse of the momentum relaxation time resulting from Fröhlich interaction [28], where k_0 is a Bessel function and $z = \beta\hbar\omega_0$, ω_0 is the dispersionless frequency of LO phonons (Einstein model, which is 5.6×10^{13} s^{-1} or ~37 meV in GaAs), $eE_0 = m_e^*e^2\hbar\omega_0(1/\epsilon_\infty - 1/\epsilon_0)/\hbar^2$ is the so-called electric force for electrons in Fröhlich potential (which is 1.07×10^{-8} erg/cm in GaAs), and we recall that $|C_{\mathbf{q}}|^2$ [cf. Eq. (84)] has the expression $|C_{\mathbf{q}}|^2 = (2\pi\hbar^2/Vm^*q^2)eE_0$ [28]. Comparison of momentum and energy relaxation times in III-nitrides is reported in Ref. [29].

In numerical calculations were used the parameters corresponding to GaAs given in Table I, and we recall that the distribution function of electrons of Eq. (100) was approximated by a Maxwell-Boltzmann distribution, which is possible, as already noticed, in the statistically nondegeneratelike limit, namely, when it is satisfied that $n_0\Lambda_{\mathrm{BT}}^3 \ll 1$, where $\Lambda_{\mathrm{BT}} = \hbar/\sqrt{m^*k_BT^*(t)}$ is the thermal de Broglie wavelength.

Accordingly, it follows that the comparison of the three values follows from

$$\frac{\theta_{I_h}}{\theta_h} = \frac{25}{2}\frac{k_BT^*}{\hbar\omega_0} = 12.5\xi, \tag{108}$$

$$\frac{\theta_{I_{h2}}}{\theta_h} = 28\left(\frac{k_BT^*}{\hbar\omega_0}\right)^2 = 28\xi^2, \tag{109}$$

$$\frac{\theta_{I_{h2}}}{\theta_{I_h}} = \frac{56}{25}\frac{k_BT^*}{\hbar\omega_0} = 2.24\xi, \tag{110}$$

and, therefore, their hierarchy depends on the ratio $\xi = \hbar\omega_0/k_BT^*$, that is, on the ratio of the energy of LO-phonon

TABLE I. Parameters characteristic of GaAs.

Parameter	Value
Electron effective mass [30], m^*	$0.067m_0$
LO-phonon energy [30], $\hbar\omega_0$	37.0 meV
Static dielectric constant [31], ε_0	12.91
Optical dielectric constant [31], ε_∞	10.91

TABLE II. Numerical values of Maxwell times for GaAs.

T^* (K)	ξ	θ_h (ps)	θ_{I_h} (ps)	$\theta_{I_{h2}}$ (ps)	θ_{I_h}/θ_h	$\theta_{I_{h2}}/\theta_h$
300	1.43	0.08	0.72	1.13	9.0	14.1
400	1.07	0.20	2.34	4.88	11.7	24.4
500	0.86	0.40	5.84	15.24	14.6	38.1
600	0.72	0.71	12.37	38.73	17.4	54.5
700	0.61	1.15	23.38	85.36	20.3	74.2
800	0.54	1.74	40.60	169.4	23.3	97.3
900	0.48	2.52	66.13	319.5	26.2	132.2
1000	0.43	3.52	102.4	534.0	29.1	151.7

modes to the nonequilibrium thermal kinetic energy of the carriers. Numerical values of the three Maxwell times for several values of the carriers' quasitemperature are given in Table II and plotted in Fig. 2. It can be noticed that these Maxwell times are on the order of picoseconds to femtoseconds.

In the case of GaAs we do have that $\hbar\omega_0 = 37$ meV and then (T_e^* in Kelvin)

$$\frac{\theta_{I_h}}{\theta_h} \simeq 0.03 T_e^*$$

and then $\theta_{I_h}/\theta_h < 1$ for $T_e^* \lesssim 34$ K and $\theta_{I_h}/\theta_h > 1$ for $T_e^* \gtrsim 34$ K. On the other hand,

$$\frac{\theta_{I_{h2}}}{\theta_h} \simeq 1.5 \times 10^{-4} (T_e^*)^2$$

and then $\theta_{I_{h2}}/\theta_h < 1$ for $T_e^* \lesssim 81$ K and $\theta_{I_{h2}}/\theta_h > 1$ for $T_e^* \gtrsim 81$ K. We stress that T_e^* is the carriers' quasitemperature, that is, the nonequilibrium temperature which is a measure in degrees Kelvin of their nonequilibrium energy [32].

It may be noticed that at such temperatures the nondegenerate distribution used for the electrons may be of dubious validity. In Table II we present the values of the three Maxwell times for carriers' temperature of 300 K and up, and it is verified that, in fact, $\theta_h < \theta_{I_h} < \theta_{I_{h2}}$, presenting an inverse ordering than in all the previous cases here considered. We conjecture that it is a consequence that in the expression for the reciprocal of Maxwell times are enhanced the contributions of the states with low crystalline momentum, particularly the contribution of Fröhlich potential. Finally it may be noticed that high electron quasitemperature T_e^* results from the application of moderate to high electric fields [33,34].

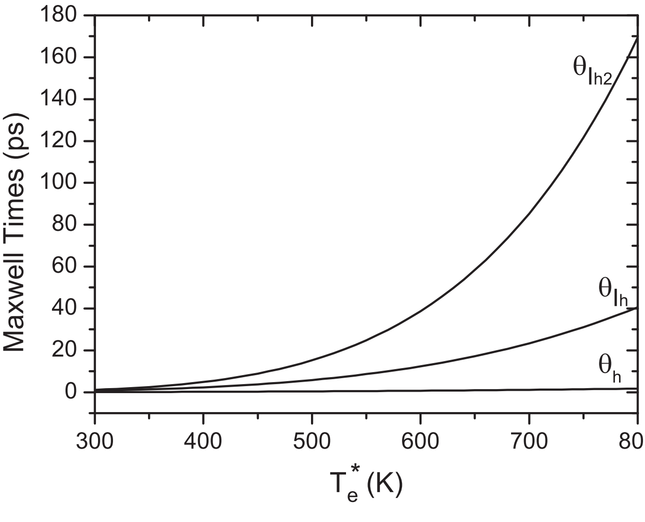

FIG. 2. Maxwell characteristic times: $\theta_h, \theta_{I_h}, \theta_{I_{h2}}$.

VI. CONCLUDING REMARKS

In the framework of mesoscopic hydrothermodynamics applied to the study of the hydrodynamic motion of a classical molecular fluid and of the "fluids" of phonons and carriers in intrinsic and doped semiconductors, we have characterized the so-called Maxwell times, or better to say generalizations of Maxwell original proposal [1] as described in the Introduction. These Maxwell times are associated with the fluxes of all orders present in MHT (fluxes of particles—or quasiparticles—and of heat). A complete characterization is obtained in the case of a classical fluid (of molecules, polymers, etc.), presented in Secs. II and III. Therefore, the quite important result is that they satisfy a hierarchy showing that they are increasingly diminishing as the order of the fluxes increases. This allows for establishing criteria for the choice of the contraction of description to be used in each case.

In other words, to introduce an appropriate—for each case—contraction of description: This contraction implies retaining the information considered as relevant for the problem at hand and disregarding irrelevant information [35].

Elsewhere [26] has been discussed the question of the contraction of description (reduction of the dimensions of the nonequilibrium thermodynamic space of states), where a criterion for justifying the different levels of contraction is derived: It depends on the range of wavelengths and frequencies which are relevant for the characterization, in terms of normal modes, of the hydrothermodynamic motion in the nonequilibrium open system. It can be shown that the truncation criterion *rests on the characteristics of the hydrodynamic motion that develops under the given experimental procedure*.

Inclusion of higher and higher-order fluxes implies describing a motion involving increasing Knudsen numbers per hydrodynamic mode, that is, governed by smaller and smaller wavelengths—larger and larger wave numbers—accompanied by higher and higher frequencies. In a qualitative manner, we can say that, as a general "rule of thumb," the criterion indicates that *a more and more restricted contraction can be used when the prevalent wavelengths in the motion* are larger and larger. It should be taken into account that application of the theory is dubious when involving wavelengths smaller than, say, ten times the mean separation distance between the molecules in a classical fluid or tens of lattice parameters in a crystal. 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. A general criterion for contraction can be conjectured; namely, a contraction of order r (meaning keeping the densities and their fluxes up to order r) can be introduced once we can show that in the spectrum of wavelengths, which characterize the motion, predominate those larger than a "frontier" one, $\lambda^2_{(r,r+1)} = v^2\theta_r\theta_{r+1}$, where v is of the order of the thermal velocity and θ_r and θ_{r+1} the corresponding *Maxwell times* associated with the r and $r+1$ order fluxes.

Section IV was devoted to the characterization of Maxwell times in the thermal motion of phonons in intrinsic semiconductors. We showed the interesting results that the Maxwell times have an expression for their inverse in the form of a weighted Mathiessen-like rule involving the inverse of the relaxation times of all phonon modes. We can say that it is expected once the hydrodynamic motion is a collective one composed of the contribution of all the phonon modes. As in the previous case, Maxwell times follow a hierarchy involving ever-decreasing values as the order of the fluxes increases.

Finally, in Sec. V, for the case of doped polar semiconductors, the Maxwell times associated with the hydrodynamic motion of the electrons in Bloch bands have been obtained. They are mainly determined by the presence of the polar Fröhlich interaction between electrons and phonons, and they follow a hierarchy of values, which is dependent on the ratio of the phonon energy $\hbar\omega_0$ with the electron thermal (kinetic) energy $k_B T^*(t)$: It implies in a series of decreasing values as long as the quasitemperature of the "hot" electrons is higher than the Einstein temperature of the phonons.

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