Gradient expansions in kinetic theory of phonons

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For simple models of the phonon transport in rigid insulators, it is demonstrated that the extended diffusional mode transforms into a second-sound mode after its coupling to a nonhydrodynamic mode at some critical value of the wave vector. This criticality shows up as a branching point of the extension of the diffusional mode within the Chapman-Enskog method, found explicitly for these models. The solution is used to test validity of several nonpolynomial approximate methods to capture this criticality. [S0163-1829(97)02510-1]

INTRODUCTION

Derivation of a hydrodynamic description from kinetic theory usually leads to formal expansions of nonhydrodynamic variables in terms of spatial gradients of relevant hydrodynamic quantities. Though the notions of ''hydrodynamic'' and ''nonhydrodynamic'' variables should be specified in each particular case, a typical situation arises: the leading term of the gradient expansion is well established, while a truncation at any further order leads to questionable and sometimes even unphysical results. Classical examples provide the Chapman-Enskog expansion (CE) in the Boltzmann kinetic theory,[1] where the first term leads to the (well-established) Navier-Stokes hydrodynamics, while the further, Burnett and super-Burnett terms result in the unphysical instability of the equilibrium.[2] Further examples can be found, e.g., in Ref. 3.

However, it should be admitted that the difficulties of the *finite*-order approximations *do not* say that the information contained in the gradient expansions *in a whole* is irrelevant or unimportant. The well-known example is the derivation of the CE expansion for Lorentz gas.[4] Another recent example of an exact and partial summation of the CE expansion in linear and nonlinear case for Grad equations[5] can be found in Ref. 6.

In this paper we address the gradient expansions arising in the problem of phonon transport in rigid insulators at low temperatures. Experiments on heat-pulse propagation through crystalline media[7] confirmed the existence of a temperature window (the Guyer-Krumhansl window[8]) with respect to which the features of heat propagation are qualitatively different: At temperatures exceeding the high-temperature edge of the window, the heat propagates in a diffusionlike way. Below the low-temperature edge of the window, the propagation goes in a ballistic way, with a constant speed of sound. Within the window, the propagation becomes wavelike. This latter regime is called second sound (see Ref. 9 for a review).

This problem has drawn some renewed attention in the last years. Models relevant for a unified description of diffusion, second sound, and ballistic regimes of heat propagation are intensively discussed (see Ref. 10 and references therein).

To be specific, recall the simplest and typical model of the phonon transport.[10] Let $e(\mathbf{x},t)$ and $\mathbf{p}(\mathbf{x},t)$ be small deviations of the energy density and of the energy flux of the phonon field from their equilibrium values, respectively. Then

$$\partial_t e = -c^2 \nabla \cdot \mathbf{p}, \tag{1a}$$

$$\partial_t \mathbf{p} = -\frac{1}{3}\nabla e - \frac{1}{\tau_R}\mathbf{p}. \tag{1b}$$

Here c is the Debye velocity of phonons, and τ_R is the characteristic time of resistive processes. Equations (1) can be derived from the Boltzmann-Peierls kinetic equation, within the relaxation time approximation, by a method similar to the Grad method.[10] Equations (1) provide the simplest model of a coupling between the hydrodynamic variable e and the nonhydrodynamic variable $\mathbf{p}$, allowing for a qualitative description of both the diffusion and the second sound. Following the standard argumentation,[10] we observe the two limiting cases: (1) As $\tau_R \to 0$, Eq. (1b) yields the Fourier relation $\mathbf{p} = -(1/3)\tau_R \nabla e$ which closes Eq. (1a) to give the diffusion equation:

$$\partial_t e + \frac{1}{3}\tau_R c^2 \Delta e = 0. \tag{2}$$

(2) As $\tau_R \to \infty$, Eq. (1b) yields $\partial_t \mathbf{p} = -(1/3)\nabla e$, and Eq. (1a) closes to give the wave equation:

$$\partial_t^2 e + \frac{1}{3}c^2 \Delta e = 0. \tag{3}$$

Here $\Delta = \nabla \cdot \nabla$ is the Laplacian. Equation (2) describes the usual diffusive regime of the heat propagation, while Eq. (3) is relevant to the (undamped) second-sound regime with the velocity $u_2 = c/\sqrt{3}$, and are both closed with respect to the variable e.

However, even within the simplest model (1), the problem of closure remains unsolved in a systematic way when τ_R is finite. The natural way of doing so is provided by the CE method.[1] In the situation under consideration, the CE method yields an extension of the diffusive transport to finite values of the parameter τ_R, and leads to an expansion of the non-hydrodynamic variable $\mathbf{p}$ in terms of the hydrodynamic variable e. With this, if we are able to make this extension of the diffusive mode exactly, we could learn more about the transition between the diffusion and second sound (within the frames of the model). Therefore, our goal here is not to investigate the properties of the system (1) as they are, but rather to proceed along the lines of the CE method to perform the closure from the standpoint of kinetic theory.

Let us briefly outline this paper. In the next section we will consider the gradient expansion for the simplest model (1). As we will see, the underlying CE method leads to a nonlinear reccurency procedure even here. Nevertheless, it will be possible to sum up the CE expansion in a closed form, and to discuss accurately the features of the CE solution for τ_R finite. In particular, we will see that the CE extension of the diffusional mode is possible only up to a certain wavelength (about the characteristic lengths of the problem, $c\tau_R$). This explicit demonstration for the simplest model (1) highlights a critical relation between the diffusional and the second-sound regimes of the phonon transport. In Sec. II, in view of the actual singularity of the exact CE solution, we also discuss the problem of nonpolynomial approximation of the CE expansion, and will test several earlier suggestions[3,11,12] with this solution. In Secs. III and IV we discuss generalizations of the simplest model (1) when the normal processes and anisotropy are taken into account. Finally, the results are discussed.

I. CRITICALITY OF THE CHAPMAN-ENSKOG SOLUTION

The CE method, as applied to the model (1), results in the following series representation:

$$\mathbf{p}^{\rm CE}=\sum_{n=0}^{\infty}\mathbf{p}^{(n)}, \tag{4}$$

where the coefficients $\mathbf{p}^{(n)}$ are due to the CE recurrence procedure,

$$\mathbf{p}^{(n)}=-\tau_R\sum_{m=0}^{n-1}\partial_t^{(m)}\mathbf{p}^{(n-1-m)}, \tag{5}$$

while the CE operators $\partial_t^{(m)}$ act on e as follows:

$$\partial_t^{(m)}e=-c^2\nabla\cdot\mathbf{p}^{(m)}. \tag{6}$$

Finally, the zero-order term reads: $\mathbf{p}^{(0)}=-(1/3)\tau_R\nabla e$, and leads to the Fourier approximation of the energy flux. Because of a somewhat involved structure of the recurrence procedure (5), (6), the CE method is a nonlinear operation even in the simplest model (1).

To *sum up* the series (4) in a closed form, we will specify the nonlinearity appearing in Eqs. (5) and (6). The coefficients $\mathbf{p}^{(n)}$ in Eqs. (4) and (5) have the following explicit structure for arbitrary order $n\geqslant 0$:

$$\mathbf{p}^{(n)}=a_n\Delta^n\nabla e, \tag{7}$$

where the real-valued and yet unknown coefficients a_n are due to the recurrence procedure (5), and (6). Indeed, the form (7) is true for $n=0$ $[a_0=-(1/3)\tau_R]$. Let us assume that Eq. (7) is proven up to the order $n-1$. Then, computing the nth order coefficient $\mathbf{p}^{(n)}$, we derive

$$\begin{aligned}\mathbf{p}^{(n)}&=-\tau_R\sum_{m=0}^{n-1}\partial_t^{(m)}a_{n-1-m}\Delta^{(n-1-m)}\nabla e\\&=-\tau_R\sum_{m=0}^{n-1}a_{n-1-m}\Delta^{(n-1-m)}\nabla(-c^2a_m\nabla\cdot\nabla\Delta^m e)\\&=\tau_Rc^2\left\{\sum_{m=0}^{n-1}a_{n-1-m}a_m\right\}\Delta^n\nabla e.\end{aligned} \tag{8}$$

The last expression has the form (7). Thus, the CE procedure for the model (1) is equivalent to the following nonlinear recurrence relation in terms of the coefficients a_n:

$$a_n=\tau_Rc^2\sum_{m=0}^{n-1}a_{n-1-m}a_m, \tag{9}$$

subject to the initial condition $a_0=-(1/3)\tau_R$. Further, it is convenient to make the Fourier transform. Using $\mathbf{p}=\mathbf{p_k}\exp\{i\mathbf{k}\cdot\mathbf{x}\}$ and $e=e_{\mathbf{k}}\exp\{i\mathbf{k}\cdot\mathbf{x}\}$, where $\mathbf{k}$ is the real-valued wave vector, we derive in Eq. (7): $\mathbf{p}_{\mathbf{k}}^{(n)}=a_ni\mathbf{k}(-k^2)^ne_{\mathbf{k}}$, and

$$\mathbf{p}_{\mathbf{k}}^{\rm CE}=i\mathbf{k}A(k^2)e_{\mathbf{k}}, \tag{10}$$

where

$$A(k^2)=\sum_{n=0}^{\infty}a_n(-k^2)^n. \tag{11}$$

Thus, the CE solution (4) amounts to finding the function $A(k^2)$ represented by the power series (11). If the function A is known, the exact CE closure of the system (1) amounts to the following dispersion relation of plane waves $\sim\exp\{\omega_{\mathbf{k}}t+i\mathbf{k}\cdot\mathbf{x}\}$:

$$\omega_{\mathbf{k}}^{\rm CE}=c^2k^2A(k^2). \tag{12}$$

Here $\omega_{\mathbf{k}}^{\rm CE}$ is a complex-valued function of the real-valued vector $\mathbf{k}$: ${\rm Re}\,\omega_{\mathbf{k}}^{\rm CE}$ is the attenuation rate, ${\rm Im}\,\omega_{\mathbf{k}}^{\rm CE}$ is the frequency.

Now we will concentrate on a problem of a computation of the function A (11) in a closed form on the basis of the recurrence relation (9). Multiplying both the equations in Eq. (9) with $(-k^2)^n$, and performing a summation in n from 1 to infinity, we get

$$A-a_0=-\tau_Rc^2k^2\sum_{n=0}^{\infty}\sum_{m=0}^{n}a_{n-m}(-k^2)^{n-m}a_m(-k^2)^m.$$

Now we notice that

$$\lim_{N\to\infty}\sum_{n=0}^{N}\sum_{m=0}^{n}a_{n-m}(-k^2)^{n-m}a_m(-k^2)^m=A^2.$$

Taking into account $a_0=-(1/3)\tau_R$, we come to a quadratic equation for the function A:

$$\tau_R c^2 k^2 A^2 + A + \frac{1}{3}\tau_R = 0. \tag{13}$$

Further, a selection procedure is required to choose the relevant root of Eq. (13). Firstly, recall that all the coefficients a_n (7) are real-valued by the sense of the CE method (5) and (6), hence the function A (11) is real valued. The conjecture is that only the real-valued roots of Eq. (13) are relevant to the CE solution. The first observation is that Eq. (13) has no real-valued solutions as soon as k is bigger than the critical value k_c, where

$$k_c = \frac{\sqrt{3}}{2\tau_R c}. \tag{14}$$

Secondly, there are two real-valued solutions to Eq. (13) at $k < k_c$. However, only one of them satisfies the CE asymptotic $\lim_{k\to 0} A(k^2) = -(1/3)\tau_R$.

With the two remarks just given, we finally derive the following exact CE dispersion relation (12):

$$\omega_{\mathbf{k}}^{\mathrm{CE}} = \begin{cases} -(2\tau_R)^{-1}[1-\sqrt{1-(k^2)/(k_c^2)}] & k < k_c \\ \text{none}, \quad k > k_c. \end{cases} \tag{15}$$

The CE dispersion relation corresponds to the extended diffusional transport, and it comes back to the standard Fourier approximation in the limit of long waves $k/k_c \ll 1$.

More interesting, however, is that the CE solution *does not exist* as soon as $k/k_c > 1$. The reason why this occurs can be found upon a closer investigation of the spectrum of the underlying system (1). In the original system, there exist three nonhydrodynamic modes which are irrelevant to the CE solution. All these nonhydrodynamic modes are characterized with a property that corresponding dispersion relations $\omega_{\mathbf{k}}$ do not go to zero as $k \to 0$. In the point k_c, the extended diffusion branch crosses one of the nonhydrodynamic branches of Eq. (1). For clear reasons, we will term this nonhydrodynamic mode the critical. For larger k, the extended diffusion mode and the critical mode produce a pair of complex conjugated solutions with the real part equal to $-1/2\tau_R$. The imaginary part of this extension after k_c has the asymptotics $\pm i u_2 k$, as $k \to \infty$, and where $u_2 = c/\sqrt{3}$ is the (undamped) second sound velocity in the model (1) [see Eq. (3)]. Though the spectrum of the original equation (1) continues indeed after k_c, the CE method does not recognize this extension as a part of the hydrodynamic branch, *while the second-sound regime is born from the extended diffusion after the coupling to the critical nonhydrodynamic mode*. Figure 1 illustrates the behavior of the extended diffusional mode.

II. OTHER METHODS

Because the opportunity to sum up the CE expansion exactly vanishes rapidly with the complexity of models, let us examine here the alternative opportunities due to approximate methods because the exact CE solution found above allows for a relevant and direct test.

First, let us come back to the CE expansion which in terms of the function A reads

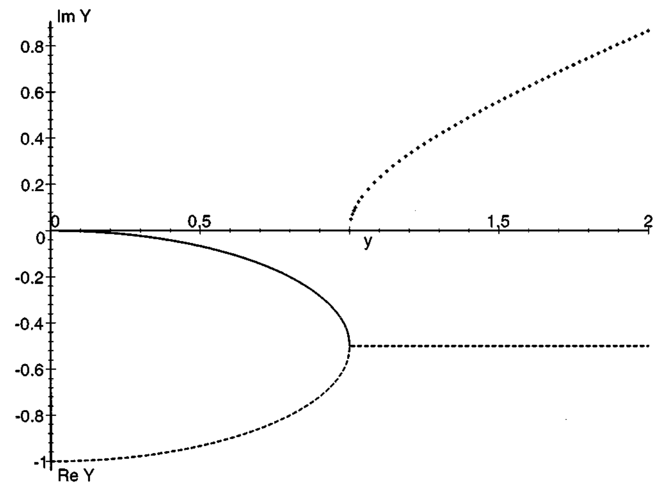

FIG. 1. Dispersion relation $Y = \tau_R \omega$ versus $y = k/k_c$. Lower case (real part): the solid line is the CE extension of the diffusion mode (15), the dashed line is the critical nonhydrodynamic mode of the phonon model (1). Upper case (imaginary part): the dashed line is the second-sound mode.

$$\tau_R^{-1} A^{\mathrm{CE}} = -\frac{1}{3}\left\{1 + \frac{1}{4}y^2 + \frac{1}{8}y^4 + \cdots\right\}, \tag{16}$$

where $y = k/k_c$. Clearly, *any* truncation of the CE expansion at a certain order will give a polynomial approximation which is unable to reproduce the singularity in the exact solution. The demand on *non*polynomial approximations becomes important because of this singularity.

The next possibility is to use the Rosenau rational approximation.[3] This approximation refers itself to the two terms in the CE expansion (16) (the Navier-Stokes and the Burnett level of description, respectively), and results in the following:

$$\tau_R^{-1} A^{\mathrm{R}} = -\frac{1}{3[1-(1/4)y^2]}. \tag{17}$$

The function A^{R} reproduces the CE expansion (16) up to the Burnett term, and has a pole at $y_R = 2$. This singularity *is* relevant, and gives an approximation to the actual branching point $y_c = 1$. However, a procedure of improving the rational approximation (17) was not discussed in Ref. 3.

Further, the result (17) coincides with the first-order partial summing of the CE expansion,[11] which amounts to the following *linear* approximation to the nonlinear recurrence relation (9):

$$a_n = \tau_R c^2 a_0 a_{n-1}. \tag{18}$$

Lastly, consider the opportunities provided by the method of invariant manifold.[12] First, the so-called invariance equation can be easily obtained in a closed form here. Consider again the expression for the heat flux in terms of the energy density (10), $\mathbf{p}_{\mathbf{k}} = i\mathbf{k}A(k^2)e_{\mathbf{k}}$, where now the function A is not thought of as the CE series (11). The invariance equation[12] is a *constraint* on the function A, expressing the form invariance of the heat flux (10) under both the dynamic equations (1a) and (1b). Indeed, computing the time derivative of the function (10) due to Eq. (1a), we obtain

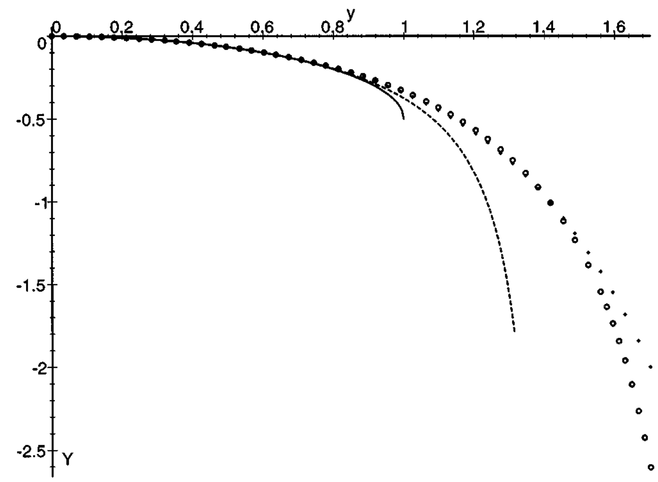

FIG. 2. Extension of the diffusion mode. The solid line is the exact CE solution (15), the dashed line is the second Newton iteration (22b), circles are the Rosenau approximation (17), dots are the super Burnett truncation of the CE expansion (16).

$$\partial_t \mathbf{p_k} = i\mathbf{k}A(k^2)\partial_t e_\mathbf{k} = c^2k^2A^2 i\mathbf{k}e_\mathbf{k}. \tag{19}$$

On the other hand, computing the time derivative of the same function due to Eq. (1b), we have

$$\partial_t \mathbf{p_k} = -\frac{1}{3}i\mathbf{k}e_\mathbf{k} - \frac{1}{\tau_R}Ai\mathbf{k}e_\mathbf{k}. \tag{20}$$

Equating expressions (19) and (20), we come to the desired invariance equation for function A. This equation, as one expects, *coincides with Eq.* (13), which was already derived above upon the exact summation of the CE expansion.

As the second step suggested by the method of invariant manifold, let us apply the Newton method to the invariance equation (13), taking the Euler approximation ($A_0^\mathrm{N}\equiv 0$) for the initial condition. Rewriting Eq. (13) in the form $F(A,k^2)=0$, we come to the following Newton iterations:

$$\left.\frac{dF(A,k^2)}{dA}\right|_{A=A_n^\mathrm{N}}(A_{n+1}^\mathrm{N}-A_n^\mathrm{N})+F(A_n^\mathrm{N},k^2)=0. \tag{21}$$

The first two iterations give

$$\tau_R^{-1}A_1^\mathrm{N} = -\frac{1}{3}, \tag{22a}$$

$$\tau_R^{-1}A_2^\mathrm{N} = -\frac{1-(1/4)y^2}{3[1-(1/2)y^2]}. \tag{22b}$$

The first Newton iteration (22a) coincides with the first term of the CE expansion (16). The second Newton iteration (22b) is a rational function with the Taylor expansion coinciding with Eq. (16) up to the super-Burnett term, and has a pole at $y_2^\mathrm{N}=\sqrt{2}$. The further Newton iterations are also rational functions with the relevant poles in the points y_n^N, and the sequence of this points tends very rapidly to the location of the actual singularity $y_c=1$ ($y_3^\mathrm{N}\approx 1.17$, $y_4^\mathrm{N}\approx 1.01$, etc.). The comparison of the extended diffusion mode due to the approximations (16), (17), and (22b) is presented in Fig. 2.

The test performed leads to the conclusion that the rational approximations provided by the methods[3,12] are much more suited to the problem of extending the diffusional transport than the polynomial approximations of the CE method in the sense that the former are able to reproduce the actual singularities of the full solution. In particular, the invariance principle leads to the result equivalent to the exact summation of the CE expansion. This fact will be explored below for other models.

III. ACCOUNT FOR NORMAL PROCESSES

The account for normal processes in frames of the semihydrodynamical models[10] leads to the following generalization of the Eq. (1) (written in Fourier variables, in the one-dimensional case):

$$\partial_t e_k = -ikc^2 p_k, \tag{23a}$$

$$\partial_t p_k = -\frac{1}{3}ike_k - ikN_k - \frac{1}{\tau_R}p_k, \tag{23b}$$

$$\partial_t N_k = -\frac{4}{15}ikc^2 p_k - \frac{1}{\tau}N_k. \tag{23c}$$

Here $\tau=\tau_N\tau_R/(\tau_N+\tau_R)$, τ_N is the characteristic time of normal processes, and N_k is the additional field variable. Following the principle of invariance as explained in the preceeding section, we write the closure relation for the nonhydrodynamic variables p_k and N_k as

$$p_k = ikA_k e_k, \quad N_k = B_k e_k, \tag{24}$$

where A_k and B_k are two unknown functions of the wave vector k. Further, following the principle of invariance as explained in the preceeding section, each of the relations (24) should be invariant under the dynamics due to Eq. (23a), and due to Eqs. (23b) and (23c). This results in two equations for the functions A_k and B_k:

$$k^2c^2A_k^2 = -\frac{1}{\tau_R}A_k - B_k - \frac{1}{3},$$

$$k^2c^2A_kB_k = -\frac{1}{\tau}B_k + \frac{4}{15}k^2c^2A_k. \tag{25}$$

When the energy balance equation (23a) is closed with the relation (24), this amounts to a dispersion relation for the extended diffusion mode, $\omega_k^\mathrm{CE}=k^2c^2A_k$, where A_k is the solution to the invariance equations (25), *subject to the condition* $A_k\to 0$ as $k\to 0$. Resolving equations (25) with respect to A_k, and introducing $\overline{A_k}=k^2c^2A_k$, we arrive at the following:

$$\Phi(\overline{A_k}) = \frac{5\overline{A_k}(1+\tau\overline{A_k})(\tau_R\overline{A_k}+1)}{5+9\tau A_k} = -\frac{1}{3}\tau_R k^2c^2. \tag{26}$$

The invariance equation (26) is completely analogous to the Eq. (13). Written in the form (26), it allows for a direct investigation of the critical points. For this purpose, we find zeroes of the derivative, $d\Phi(A_k)/dA_k=0$. When the roots of the latter equation, $\overline{A_k^c}$, are found, the critical values of the wave vector are given as $-(1/3)k_c^2c^2=\Phi(\overline{A_k^c})$. The condition $d\Phi(\overline{A_k})/d\overline{A_k}=0$ reads

$$18\tau^2\tau_R\overline{A_k^3}+3\tau(3\tau+8\tau_R)\overline{A_k^2}+10(\tau+\tau_R)\overline{A_k}+5=0. \tag{27}$$

Let us consider the particularly interesting case, $\epsilon=\tau_N/\tau_R\ll 1$ (the normal events are less frequent than resistive). Then the real-valued root of Eq. (27), $\overline{A_k}(\epsilon)$, corresponds to the coupling of the extended diffusion mode to the critical nonhydrodynamic mode. The corresponding modification of the critical wave vector k_c (14) due to the normal processes amounts to a shifts towards shorter waves, and we derive

$$[k_c(\epsilon)]^2=k_c^2+\frac{3\epsilon}{10\tau_R^2c^2}. \tag{28}$$

IV. ACCOUNT FOR ANISOTROPY

The above examples concerned the isotropic Debye model. Let us consider the simplest anisotropic model of a cubic media with a longitudinal (L) and two degenerated transverse (T) phonon modes, taking into account resistive processes only. Introduce the Fourier variables, $e_{\mathbf{k}}$, $e_{\mathbf{k}}^T$, $\mathbf{p}_{\mathbf{k}}^T$, and $\mathbf{p}_{\mathbf{k}}^L$, where $e_{\mathbf{k}}=e_{\mathbf{k}}^L+2e_{\mathbf{k}}^T$ is the Fourier transform of the total energy of the three phonon modes (the only conserving quantity), while the rest of variables are specific quantities. The isotropic model (1) generalizes to give[10]

$$\partial_t e_{\mathbf{k}}=-ic_L^2\mathbf{k}\cdot\mathbf{p}_{\mathbf{k}}^L-2ic_T^2\mathbf{k}\cdot\mathbf{p}_{\mathbf{k}}^T, \tag{29a}$$

$$\partial_t e_{\mathbf{k}}^T=-ic_T^2\mathbf{k}\cdot\mathbf{p}_{\mathbf{k}}^T+\frac{1}{\lambda}[c_L^3(e_{\mathbf{k}}-2e_{\mathbf{k}}^T)-c_T^3e_{\mathbf{k}}^T], \tag{29b}$$

$$\partial_t\mathbf{p}_{\mathbf{k}}^L=-\frac{1}{3}i\mathbf{k}(e_{\mathbf{k}}-2e_{\mathbf{k}}^T)-\frac{1}{\tau_R^L}\mathbf{p}_{\mathbf{k}}^L, \tag{29c}$$

$$\partial_t\mathbf{p}_{\mathbf{k}}^T=-\frac{1}{3}i\mathbf{k}e_{\mathbf{k}}^T-\frac{1}{\tau_R^T}\mathbf{p}_{\mathbf{k}}^T, \tag{29d}$$

where $\lambda=\tau_R^Tc_T^3+2\tau_R^Lc_L^3$. The term containing the factor λ^{-1} corresponds to the energy exchange between the L and T phonon modes. The invariance constraint for the closure relations,

$$\mathbf{p}_{\mathbf{k}}^L=i\mathbf{k}A_{\mathbf{k}}e_{\mathbf{k}},\quad \mathbf{p}_{\mathbf{k}}^T=i\mathbf{k}B_{\mathbf{k}}e_{\mathbf{k}},\quad e_{\mathbf{k}}^T=X_{\mathbf{k}}e_{\mathbf{k}}, \tag{30}$$

result in the following invariance equations for the $\mathbf{k}$-dependent functions $A_{\mathbf{k}}$, $B_{\mathbf{k}}$, and $X_{\mathbf{k}}$:

$$k^2c_L^2A_{\mathbf{k}}^2+2k^2c_T^2A_{\mathbf{k}}B_{\mathbf{k}}=-\frac{1}{\tau_R^L}A_{\mathbf{k}}-\frac{1}{3}(1-2X_{\mathbf{k}}), \tag{31a}$$

$$2k^2c_T^2B_{\mathbf{k}}^2+k^2c_LB_{\mathbf{k}}A_{\mathbf{k}}=-\frac{1}{\tau_R^T}B_{\mathbf{k}}-\frac{1}{3}X_{\mathbf{k}}, \tag{31b}$$

$$X_{\mathbf{k}}(k^2c_L^2A_{\mathbf{k}}+2k^2c_T^2B_{\mathbf{k}})=c_T^2k^2B_{\mathbf{k}}+\frac{1}{\lambda}[c_L^3-X_{\mathbf{k}}(2c_L^3+c_T^3)]. \tag{31c}$$

When the energy balance equation (29a) is closed with the relations (30), this leads to the dispersion relation for the extended diffusion mode, $\omega_{\mathbf{k}}^{\mathrm{CE}}=\overline{A_{\mathbf{k}}}+2\overline{B_{\mathbf{k}}}$, where the functions $\overline{A_{\mathbf{k}}}=k^2c_L^2A_{\mathbf{k}}$, and $\overline{B_{\mathbf{k}}}=k^2c_T^2B_{\mathbf{k}}$, satisfy the condition: $\overline{A_{\mathbf{k}}}\to 0$, and $\overline{B_{\mathbf{k}}}\to 0$, as $k\to 0$. The resulting dispersion relation is rather complicated in the general case of the four parameters of the problem, c_L, c_T, τ_R^L, and τ_R^T. Therefore, introducing a function $\overline{Y_{\mathbf{k}}}=\overline{A_{\mathbf{k}}}+2\overline{B_{\mathbf{k}}}$, let us consider the following specific situations of closed equations for the $\overline{Y_{\mathbf{k}}}$ on the basis of the invariance equations (31):

(i) $c_L=c_T=c$, $\tau_R^L=\tau_R^T=\tau_R$ (complete degeneration of the parameters of the L and T subsystems): The system (31) results in two decoupled equations:

$$\overline{Y_{\mathbf{k}}}(\tau_R\overline{Y_{\mathbf{k}}}+1)+\frac{1}{3}k^2c^2\tau_R=0, \tag{32a}$$

$$(\tau_R\overline{Y_{\mathbf{k}}}+1)^2+\frac{1}{3}k^2c^2\tau_R^2=0. \tag{32b}$$

Equation (32a) coincides with Eq. (13) for the isotropic case, and its solution defines the coupling of the extended diffusion to a nonhydrodynamic mode. Equation (32b) does not have a solution with the required asymptotic $\overline{Y_{\mathbf{k}}}\to 0$ as $k\to 0$, and is therefore irrelevant to the features of the diffusion mode in this completely degenerated case. It describes the two further propagating and damped nonhydrodynamic modes of Eqs. (29). The nature of these modes, as well of the mode which couples to the diffusional mode will be seen below.

(ii) $c_L=c_T=c$, $\tau_R^L\neq\tau_R^T$ (nondegenerate characteristic time of resistive processes in the L and the T subsystems):

$$\left[\overline{Y_{\mathbf{k}}}(\tau_R^L\overline{Y_{\mathbf{k}}}+1)+\frac{1}{3}k^2c^2\tau_R^L\right]\times\left[(\tau_R'\overline{Y_{\mathbf{k}}}+3)(\tau_R^T\overline{Y_{\mathbf{k}}}+1)+\frac{1}{3}k^2c^2\tau_R^T\tau_R'\right]=-\frac{2}{3}k^2c^2(\tau_R^T-\tau_R^L), \tag{33}$$

where $\tau_R'=2\tau_R^L+\tau_R^T$. As $\tau_R^T-\tau_R^L\to 0$, Eq. (33) tends to the degenerated case (32). At $k=0$, $\tau_R^L\neq\tau_R^L$, there are four solutions to Eq. (33). The $\overline{Y_0}=0$ is the hydrodynamic solution indicating the beginning of the diffusion mode. The two nonhydrodynamic solutions, $\overline{Y_0}=-1/\tau_R^L$, and $\overline{Y_0}=-1/\tau_R^T$, $\overline{Y_0}=-3/\tau_R'$, are associated with the longitudinal and the transverse phonons, respectively. The difference in relaxational times makes the latter transverse root nondegenerate, instead there appears a third nonhydrodynamic mode, $\overline{Y_0}=-3/\tau_R'$

(iii) $c_L\neq c_T$, $\tau_R^L=\tau_R^T=\tau_R$ (nondegenerate speed of the L and the T sound):

$$\left[\overline{Y_{\mathbf{k}}}(\tau_R\overline{Y_{\mathbf{k}}}+1)+\frac{1}{3}k^2c_L^2\tau_R\right]\left[(\tau_R\overline{Y_{\mathbf{k}}}+1)^2+\frac{1}{3}k^2c_T^2\tau_R^2\right]$$
$$=-\frac{2}{3}k^2\tau_R\frac{c_L^3(c_T^2-c_L^2)}{2c_L^3+c_T^3}(\tau_R\overline{Y_{\mathbf{k}}}+1). \quad (34)$$

As $c_T-c_L\to 0$, Eq. (34) tends to the degenerated case (32). However, this time the nonhydrodynamic mode associated with the transverse phonons is degenerated at $k=0$.

Thus, we are able to identify the modes in equations (32a) and (32b). The nonhydrodynamic mode which couples to the extended diffusion mode is associated with the longitudinal phonons, and is the case of Eq. (32a). Equation (32b) is due to the transverse phonons. In the nondegenerate cases, Eqs. (33) and (34), both pairs of modes become propagating after certain critical values of k, and the behavior of the extended diffusion mode is influenced by all three nonhydrodynamic modes just mentioned. It should be stressed, however, that the second-sound mode, which is the continuation of the diffusion mode,[7] is due to Eq. (32a).

DISCUSSION

The results of the above analysis lead to the following discussion:

(i) The examples considered above indicate an interesting mechanism of a *kinetic* formation of the second-sound regime from the extended diffusion with the participation of the nonhydrodynamic mode. The onset of the propagating mode shows up as the critical point of the extension of the hydrodynamic solution into the domain of finite k, which was found within the Chapman-Enskog and equivalent approaches. These results concern the situation at the high-temperature edge of the Guyer-Krumhansl window, and are complementary to the coupling between the transversal ballistic mode and second sound at the low-temperature edge.[13]

(ii) The crossover from the diffusionlike to the wavelike propagation was previously found in Ref. 14 in frames of the exact CE solution to the Boltzmann equation for the Lorentz gas model,[4] and for similar models of phonon scattering in anisotropic disordered media.[15] The characteristic common feature of the models studied in Refs. 4, 14, 15 and the models[10] is the existence of a gap between the hydrodynamic (diffusive) and the nonhydrodynamic components of the spectrum. Therefore, one can expect that the destruction of the extended diffusion is solely due to the *existence* of this gap. In applications to the phonon kinetic theory this amounts to the introduction of the relaxation time approximation. In other words, we may expect that the mechanism of crossover from diffusion to second sound in the simple models[10] is identical to what could be found from the phonon-Boltzmann kinetic equation within the relaxation time approximation. However, a remark is in order since the original (i.e., without the relaxation time approximation) phonon kinetic equations are *gapless* (cf., e.g., Ref. 9). On the other hand, most of the work on heat propagation in solids *do* explore the idea of the gap, since it is only possible to speak of the diffusion if such a gap exists. To conclude this point, the following general hypothesis can be expressed: *the existence of the diffusion (and hence of the gap in the relaxational spectrum) leads to its destruction through the coupling to a nonhydrodynamic mode.*

(iii) In addition to the methods compared in Sec. II, it should be mentioned that the continuous-fraction method (see elsewhere, e.g., Ref. 16) provides a very good tool of approximation techniques for the gradient expansions in the Lorentz gas model.[14,15]

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