Time-Dependent Thermal Conductivity of Ideal Anharmonic Dielectric Crystal within Poiseuille Flow Regime[1]

A.S.Rudy[2,3]

[1] Paper presented at the Thirteenth Symposium on Thermophysical Properties, June 22-27, Boulder, Colorado, U.S.A.

[2] Division of Physics, Institute for Basic Research, I-86075 Monteroduni (IS), Molise, Italy.

[3] Permanent address: Yaroslavl State University, Sovetskaya, 14, Yaroslavl, 150000,

ABSTRACT

The dynamic (**w**-dependent) thermal conductivity of a perfect anharmonic dielectric crystal is considered within a temperature range corresponding to Poiseuille flow “window”. The weak perturbations of uniform flow are calculated conformably to idealised model of phonon fluid with assumption that crystal surfaces are molecularly smooth, while ***U***-processes are completely frozen. The model of such fluid in a local temperature approximation is a set of hydrodynamic equations, one of which is of Eulerian type, while two others are energy and entropy continuity equations. In the case of wave perturbations the set reduces to a single wave equation featuring parametrical dependence on phonon flow velocity. Its solutions describe temperature waves with linear but anisotropic dispersion. The latter determines the range of flow velocities within which the wave motion is allowed. Thus temperature wave may propagate against phonon flow only when its velocity u is less than its first critical value $u_1 = 0,3443\ v$, where v is first sound velocity. Above the second critical value $u_2 = 0,3644\ v$ no wave motion is possible. Such behaviour of wave perturbations determines dynamic thermal conductivity anisotropic with $u \neq 0$ and vanishing when u reaches the first critical value. Thermal conductivity dependence on frequency is analogous to that of dynamic electrical conductivity in Drude-Lorentz model.

KEY WORDS: phonon fluid, second sound, thermal conductivity, Poiseuille flow, anisotropic dispersion.

1. INTRODUCTION

The concept phonon fluid is an approach often resorted for description of thermal properties of a perfect dielectric crystal. At macroscopic level of consideration phonon fluid behaviour is modelled by the set of hydrodynamic equations manifesting the balance of one of dynamic variables (energy, quasimomentum, etc.). The most general form of quasimomentum balance equation

$$\frac{\vec{q}}{\tau_z} + \frac{\partial \vec{q}}{\partial t} - \frac{\tau_N v^2}{5}\left(\nabla^2 + 2\nabla\nabla\times\right)\vec{q} = -\frac{1}{3}c_v v^2 \nabla T \qquad (1)$$

obtained by R.Guyer and J.Krumhansl [1] presents the linearised analogue of Navier-Stokes equation. In Poiseuille flow temperature region the quasimomentum loss is due to wall scattering and if crystal walls are molecularly smooth Eq. (1) allows homogeneous solutions $T = const$, $\vec{q} = const$ corresponding to equilibrium phonon distribution

$$n_s^u(\vec{k}) = \frac{1}{\exp\beta\hbar[\omega_s(\vec{k}) - (\vec{u},\vec{k})] - 1}, \qquad (2)$$

where $\vec{k}$ is a wave vector, $\beta = 1/k_B T$, $\omega_s(\vec{k})$ is a cyclic frequency of $\vec{k}$ phonon from *s-th* brunch of spectrum, $\vec{u}$ is a flow velocity of phonon aggregate. In the framework of this approach phonon flow may reach velocity comparable with that of first sound $u/v \sim 1$. The unattainability of such velocity, directly ensuing from (2), by no means follows from (1). Thus hydrodynamic equations of phonon fluid drifting under

propagation of perturbations to a certain critical value of flow velocity. The thermal properties of such “relativistic” phonon fluid should parameterically depend on fluid velocity and contain singularities at $u = v$. The purpose of present paper is to obtain hydrodynamic equations for nonviscous phonon fluid within Poiseuille window and define thermal properties of ideal anharmonic crystal as a functions of phonon fluid velocity.

2. EQUILIBRIUM AND PERTURBED STATES OF NONVISCOUS PHONON FLOW

The internal energy of uniform phonon flow which distribution function is Eq. (2) was calculated in [2] in Debye approximation. It depends on normalised phonon fluid velocity $s_0 = u_0 / v$ as

$$U_v = \frac{1}{4} c_v T \frac{1 + s_0^2/3}{(1 - s_0^2)^3}, \tag{4}$$

where c_v is specific heat of unit volume, n is density of atoms in lattice, k_B is Boltsmann constant, Θ_D is Debye temperature, v first sound velocity, subscript ***“0”*** indicates an equilibrium magnitudes of variables. According to Eq. (4) specific heat of drifting phonons depends on normalised fluid velocity as

$$c_v^u = c_v \frac{1 + s_0^2/3}{(1 - s_0^2)^3}. \tag{5}$$

Analogous calculation for energy reveals that energy flux j is related to normalised flow velocity as

$$j = \frac{1}{3} c_v T \frac{u}{(1 - s_0^2)^3} = \frac{q}{(1 - s_0^2)^3}. \tag{6}$$

where $q = c_v T u / 3$ is a heat flux. According to distribution (2) the density of phonons moving along flux tends to infinity with fluid velocity tending to phonon group velocity. In agreement with this fact expressions (5), (6) have singularities at $s = 1$, signifying unattainability of group velocity by phonon fluid.

To obtain expressions describing the motion of nonviscous phonon fluid in [2] a small local perturbation of Eq. (2) was considered. The calculations, carried out in a framework of local temperature approximation employing Debye interpolation scheme, have brought to the generalised equation of heat conduction. Its projection onto phonon flow direction $\vec{u} \| \vec{e}_z$ has the form

$$\frac{\partial j}{\partial t} + \frac{1}{2} c_v T \frac{1 + s_0^2}{(1 - s_0^2)^4} \frac{\partial u^2}{\partial z} = - \frac{1}{3} c_v v^2 \frac{1 + 3 s_0^2}{(1 - s_0^2)^3} \frac{\partial T}{\partial z}. \tag{7}$$

Eq. (7) is Eulerian equation relating local and continual rates of energy flux alteration to thermodynamic force.

To form a closed set of equations Eq. (7) is supplemented by energy conservation

$$\frac{\partial j}{\partial t} + 3\,\frac{c_v}{c_v^u}\,\frac{1+\sigma_0^2}{(1-\sigma_0^2)^4}\,u_0\,\frac{\partial j}{\partial z} = -\,\frac{1}{3}\,c_v v^2\,\frac{1}{(1-\sigma_0^2)^3}\,\cdot$$

$$\cdot\left\{1 + 3\sigma_0^2 - 9\sigma_0^2\,\frac{1+\sigma_0^2}{1-\sigma_0^2}\right\}\frac{\partial T}{\partial z}, \tag{8}$$

$$c_v^u\,\frac{\partial T}{\partial t} = -\,\frac{\partial j}{\partial z}. \tag{9}$$

In the case of small harmonic oscillations $T = V(z)\exp(i\omega t)$ the set (8), (9) reduces to single expression

$$\frac{\partial^2 T}{\partial t^2} = a\,\frac{v^2}{3}\,\frac{\partial^2 T}{\partial z^2} - i\omega b\,\frac{\partial T}{\partial z},$$

$$a = \frac{1}{1+\sigma_0^2/3}\left\{1 + 3\sigma_0^2 - 9\sigma_0^2\,\frac{1+\sigma_0^2}{1-\sigma_0^2}\right\}, \tag{10}$$

$$b = \frac{3\sigma_0}{1+\sigma_0^2/3}\,\frac{1+\sigma_0^2}{1-\sigma_0^2}.$$

The characteristic equation of Eq. (10)

$$\frac{v^2}{3} a k^2 + \omega b v k - \omega^2 = 0 \tag{11}$$

yields the expressions for wave vectors projections

$$k_D = \frac{\omega}{2a}\frac{3b}{v}(\gamma - 1), \quad \gamma = \sqrt{1 + \frac{4a}{3b^2}},$$

$$k_R = -\frac{\omega}{2a}\frac{3b}{v}(\gamma + 1). \tag{12}$$

corresponding two waves running along and against phonon flow respectively. Graphs displaying wave vectors dependence on phonon fluid velocity are shown in Fig. 1.

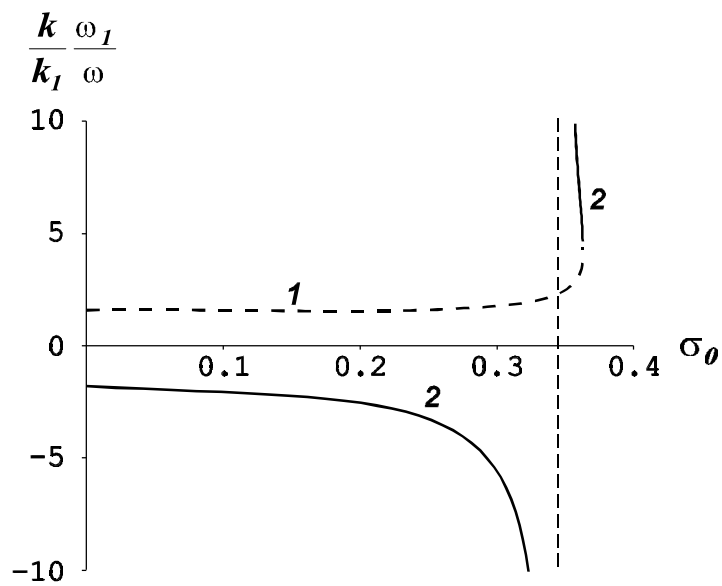

Fig.1. Projections of wave vectors onto direction of phonon flow normalised to first sound wave number and first to second sounds frequencies ratio. Curves 1 and 2

Introducing notation $v_j = w / k$ and rewriting characteristic equation (12) as

$$v_j^2 - bvv_j - \frac{v^2}{3} a = 0 \tag{13}$$

one can find direct and reverse wave phase velocities. Their resolutions onto flow direction

$$v_D = \frac{bv}{2} (g + 1),$$

$$v_R = - \frac{bv}{2} (g - 1), \tag{14}$$

depends on fluid velocity as shown in Fig. 2. These graphs reveal the driftage of both waves by phonon flow due to which the reverse wave at first critical value of flow velocity $s_0 = 0,3443$ changes its direction. In inversion point $(a = 0)$ wave velocity vanishes while the wave vector suffers the break. In the region $a < 0$ the wave motion, allowed only along phonon flow, is forbiden above its second critical velocity $s_0 = 0,3644$, as no wave may propagate with $n_j < u / \sqrt{3}$. Thus any wave motion is ceased long before the flow reaches the second sound velocity $s_0 = 1 / \sqrt{3}$.

3. DYNAMIC THERMAL CONDUCTIVITY

The dynamic (ω-dependent) thermal conductivity of ideal phonon fluid may be calculated in assumption of momentum loss scattering process possibility, implying that the required expression is obtained when relaxation time τ_R tends to infinity. As mo

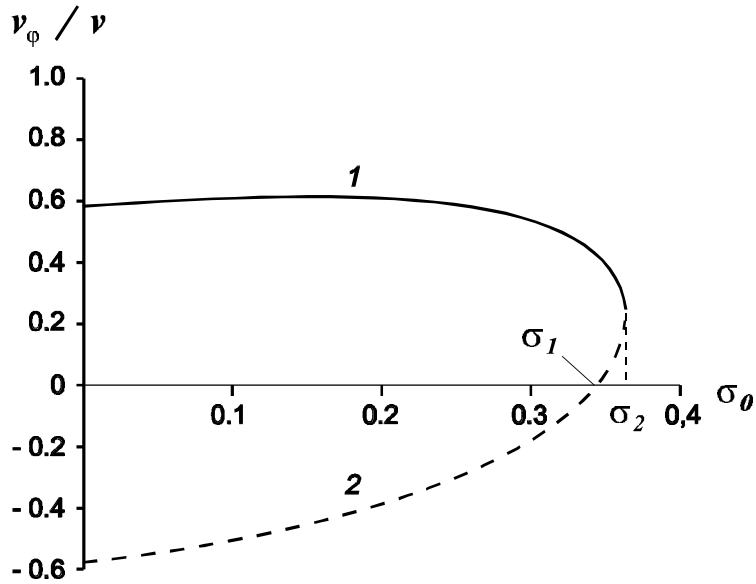

Fig. 2. Velocities of direct 1 and reverse 2 waves in a scale of first sound velocity. Parameters σ_1 and σ_2 are first and second flow critical velocities.

mentum loss is equivalent of first viscosity its account in Eq. (8) results in the additional term $-j/\tau_R$. After Eq. (9) substitution into Eq. (8) we obtain

$$\frac{\partial j}{\partial t} - 3c_v \frac{1+\sigma_0^2}{(1-\sigma_0^2)^4} u_0 \frac{\partial T}{\partial t} = -\frac{1}{3} c_v v^2 \frac{1}{(1-\sigma_0^2)^3} \cdot$$

$$\cdot \left\{ 1 + 3\sigma_0^2 - 9\sigma_0^2 \frac{1+\sigma_0^2}{1-\sigma_0^2} \right\} \frac{\partial T}{\partial z} - \frac{j}{\tau_z}. \qquad (15)$$

For wave perturbations of temperature field $T = C_1 \exp i(\omega t - k_D z)$ of infinite crystal Eq. (15) with respect to $\partial j / \partial t = i\omega j$, $\partial T / \partial t = -v_D(\partial T / \partial z)$ and Eq. (6) converts into generalised Fourier law

$$q = -\frac{\lambda(\sigma_0)}{1 + i\omega\tau_R} T'(z,t). \tag{16}$$

Coefficient attached to temperature gradient makes the significance of dynamic thermal conductivity $\lambda(\omega,\sigma_0) = \lambda'(\omega,\sigma_0) - i\lambda''(\omega,\sigma_0)$, where

$$\lambda'(\omega,\sigma_0) = \frac{\lambda(\sigma_0)}{1 + \omega^2\tau_R^2}, \quad \lambda''(\omega,\sigma_0) = \frac{\lambda(\sigma_0)\omega\tau_R}{1 + \omega^2\tau_R^2} \tag{17}$$

$$\lambda(\sigma_0) = \lambda\left[1 + 3\sigma_0^2 + 9\sigma_0\frac{1+\sigma_0^2}{1-\sigma_0^2}\left(\frac{v_D(\sigma_0)}{v} - \sigma_0\right)\right], \tag{18}$$

and $\lambda = c_v v^2 \tau_R / 3$ is kinetic thermal conductivity. With $\tau_R \to \infty$ stationary thermal conductivity is real and infinite $\lambda'(0,\sigma_0) = \infty$, $\lambda''(0,\sigma_0) = 0$, while dynamic thermal conductivity is purely imaginary

$$\lambda''(\omega,\sigma_0) = \frac{c_v v^2}{3}\frac{1}{\omega}\left[1 + 3\sigma_0^2 + 9\sigma_0\frac{1+\sigma_0^2}{1-\sigma_0^2}\left(\frac{v_D(\sigma_0)}{v} - \sigma_0\right)\right]. \tag{19}$$

The plots of dynamic thermal conductivity as a function of frequency are shown in Fig. 3. Fig. 4 illustrates the dependence of parameter $l(s_0)$ on fluid velocity. It is noteworthy that Eq. (7) is isomorphous to the first of F.London and H.London equations, therefore dynamic thermal conductivity ideal phonon liquid is the analogue of complex conductivity of superconductors [3].

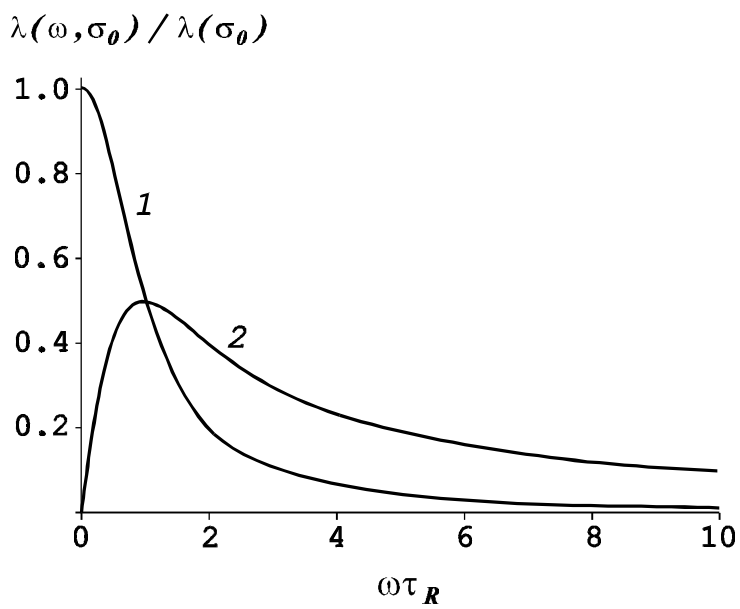

Fig.3. Real 1 and imaginary 2 parts of dynamic thermal conductivity.

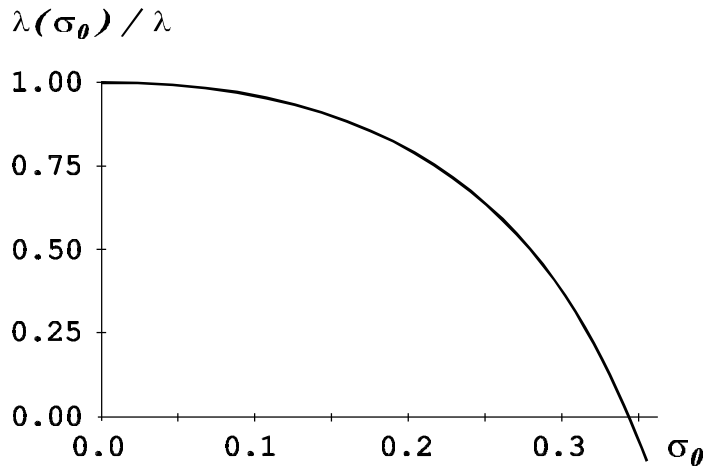

Fig.4. Parameter $l(s_0)$ normalised to kinetic thermal conductivity l as a function of phonon flow velocity.

SUMMARY

The above performed calculation proves that weak density perturbations of phonon aggregate drifting under its own momentum obey the variety of Eulerian equation for ideal liquid. The latter as applied to periodic perturbations converts into a wave equation which parameters depend on phonon fluid velocity. Therefore temperature waves dispersion is anisotropic while the region of wave motions is limited due to the driftage of phonon density perturbations. Within the region where wave motion is allowed the set of equations under consideration acquires the form of generalised Fourier law. This fact permits to introduce a complex thermal conductivity, which in many respects is analogous to dynamic electrical conductivity in Drude-Lorentz model. However, due to restriction imposed on the second sound velocity in phonon flow, thermal conductivity in contrast to electrical one monotonously decays with flow

LITERATURE

1. R.A.Guyer, J.A.Krumhansl, *Phys. Rev.* **148**: 766 (1965).

2. A.S.Rudy, *Physica Scripta.* (1997) to be published

3. V.V.Shmidt, *Vvedenie v Fiziku Sverhprovodnikov* (Nauka, Moscow, 1982), pp. 51-52. *(in Russian)*