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A RELAXATION MODEL OF PHONON GAS INTERACTION WITH AN EXTERNAL FIELD

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In the paper, a kinetic model of interactiona of optical and acoustical phonons is discussed, basing on four life-times. Equations of non-diffusive transfer of heat perturbations, induced by an external field acting upon an assembly of optical phonons, are derived form the proposed model.

1. Introduction

In phenomenological description of heat conduction, the Fourier law of heat conduction is usually applied. According to this law, heat flux is a linear function of temperature gradient. Processes of heat transfer may be also described by microscopic models, deduced from solid state physics. They lead, in the case of dielectrics, to description of heat transfer in terms of mutual interactions of elementary excitations, called phonons [1, 2]. In this paper, we limit ourselves to discussion of a model in which dynamics of a phonon gas is described by the kinetic Boltzmann-Peierls equation [2]. As it is known, the Fourier law of heat conduction may be deduced from kinetic equations for phonons if the relevant modification of Chapman-Enskog method is applied. This derivation is based on the search of such solutions of phonon kinetic equations which may be expressed in the form of asymptotic expansions in terms of temperature gradients [2]. The scope of applications of the Chapman-Enskog method is, however, limited to those states of the system only which differ insignificantly from local thermodynamical equilibrium. For states significantly different from local thermodynamical equlibrium, conditions required by Chapman-Enskog method are not satisfied and heat transfer due to phonon interactions may not be approximated by the Fourier law of heat conduction. Conditions in which the state of phonons assembly is far from local thermodynamical equilibrium may correspond to situation in a dielectric treated, for instance, by laser radiation. Strickly speaking, description of heat transfer in such conditions requires solving kinetic equation. In the limits of approximations stated further and based on a relaxation model of phonon interactions, it is possible to deduce equations of heat transfer in the form of a closed system of differential equations. In the paper, we consider a dielectric in which optical, as well as acoustic, vibration modes exist. For simplicity we limit ourselves to the case when only one branch of each type of vibrations exists. For such a system, the kinetic Boltzmann-Peierls description reduces to a set of two coupled kinetic equations for one-point distribution functions for optical and acoustic phonons.

We assume that energy is transmitted from outside directly to the assembly of optical phonons and then, as a result of mutual phonon interactions, transformed into phonon excitations in the acoustic branch. We also assume that the dominating contribution to energy transport processes comes from the assembly of acoustic phonons. It is known, from solid state physics, that interactions of phonons, ocurring under the influence of electromagnetic radiation, depend on radiation frequency. These effects may be taken into account by assuming that collision integrals in phonon kinetic equations depend on history of external fields. From the processes of phonons interactions, we can separate processes of mutual energy exchange between optical and acoustical phonons assemblies, relaxation processes in optical phonons gas and relaxation process in acoustical phonons gas. The description of these processes by four life-times is introduced, and conformance of the model to the second principle of thermodynamics is shown. Next, basing on moment equations, a set of field equations is educed, which couples energy densities of optical and acoustic phonons with heat flux of acoustic phonons. In the limits of the proposed model, influence of external field reduces to apparition of a time-dependent source in energy balance for optical phonons. From the relations obtained, a set of two equations which connect densities of optical and acoustic phonons, follows.

The microscopic model of transport phenomena, used in this paper, is based on description of phonon interactions in a rigid dielectric. Hence, it does not give the possibility of discussion of effects of coupling thermal and deformation fields. Discussion of such effects, based on microscopic description of phonon assembly and deformation field interaction, will be the subject of a separate paper.

2. Relaxation model of phonon heat transfer

Let us consider a microscopic model of heat transfer in a dielectric, based on the following system of coupled kinetic equations for optical and acoustic phonons

$$\begin{aligned} &\frac{\partial}{\partial t} f_0(\mathbf{x}, \mathbf{k}, t) + \frac{\partial \omega_0(\mathbf{k})}{\partial k_i} \frac{\partial f_0(\mathbf{x}, \mathbf{k}, t)}{\partial x_i} = J_0\big(f_0(\mathbf{x}, \mathbf{k}, t), f_a(\mathbf{x}, \mathbf{k}, t), E_s(t)\big) \\ &\frac{\partial}{\partial t} f_a(\mathbf{x}, \mathbf{k}, t) + \frac{\partial \omega_a(\mathbf{k})}{\partial k_i} \frac{\partial f_a(\mathbf{x}, \mathbf{k}, t)}{\partial x_i} = J_a\big(f_0(\mathbf{x}, \mathbf{k}, t), f_a(\mathbf{x}, \mathbf{k}, t), E_s(t)\big) \end{aligned} \tag{2.1}$$

where $\mathbf{x}$ is a space variable, $\mathbf{k}$ is a phonon wave vector, t mean time, $f_0(\mathbf{x}, \mathbf{k}, t)$ is a distribution function of optical phonons, $f_a(\mathbf{x}, \mathbf{k}, t)$ is a distribution function of acoustic phonons; $\omega_0(\mathbf{k})$ and $\omega_a(\mathbf{k})$ are dispersion curves for optical and acoustic phonons, respectively; $J_0\big(f_0(\mathbf{x}, \mathbf{k}, t), f_a(\mathbf{x}, \mathbf{k}, t), E_s(t)\big)$ is the collision integral in the kinetic equation for optical phonons, $J_a\big(f_0(\mathbf{x}, \mathbf{k}, t), f_a(\mathbf{x}, \mathbf{k}, t), E_s(t)\big)$ is the collision integral in the kinetic equation for acoustic phonons; $E_s(t) = E(t-s)$, $s \geqslant 0$ describes history of an external field acting upon the whole system; x_i and k_i are cartesian coordinates of vectors $\mathbf{x}$ and $\mathbf{k}$. In the above model, it is assumed for simplicity that there exists only one branch for each type of phonon excitations.

From solid state physics, it is known that functions $\hbar\omega_0(k)$ and $\hbar\omega_a(k)$ have a meaning of energy of a single phonon from the corresponding branch ($2\pi\hbar$ is the Planck constant) [2]. After multiplying Eqs. $(2.1)_1$ and $(2.1)_2$ by $\hbar\omega_0(\mathbf{k})$ and $\hbar\omega_a(\mathbf{k})$, respectively, integrating equations obtained with respect to $\mathbf{k}$ and changing the order of integration and differentiation, we obtain energy balance equations for optical and acoustical phonons

$$\begin{gathered}\frac{\partial}{\partial t}\varepsilon_0(\mathbf{x}, t) + \operatorname{div}\mathbf{q}_0(\mathbf{x}, t) = P_0(\mathbf{x}, t)\\ \frac{\partial}{\partial t}\varepsilon_a(\mathbf{x}, t) + \operatorname{div}\mathbf{q}_a(\mathbf{x}, t) = P_a(\mathbf{x}, t)\end{gathered} \tag{2.2}$$

where

$$\begin{gathered}\varepsilon_0(\mathbf{x}, t) = \int \hbar\omega_0(\mathbf{k})\, f_0(\mathbf{x}, \mathbf{k}, t)\frac{d^3\mathbf{k}}{(2\pi)^3}\\ \mathbf{q}_0(\mathbf{x}, t) = \int [\hbar\omega_0(\mathbf{k})\nabla_{\mathbf{k}}\omega_0(\mathbf{k})]\, f_0(\mathbf{x}, \mathbf{k}, t)\frac{d^3\mathbf{k}}{(2\pi)^3}\\ P_0(\mathbf{x}, t) = \int \hbar\omega_0(\mathbf{k}) J_0\big(f_0(\mathbf{x}, \mathbf{k}, t), f_a(\mathbf{x}, \mathbf{k}, t), E_s(t)\big)\frac{d^3\mathbf{k}}{(2\pi)^3}\end{gathered} \tag{2.3}$$

are energy density of optical phonons, heat flux carried by the gas of optical phonons, and a source in the energy balance for optical phonons, while

$$\begin{gathered}\varepsilon_a(\mathbf{x}, t) = \int \hbar\omega_a(\mathbf{k})\, f_a(\mathbf{x}, \mathbf{k}, t)\frac{d^3\mathbf{k}}{(2\pi)^3}\\ \mathbf{q}_a(\mathbf{x}, t) = \int [\hbar\omega_a(\mathbf{k})\nabla_{\mathbf{k}}\omega_a(\mathbf{k})]\, f_a(\mathbf{x}, \mathbf{k}, t)\frac{d^3\mathbf{k}}{(2\pi)^3}\\ P_a(\mathbf{x}, t) = \int \hbar\omega_a(\mathbf{k}) J_a\big(f_0(\mathbf{x}, \mathbf{k}, t), f_a(\mathbf{x}, \mathbf{k}, t), E_s(t)\big)\frac{d^3\mathbf{k}}{(2\pi)^3}\end{gathered} \tag{2.4}$$

are energy density of acoustic phonons, heat flux carried by the gas of acoustic phonons and source in the energy balance for acoustic phonons.

In Eqs. (2.3), (2.4) we make use of the convention of normalization of phonon distribution functions which in usually applied in solid state physics [2]. Symbols $\nabla_{\mathbf{k}}$ and div mean gradient in respect to $\mathbf{k}$ and space divergence, respectively.

Adding the two balance equations $(2.2)_1$ and $(2.2)_2$ gives the balance equation for the total energy.

$$\frac{\partial}{\partial t}\varepsilon + \operatorname{div}\mathbf{q} = P \tag{2.5}$$

where

$$\begin{aligned} \varepsilon &= \varepsilon_0 + \varepsilon_a \\ \mathbf{q} &= \mathbf{q}_0 + \mathbf{q}_a \\ P &= P_0 + P_a \end{aligned} \tag{2.6}$$

are total energy density, total energy flux and a source component, respectively.

Let us assume that collision integrals in Eqs. $(2.1)_1$, $(2.1)_2$ have the form of the following sums

$$\begin{aligned} J_0\big(f_0(\mathbf{x}, \mathbf{k}, t), f_a(\mathbf{x}, \mathbf{k}, t), E_s(t)\big) &= J_{0,E}\big(f_0(\mathbf{x}, \mathbf{k}, t), E_s(t)\big) \\ &\quad + J_{0,R}\big(f_0(\mathbf{x}, \mathbf{k}, t)\big) + J_{0,I}\big(f_0(\mathbf{x}, \mathbf{k}, t), f_a(\mathbf{x}, \mathbf{k}, t)\big) \\ J_a\big(f_0(\mathbf{x}, \mathbf{k}, t), f_a(\mathbf{x}, \mathbf{k}, t), E_s(t)\big) &= J_{a,R}\big(f_a(\mathbf{x}, \mathbf{k}, t)\big) + J_{a,I}\big(f_0(\mathbf{x}, \mathbf{k}, t), f_a(\mathbf{x}, \mathbf{k}, t)\big). \end{aligned} \tag{2.7}$$

The component $J_{0,E}\big(f_0(\mathbf{x}, \mathbf{k}, t), E_s(t)\big)$ of the collision integral $(2.7)_1$ describes processes in which an external field transmits energy to the assembly of acoustic phonons. We assume that these processes may depend on the form of optical phonon distribution $f_0(\mathbf{x}, \mathbf{k}, t)$.

Expressions $J_{0,I}\big(f_0(\mathbf{x}, \mathbf{k}, t), f_a(\mathbf{x}, \mathbf{k}, t)\big)$ and $J_{a,I}\big(f_0(\mathbf{x}, \mathbf{k}, t), f_a(\mathbf{x}, \mathbf{k}, t)\big)$ describe processes of mutual energy exchange between the assemblies of optical and acoustic phonons. The principle of conservation of energy requires that the sum of contributions of these processes to the total energy source is equal to zero

$$\begin{aligned} &\int \hbar\omega_0(\mathbf{k}) J_{0,I}\big(f_0(\mathbf{x}, \mathbf{k}, t), f_a(\mathbf{x}, \mathbf{k}, t)\big)\frac{d^3\mathbf{k}}{(2\pi)^3} \\ &\qquad + \int \hbar\omega_a(\mathbf{k}) J_{a,I}\big(f_0(\mathbf{x}, \mathbf{k}, t), f_0(\mathbf{x}, \mathbf{k}, t)\big)\frac{d^3\mathbf{k}}{(2\pi)^3} = 0. \end{aligned} \tag{2.8}$$

Expression $J_{0,R}\big(f_0(\mathbf{x}, \mathbf{k}, t)\big)$ describes relaxation processes in the optical phonons assembly; i.e. processes in which acoustic phonons do not participate, and which describe the tendency of optical phonons assembly towards thermodynamical equilibrium if only processes of mutual transmutations of optical and acoustic phonons are eliminated and if $J_{0,E}\big(f_0(\mathbf{x}, \mathbf{k}, t), E_s(t)\big)$ equals zero.

It follows, from the principle of conservation of energy, that the energy source related to relaxation processes described by $J_{0,R}(f_0(\mathbf{x}, \mathbf{k}, t))$ must be to equal zero

$$\int \hbar\omega_0(\mathbf{k}) J_{0,R}(f_0(\mathbf{x}, \mathbf{k}, t)) \frac{d^3\mathbf{k}}{(2\pi)^3} = 0. \tag{2.9}$$

Expression $J_{a,R}(f_0(\mathbf{x}, \mathbf{k}, t))$ describes relaxation processes in the acoustic phonons assembly and, like $J_{0,R}(f_0(\mathbf{x}, \mathbf{k}, t))$, satisfies the identity corresponding to energy conservation

$$\int \hbar\omega_0(\mathbf{k}) J_{a,R}(f_a(\mathbf{x}, \mathbf{k}, t)) \frac{d^3\mathbf{k}}{(2\pi)^3} = 0 \tag{2.10}$$

According to the general rules of constructing relaxational models for multiple "competing" dissipation processes, we substitute the components of collision integrals separated above by their relaxation equivalents, in which processes of mutual phonon transmutations are approximately described by life-times dependent, in general, on the wave vector $\mathbf{k}$ [3].

The relaxation model of the $J_{0R}(f_0(\mathbf{x}, \mathbf{k}, t))$ component of the collision integral $(2.7)_1$ is described by

$$C_{0,R}(f_0(\mathbf{x}, \mathbf{k}, t)) = -(\tau_{0,R}(\mathbf{k}))^{-1}\big(f_0(\mathbf{x}, \mathbf{k}, t) - \Phi_{0,R}(\alpha(\mathbf{x}, t))\big) \tag{2.11}$$

where $\tau_{0,R}(\mathbf{k})$ is a life-time, modelling dissipation processes described by $J_{0,R}(f_0(\mathbf{x}, \mathbf{k}, t))$; function $\alpha(\mathbf{x}, t)$ is given as the solution of the following identity

$$\int \frac{\hbar\omega_0(\mathbf{k})}{\tau_{0,R}(\mathbf{k})} \left[f_0(\mathbf{x}, \mathbf{k}, t) - \frac{1}{e^{\alpha(\mathbf{x},t)\hbar\omega_0(\mathbf{k})} - 1} \right] \frac{d^3\mathbf{k}}{(2\pi)^3} = 0 \tag{2.12}$$

while

$$\Phi_{0,R}(\alpha(\mathbf{x}, t)) = \frac{1}{e^{\alpha(\mathbf{x},t)\hbar\omega_0(\mathbf{k})} - 1} \tag{2.13}$$

(Because the life-time is positive, it follows that the above definition of $\alpha(\mathbf{x}, t)$ is unambiguous).

It can is seen that the expression (2.11), defined in such a way, satisfies condition of conservation of energy. Similarly, dissipation processes described by $J_{a,R}(f_a(\mathbf{x}, \mathbf{k}, t))$, which are responsible for relaxation to thermodynamical equilibrium of the acoustical phonons assembly, are modelled by the life-time $\tau_{a,R}(\mathbf{k})$ dependent on the wave vector. The relevant contribution to the collision integral has the form

$$C_{a,R}(f_a(\mathbf{x}, \mathbf{k}, t)) = -(\tau_{a,R}(\mathbf{k}))^{-1}\big(f_a(\mathbf{x}, \mathbf{k}, t) - \Phi_{a,R}(\beta(\mathbf{x}, t))\big) \tag{2.14}$$

where

$$\Phi_{a,R}(\beta(\mathbf{x},t)) = \frac{1}{e^{\beta(\mathbf{x},t)\hbar\omega_a(\mathbf{k})}-1} \tag{2.15}$$

and the condition of energy conservation

$$\int \frac{\hbar\omega_a(\mathbf{k})}{\tau_{a,R}(\mathbf{k})}\big(f_a(\mathbf{x},\mathbf{k},t)-\Phi_{a,R}(\beta(\mathbf{x},t))\big)\frac{d^3\mathbf{k}}{(2\pi)^3} = 0 \tag{2.16}$$

determines the value of $\beta(\mathbf{x}, t)$ which appears in (2.14) and (2.15) as a parameter.

Expressions $J_{0,I}(f_0(\mathbf{x},\mathbf{k},t), f_a(\mathbf{x},\mathbf{k},t))$ and $J_{a,I}(f_0(\mathbf{x},\mathbf{k},t), f_a(\mathbf{x},\mathbf{k},t))$, describing mutual transmutation processes of optical and acoustic phonons, are approximated by

$$\begin{aligned} C_{0,I}(f_0(\mathbf{x},\mathbf{k},t), f_a(\mathbf{x},\mathbf{k},t)) &= -(\tau_{0,I}(\mathbf{k}))^{-1}\big(f_0(\mathbf{x},\mathbf{k},t)-\Phi_{0,I}(\gamma(\mathbf{x},t))\big)\\ C_{a,I}(f_0(\mathbf{x},\mathbf{k},t), f_a(\mathbf{x},\mathbf{k},t)) &= -(\tau_{a,I}(\mathbf{k}))^{-1}\big(f_a(\mathbf{x},\mathbf{k},t)-\Phi_{a,I}(\gamma(\mathbf{x},t))\big), \end{aligned} \tag{2.17}$$

respectively, where

$$\begin{aligned} \Phi_{0,I}(\gamma(\mathbf{x},t)) &= \frac{1}{e^{\gamma(\mathbf{x},t)\hbar\omega_0(\mathbf{k})}-1}\\ \Phi_{a,I}(\gamma(\mathbf{x},t)) &= \frac{1}{e^{\gamma(\mathbf{x},t)\hbar\omega_a(\mathbf{k})}-1} \end{aligned} \tag{2.18}$$

while the condition of energy conservation in energy transfer processes between the optical and acoustic phonons assemblies takes the form of equality

$$\begin{aligned} 0 = &\int \frac{\hbar\omega_0(\mathbf{k})}{\tau_{0,I}(\mathbf{k})}\big(f_0(\mathbf{x},\mathbf{k},t)-\Phi_{0,I}(\gamma(\mathbf{x},t))\big)\frac{d^3\mathbf{k}}{(2\pi)^3}\\ &+\int \frac{\hbar\omega_a(\mathbf{k})}{\tau_{a,I}(\mathbf{k})}\big(f_a(\mathbf{x},\mathbf{k},t)-\Phi_{a,I}(\gamma(\mathbf{x},t))\big)\frac{d^3\mathbf{k}}{(2\pi)^3}. \end{aligned} \tag{2.19}$$

This equality determines the value of $\gamma(\mathbf{x}, t)$. It is easily verified that, for any pair of distribution functions $f_0(\mathbf{x}, \mathbf{k}, t)$ and $f_a(\mathbf{x}, \mathbf{k}, t)$, the quantity $\gamma(\mathbf{x}, t)$ is determined unambigously.

Hence, the proposed system of kinetic equations takes the form

$$\begin{aligned} \frac{\partial}{\partial t} f_0(\mathbf{x},\mathbf{k},t) + \frac{\partial\omega_0(\mathbf{k})}{\partial k_i}\frac{\partial f_0(\mathbf{x},\mathbf{k},t)}{\partial x_i} &= -(\tau_{0,R}(\mathbf{k}))^{-1}\big(f_0(\mathbf{x},\mathbf{k},t)-\Phi_{0,R}(\alpha(\mathbf{x},t))\big)\\ &\quad -(\tau_{0,I}(\mathbf{k}))^{-1}\big(f_0(\mathbf{x},\mathbf{k},t)-\Phi_{0,I}(\gamma(\mathbf{x},t))\big)+J_{0,E}(f_0(\mathbf{x},\mathbf{k},t), E_s(t))\\ \frac{\partial}{\partial t} f_a(\mathbf{x},\mathbf{k},t) + \frac{\partial\omega_a(\mathbf{k})}{\partial k_i}\frac{\partial f_a(\mathbf{x},\mathbf{k},t)}{\partial x_i} &= -(\tau_{a,R}(\mathbf{k}))^{-1}\big(f_a(\mathbf{x},\mathbf{k},t)-\Phi_{a,R}(\beta(\mathbf{x},t))\big)\\ &\quad -(\tau_{a,I}(\mathbf{k}))^{-1}\big(f_a(\mathbf{x},\mathbf{k},t)-\Phi_{a,I}(\gamma(\mathbf{x},t))\big). \end{aligned} \tag{2.20}$$

The functions $\Phi_{0,R}$, $\Phi_{0,I}$, $\Phi_{a,I}$, $\Phi_{a,R}$ are given by the formulae (2.13), (2.18) and (2.15), while their arguments, functions $\alpha(\mathbf{x}, t)$, $\gamma(\mathbf{x}, t)$ and $\beta(\mathbf{x}, t)$, are defined as the solutions of Eqs. (2.12), (2.19) and (2.16).

The functions $\Phi_{0,R}$, $\Phi_{0,I}$, $\Phi_{a,I}$, $\Phi_{a,R}$ have the form of local equilibrium Planck distributions in which the inverse of product of temperature and the Boltzmann constant is identified with the functions $\alpha(\mathbf{x}, t)$, $\gamma(\mathbf{x}, t)$ and $\beta(\mathbf{x}, t)$, respectively.

Hence, $\alpha(\mathbf{x}, t)$ may be assigned such a temperature field which determines the local equilibrium state to which the distribution of optical phonons tends if all the interaction, but optical phonon relaxation processes, are "turned off". The functions $\beta(\mathbf{x}, t)$ and $\gamma(\mathbf{x}, t)$ may be interpreted in a similar way.

3. Entropy balance

We will show that the proposed system of kinetic equations (2.20) conforms to thermodynamics in the sense that its solutions satisfy entropy balance. In the entropy balance, the source term is a sum of two components; the first, always non-negative, describes dissipation processes inside the assembly while the second describes an entropy source due to the influence of external field. The entropy source related to external field depends only on processes described by the component $J_{0,E}(f_0(\mathbf{x}, \mathbf{k}, t), E_s(t))$ of the collision integral. The term is non-negative if the source of optical phonons described by $J_{0,E}(f_0(\mathbf{x}, \mathbf{k}, t), E_s(t))$ is non-negative for any values of the wave vector, i.e., if interaction with the external field does not diminish the number of optical phonons, independently of their spectrum range.

It is known from solid state physics that entropy densities of optical and acoustic phonons are given, respectively, by the formulae

$$S_0(\mathbf{x}, t) = \int \{(f_0+1)\ln(f_0+1) - f_0 \ln f_0\} \frac{d^3\mathbf{k}}{(2\pi)^3}$$

$$S_a(\mathbf{x}, t) = \int \{(f_a+1)\ln(f_a+1) - f_a \ln f_a\} \frac{d^3\mathbf{k}}{(2\pi)^3}. \tag{3.1}$$

(From now on, to simplify the notation, arguments on which phonon distribution functions depend will not be written explicitly.) Total entropy density S is a sum of expressions $(3.1)_1$ and $(3.1)_2$

$$S(\mathbf{x}, t) = S_0(\mathbf{x}, t) + S_a(\mathbf{x}, t). \tag{3.2}$$

It can be seen, on differentiating (3.2) with respect to time and using Eq. (2.20), that the total entropy balance of the assembly being considered has the form

$$\frac{\partial}{\partial t} S(\mathbf{x}, t) + \operatorname{div}\mathbf{S} = P_S \tag{3.3}$$

where

$$\mathbf{S}(\mathbf{x}, t) = \int \{(f_0+1)\ln(f_0+1) - f_0 \ln f_0\} \nabla_{\mathbf{k}} \omega_0(\mathbf{k}) \frac{d^3\mathbf{k}}{(2\pi)^3} + \int \{(f_a+1)\ln(f_a+1) - f_a \ln f_a\} \nabla_{\mathbf{k}} \omega_a(\mathbf{k}) \frac{d^3\mathbf{k}}{(2\pi)^3} \tag{3.4}$$

is the total entropy flux, and

$$P_S(\mathbf{x}, t) = \int \left(\ln \frac{f_0+1}{f_0}\right) C_{0,R}(f_0) \frac{d^3\mathbf{k}}{(2\pi)^3} + \int \left(\ln \frac{f_a+1}{f_a}\right) C_{a,R}(f_a) \frac{d^3\mathbf{k}}{(2\pi)^3} + \int \left(\ln \frac{f_0+1}{f_0}\right) C_{0,I}(f_0, f_a) \frac{d^3\mathbf{k}}{(2\pi)^3} + \int \left(\ln \frac{f_a+1}{f_a}\right) C_{a,I}(f_0, f_a) \frac{d^3\mathbf{k}}{(2\pi)^3} + \int \left(\ln \frac{f_0+1}{f_0}\right) J_{0,E}(f_0, E_s(t)) \frac{d^3\mathbf{k}}{(2\pi)^3} \tag{3.5}$$

is the source of entropy. To investigate signs of components appearing in (3.5), we use the well-known identity stating that, for any positive numbers y, z, the following inequality holds [2]

$$(y-z)\ln\frac{y}{z} \geqslant 0. \tag{3.6}$$

On substituting $y = (f_0)^{-1}(f_0+1)$, $z = (\Phi_{0,I})^{-1}(\Phi_{a,I}+1)$ and $y = (f_a)^{-1}(f_a+1)$, $z = (\Phi_{a,I})^{-1}(\Phi_{a,I}+1)$ we obtain, after multiplied by $\Phi_{a,I} f_0$ and $\Phi_{a,I} f_a$, respectively,

$$\begin{aligned} &(\Phi_{0,I} - f_0)\ln\frac{(f_0+1)\Phi_{0,I}}{f_0(\Phi_{0,I}+1)} \geqslant 0 \\ &(\Phi_{a,I} - f_a)\ln\frac{(f_a+1)\Phi_{a,I}}{f_a(\Phi_{a,I}+1)} \geqslant 0. \end{aligned} \tag{3.7}$$

After multiplying the inequalities $(3.7)_1$ by $(2\pi)^{-3}\left(\tau_{0,I}(\mathbf{k})\right)^{-1}$ and $(3.7)_2$ by $(2\pi)^{-3}\left(\tau_{a,I}(\mathbf{k})\right)^{-1}$, adding the results, integrating the sum in respect to $\mathbf{k}$, and taking into account (2.19) we arrive at the inequality

$$\begin{aligned} &-\int (f_0 - \Phi_{0,I})\ln\frac{f_0+1}{f_0}\frac{d^3\mathbf{k}}{(2\pi)^3} - \int (f_a - \Phi_{a,I})\ln\frac{f_a+1}{f_a}\frac{d^3\mathbf{k}}{(2\pi)^3} = \\ &= \int \left(\ln\frac{f_0+1}{f_0}\right) C_{0,I}(f_0, f_a)\frac{d^3\mathbf{k}}{(2\pi)^3} + \int \left(\ln\frac{f_a+1}{f_a}\right) C_{a,I}(f_0, f_a)\frac{d^3\mathbf{k}}{(2\pi)^3} \geqslant 0. \end{aligned} \tag{3.8}$$

From (3.8) it follows that the sum of the third and fourth components of (3.5) is non-negative. It testifies that, in the scope of the model assumed, processes of mutual transmutations of optical and acoustic phonons give a non-negative contribution to the entropy source. In a similar way, it can be is demonstrated that the contributions from the first two components on the right side of (3.5) are non-negative, as well. The last component of the sum (3.5) describes the entropy source due to external interaction upon the systems. As we mentioned, if the external interaction, independently of spectrum range of optical phonons, increases the number of excitations then their contribution to the total entropy source is also non-negative.

4. Education of field equations

In order to derive the system of field equations describing heat transport processes, we additionally assume that the life-times $\tau_{0,I}(\mathbf{k})$, $\tau_{a,I}(\mathbf{k})$, $\tau_{0,R}(\mathbf{k})$ and $\tau_{a,R}(\mathbf{k})$ do not depend on the wave vector, and that dispersion curve of acoustic phonons is described by the formula

$$\omega_a(\mathbf{k}) = c|\mathbf{k}| \tag{4.1}$$

where c is interpreted as the velocity of sound [2]. On multiplying Eq. $(2.20)_1$ by $(2\pi)^{-3}\hbar\omega_0(\mathbf{k})$ and integrating it with respect to $\mathbf{k}$, we obtain an equation for energy balance of acoustic phonons

$$\frac{\partial}{\partial t}\varepsilon_0 + \operatorname{div}\mathbf{q}_0 = -(\tau_{0,I})^{-1}(\varepsilon_0 - \varepsilon_0(\gamma)) + P_E \tag{4.2}$$

where ε_0 and $\mathbf{q}_0$ are described by the formulae $(2.3)_{1,2}$ while

$$P_E = \int \hbar\omega_0(\mathbf{k}) J_{0,E}(f_0, E_s)\frac{d^3\mathbf{k}}{(2\pi)^3}. \tag{4.3}$$

Next, after multiplying $(2.20)_2$ consecutively by $(2\pi)^{-3}\hbar\omega_a(\mathbf{k})$ and $(2\pi)^{-3}\hbar\omega_a(\mathbf{k})\nabla_{\mathbf{k}}\omega_a(\mathbf{k})$, integrating with respect to $\mathbf{k}$ and substituting (4.1), we obtain equations for energy balance and heat flux of acoustic phonons

$$\begin{aligned} &\frac{\partial}{\partial t}\varepsilon_a + \operatorname{div}\mathbf{q}_a = -(\tau_{a,I})^{-1}(\varepsilon_a - \varepsilon_a(\gamma)) \\ &\frac{\partial}{\partial t}\mathbf{q}_a + \operatorname{div}\mathbf{Q}_a = -\mathbf{q}_a[(\tau_{a,R})^{-1} + (\tau_{a,I})^{-1}] \end{aligned} \tag{4.4}$$

where

$$\begin{aligned} \mathbf{Q}_a &= \int \hbar\omega_a(\mathbf{k})[\nabla_{\mathbf{k}}\omega_a(\mathbf{k})]\otimes[\nabla_{\mathbf{k}}\omega_a(\mathbf{k})]\, f_a \frac{d^3\mathbf{k}}{(2\pi)^3} = \hbar c^3 \int \frac{\mathbf{k}}{|\mathbf{k}|}\otimes\mathbf{k} f_a \frac{d^3\mathbf{k}}{(2\pi)^3} \\ \varepsilon_0(\gamma(\mathbf{x}, t)) &= \int \hbar\omega_0(\mathbf{k})\frac{1}{e^{\gamma(\mathbf{x},t)\hbar\omega_0(\mathbf{k})} - 1}\frac{d^3\mathbf{k}}{(2\pi)^3} \\ \varepsilon_a(\gamma(\mathbf{x}, t)) &= \hbar c \int |\mathbf{k}| \frac{1}{e^{\gamma(\mathbf{x},t)\hbar c|\mathbf{k}|} - 1}\frac{d^3\mathbf{k}}{(2\pi)^3} \end{aligned} \tag{4.5}$$

while, as it follows from (2.19), the value of $\gamma(\mathbf{x}, t)$ is related to energy densities of optical and acoustic phonons by the formula

$$\tau_{a,I}\big(\varepsilon_0(\mathbf{x}, t))\big) - \varepsilon_0\big(\gamma(\mathbf{x}, t)\big) = \tau_{0,I}\big(\varepsilon_a(\mathbf{x}, t) - \varepsilon_a\big((\gamma(\gamma(x, t))\big)\big) \tag{4.6}$$

(It can be easily verified that, for any pair of non-negative values ε_0, ε_a, the formula (4.6) determines unambigously the value of γ).

To obtain a closed set of equations from the relations deduced above, we assume that the heat flux transferred by optical phonons is negligibly small as compared with the heat flux transferred by acoustic phonons, and that the dominating contribution to the change in time of energy density of optical phonons is related to processes described by the source component in Eq. (4.2) (this assumption conforms to estimates known in literature, eg. cf. [4]).

The tensor $\mathbf{Q}_a$, which has a meaning of a heat flux tensor may be uniquely expressed as a sum of a spherical and a traceless tensors

$$\mathbf{Q}_a = \tfrac{1}{3}\hat{I}\cdot \mathrm{Tr}\,\mathbf{Q}_a + \langle \mathbf{Q}_a \rangle \tag{4.7}$$

where $\hat{I}$ is the unit tensor, Tr means trace operation, and $\langle Q_a \rangle$ is the traceless part of Q_α. We assume that the dominant part of the tensor Q_a is the spherical one and that $\langle Q_a \rangle$ may be neglected we repeat the argumentation used by Peierls [5]. This assumption holds when the dominant part of the distribution function is invariant in respect to rotations of $\mathbf{k}$. In particular, it is true when the distribution function of acoustic phonons has the shape approaching that of local equilibrium Planck distribution.

The above approximations imply a closed set of relations, describing propagation of perturbations in a coupled system of optical and acoustic phonons:

$$\begin{aligned}
&\frac{\partial}{\partial t}\varepsilon_0 = -(\tau_{0,I})^{-1}\big(\varepsilon_0 - \varepsilon_0(\gamma)\big) + P_E \\
&\frac{\partial}{\partial t}\varepsilon_a + \mathrm{div}\,\mathbf{q}_a = -(\tau_{a,R})^{-1}\big(\varepsilon_a - \varepsilon_a(\gamma)\big) \\
&\frac{\partial}{\partial t}\mathbf{q}_a + \mathrm{div}\big(\hat{I}\cdot\tfrac{1}{3}c^2\varepsilon_a\big) = -\mathbf{q}_a\big((\tau_{a,R})^{-1} + (\tau_{a,I})^{-1}\big) \\
&\tau_{a,I}\big(\varepsilon_0 - \varepsilon_0(\gamma)\big) = \tau_{0,I}\big(\varepsilon_a - \varepsilon_a(\gamma)\big)
\end{aligned} \tag{4.8}$$

where $\varepsilon_0(\gamma)$ and $\varepsilon_a(\gamma)$ are determined by the formulae $(4.5)_2$, $(4.5)_3$ and (4.6). In the above description, the function P_E, describing velocity with which an external field transfers energy to the optical phonons, is regarded as given. It is seen that the life-time $\tau_{0,R}$, describing relaxation velocity of optical phonons to an equilibrium state, does not appear in the set (4.8).

Taking divergence of Eq. $(4.8)_3$ gives

$$\frac{\partial}{\partial t}\mathrm{div}\,\mathbf{q}_a + \frac{c^2}{3}\Delta\varepsilon_a = -\mathrm{div}\,\mathbf{q}_a\big((\tau_{a,R})^{-1} + (\tau_{a,I})^{-1}\big) \tag{4.9}$$

After substituting in (4.9) expressions for $\operatorname{div}\mathbf{q}_a$ and $\frac{\partial}{\partial t}\operatorname{div}\mathbf{q}_a$ determined from $(4.8)_2$ and its time derivative, we obtain a set of two equations, relating space densities of energies of optical and acoustic phonons

$$\begin{cases} -\dfrac{\partial^2}{\partial t^2}\varepsilon_a+\dfrac{c^2}{3}\Delta\varepsilon_a = \left((\tau_{a,R})^{-1}+(\tau_{a,I})^{-1}\right)\left[\dfrac{\partial}{\partial t}\varepsilon_a+(\tau_{a,R})^{-1}\left(\varepsilon_a-\varepsilon_a(\gamma)\right)\right] \\ \qquad\qquad\qquad\qquad\qquad\qquad +(\tau_{a,R})^{-1}\dfrac{\partial}{\partial t}\left(\varepsilon_a-\varepsilon_a(\gamma)\right) \\ \dfrac{\partial}{\partial t}\varepsilon_0 = -(\tau_{0,I})^{-1}\left(\varepsilon_0-\varepsilon_0(\gamma)\right)+P_E \end{cases} \tag{4.10}$$

Processes of heat transfer, described by (4.10), have a different character than processes described by the Fourier law of heat conductivity. We may notice that in the set (4.10) we can assume different primitive fields which can be easily physically interpreted. Namely, one of the variables may be taken to be the field γ (proportional to the inverse of the (temperature to which the system relaxes locally), while the other one may be the $\varepsilon_a-\varepsilon_a(\gamma)$ (or, equivalently, $\varepsilon_0-\varepsilon_0(\gamma)$), describing the measure of deviation of the system from local thermodynamical equilibrium.

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