

Kinetic and Hydrodynamic Equations for Phonons Interacting with High-Frequency Sound

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A kinetic equation for phonons interacting with sound whose frequency is much greater than their inverse relaxation time is obtained by the method of decoupling of the Bogolyubov chain of equations for the quantum distribution functions. In addition to the usual Peierls-Boltzmann collision integral, this equation contains an additional collision term which is proportional to the intensity of the sound wave. The laws of conservation of the total quasimomentum and energy of the phonon gas are derived on the basis of the kinetic equation with account of phonon drag and heating by the sound. Conditions are formulated under which the state of the gas of thermal phonons interacting with high-frequency sound is quasiequilibrium and hence the conservation laws may be regarded as phonon hydrodynamic equations.

IN very pure dielectric samples, the propagation of high-frequency sound at low temperatures is accompanied by dragging of the thermal phonons by the sound wave, and by the appearance of a drift of the phonon gas. By high frequency (HF) here we mean sound whose frequency is much greater than the inverse relaxation time of the thermal phonons. This acousto-thermal effect has been studied previously by the author.^[1,2] Consideration in^[1,2] was based on the hydrodynamic equations, which describe the motion of the phonon gas in the limit $l_N \ll l_U$, where l_N and l_U are the main path lengths of the phonon relative to normal processes and Umklapp processes, respectively. The dragging and heating of the phonons by the sound have been considered purely phenomenologically, by adding to the hydrodynamic equations additional terms whose form was established by means of simple physical considerations.

The purpose of the present research is the systematic microscopic derivation of the kinetic and hydrodynamic equations for phonons interacting with high-frequency sound waves. A detailed analysis of the effect of the sound on the state of the phonon gas in the crystal allows us to establish the limits of applicability of the equations of phonon hydrodynamics used in^[1,2]. It will be shown below, in particular, that the usual condition of the predominance of N processes over all forms of scattering with losses of quasimomentum in the given case no longer guarantees the legitimacy of the hydrodynamic approach. Furthermore, the derivation of the kinetic equation for phonons interacting with high-frequency sound is of interest in its own right. On the basis of this equation, we can compute the sound absorption coefficient in those cases in which the sound wave brings about an appreciable departure of the state of the phonon gas from equilibrium. Such a situation arises, for example, in the propagation of longitudinal sound in dielectrics at low temperatures.^[3,4]

In what follows, we shall assume that the sound frequency $\Omega \ll T/\hbar$ and $l_N \Gamma \ll 1$, where T is the temperature of the crystal and Γ the sound absorption coefficient.

1. THE HAMILTONIAN

Since we are interested in low temperature effects, we shall consider the crystal as an anisotropic elastic

continuum and limit ourselves to account of anharmonicity of third order only. Then the energy density of the elastic deformations will have the form

$$W = \frac{1}{2} \lambda_{ijkl} u_{ij} u_{kl} + \frac{1}{3} \kappa_{ijklmn} u_{ij} u_{kl} u_{mn}, \tag{1}$$

where λ_{ijkl} is the elastic modulus tensor and κ_{ijklmn} the tensor of anharmonic elastic constants. The components of the deformation tensor u_{ij} are expressed in well known fashion by the deformation vector $u(\mathbf{r})$:

$$u_{ij} = \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} + \frac{\partial u_k}{\partial x_i} \frac{\partial u_k}{\partial x_j} \right), \tag{2}$$

where the x_i are the components of the radius vector \mathbf{r} . We introduce the phonon Bose operators $a_\lambda(\mathbf{q})$ and $a_\lambda^\dagger(\mathbf{q})$:

$$u(\mathbf{r}) = \sum_{\mathbf{q}\lambda} \left[\frac{\hbar}{2\rho V\omega_\lambda(\mathbf{q})} \right]^{1/2} e^{i\mathbf{q}\cdot\mathbf{r}} [a_\lambda(\mathbf{q}) e^{i\mathbf{q}\cdot\mathbf{r}} + a_\lambda^\dagger(\mathbf{q}) e^{-i\mathbf{q}\cdot\mathbf{r}}]. \tag{3}$$

Here \mathbf{q} , $\omega_\lambda(\mathbf{q})$ and $e^\lambda(\mathbf{q})$ are the wave vector, frequency and polarization vector of the phonon mode, λ the index of polarization, ρ the density of the crystal and V the normalized volume. Using (1) and (3), and after some transformations, we can obtain the Hamiltonian in the form

$$H = \sum_{\mathbf{q}\alpha} \hbar\omega_\alpha(\mathbf{q}) [a_\alpha^\dagger(\mathbf{q}) a_\alpha(\mathbf{q}) + 1/2] + \frac{i}{V^{1/2}} \left(\frac{\hbar}{2\rho} \right)^{3/2} \times \sum_{\alpha\beta\gamma} \sum_{\mathbf{q}\mathbf{q}'\mathbf{q}''} M^{\alpha\beta\gamma}(\mathbf{q}, \mathbf{q}', \mathbf{q}'') \Delta(\mathbf{q} - \mathbf{q}' - \mathbf{q}'') [a_\alpha^\dagger(\mathbf{q}) a_\beta(\mathbf{q}') a_\gamma(\mathbf{q}'') - \text{H.c.}], \tag{4}$$

where H.c. denotes the Hermitian conjugate, $\Delta(\xi) \equiv \delta_{0\xi}$ is the Kronecker symbol and

$$2M^{\alpha\beta\gamma}(\mathbf{q}, \mathbf{q}', \mathbf{q}'') = L^{2\beta\gamma}(\mathbf{q}, \mathbf{q}', \mathbf{q}'') + L^{2\gamma\beta}(\mathbf{q}, \mathbf{q}', \mathbf{q}'') + L^{3\alpha\gamma}(\mathbf{q}, \mathbf{q}', \mathbf{q}'') + L^{3\gamma\alpha}(\mathbf{q}, \mathbf{q}', \mathbf{q}'') + L^{3\alpha\beta}(\mathbf{q}, \mathbf{q}', \mathbf{q}'') + L^{3\beta\alpha}(\mathbf{q}, \mathbf{q}', \mathbf{q}''), \tag{5}$$

$$L^{\alpha\beta\gamma}(\mathbf{q}, \mathbf{q}', \mathbf{q}'') = \frac{e_i^\alpha(\mathbf{q}) q_j + e_j^\alpha(\mathbf{q}) q_i}{4[\omega_\alpha(\mathbf{q}) \omega_\beta(\mathbf{q}') \omega_\gamma(\mathbf{q}'')]^{1/2}} [\lambda_{ijkl} e_m^\beta(\mathbf{q}') q_k' e_n^\gamma(\mathbf{q}'') q_l'' + 1/6 \kappa_{ijklmn} (e_k^\beta(\mathbf{q}') q_l' + e_l^\beta(\mathbf{q}') q_k') (e_m^\gamma(\mathbf{q}'') q_n'' + e_n^\gamma(\mathbf{q}'') q_m'')].$$

We note that the coefficients $M^{\alpha\beta\gamma}(\mathbf{q}, \mathbf{q}', \mathbf{q}'')$ are not altered by any permutation of their arguments.

In high-frequency sound propagation in the crystal, the field of deformations has a coherent (acoustical) component and an incoherent (thermal component). We take this fact into account by means of a transformation suggested by Tyablikov.^[5]

$$a_\lambda(\mathbf{q}) = b_\lambda(\mathbf{q}) + B_\lambda(\mathbf{q}), \quad a_\lambda^+(\mathbf{q}) = b_\lambda^+(\mathbf{q}) + B_\lambda^*(\mathbf{q}). \quad (7)$$

The operators $b_\lambda(\mathbf{q})$ and $b_\lambda^+(\mathbf{q})$ correspond to the field of thermal phonons and obey the usual Bose commutation relations. Furthermore,

$$\langle b_\lambda(\mathbf{q}) \rangle = \langle b_\lambda^+(\mathbf{q}) \rangle = 0, \quad (8)$$

where $\langle \xi \rangle = \text{Tr}(\xi \rho)$, ρ is the density matrix of the system. The amplitudes $B_\lambda(\mathbf{q})$ and $B_\lambda^*(\mathbf{q})$ are c-numbers and describe the coherent sound field, and

$$B_\lambda(\mathbf{q}) = \langle a_\lambda(\mathbf{q}) \rangle, \quad B_\lambda^*(\mathbf{q}) = \langle a_\lambda^+(\mathbf{q}) \rangle. \quad (9)$$

The Hamiltonian (4) does not contain a term corresponding to Umklapp processes; however, this is not essential for us. Actually, at low temperatures, the collisions of sound phonons with the thermal ones, which is accompanied by the Umklapp, take place much more rarely than the normal collisions. So far as U processes with the participation of thermal phonons only are concerned, the derivation of the corresponding collision integral in the kinetic equations does not have much intrinsic interest, inasmuch as it is entirely similar to the derivation of the collision term for N processes, which will be given below.

2. THE KINETIC EQUATION

For the description of the state of thermal phonons in a crystal, we use the Wigner distribution function:

$$n_\alpha(\mathbf{r}, \mathbf{q}) = \sum_{\mathbf{k}} e^{i\mathbf{k}\mathbf{r}} \left\langle b_\alpha^+ \left(\mathbf{q} - \frac{\mathbf{k}}{2} \right) b_\alpha \left(\mathbf{q} + \frac{\mathbf{k}}{2} \right) \right\rangle. \quad (10)$$

Using the equations of motion for single-particle density matrices (SDM) $\langle b_\alpha^+(\mathbf{q} - \mathbf{k}/2) b_\alpha(\mathbf{q} + \mathbf{k}/2) \rangle$, it is easy to obtain the first equation of the Bogolyubov chain:

$$\begin{aligned} \frac{\partial n_\alpha(\mathbf{r}, \mathbf{q})}{\partial t} + \frac{\partial \omega_\alpha(\mathbf{q})}{\partial \mathbf{q}} \frac{\partial n_\alpha(\mathbf{r}, \mathbf{q})}{\partial \mathbf{r}} &= \left(\frac{\hbar}{8V\rho^2} \right)^{1/2} \sum_{\mathbf{x}} e^{i\mathbf{x}\mathbf{r}} \\ &\times \sum_{\mathbf{p}, \mathbf{p}'} \left[M^{\alpha\beta\gamma} \left(\mathbf{q} - \frac{\mathbf{k}}{2}, \mathbf{q} - \mathbf{p} - \frac{\mathbf{k}}{2}, \mathbf{p} \right) \left\langle a_\gamma^+(\mathbf{p}) a_\beta^+ \left(\mathbf{q} - \mathbf{p} - \frac{\mathbf{k}}{2} \right) \right. \right. \\ &\quad \times b_\alpha \left(\mathbf{q} + \frac{\mathbf{k}}{2} \right) \rangle + M^{\alpha\beta\gamma} \left(\mathbf{q} + \frac{\mathbf{k}}{2}, \mathbf{q} - \mathbf{p} + \frac{\mathbf{k}}{2}, \mathbf{p} \right) \\ &\quad \times \left\langle b_\alpha^+ \left(\mathbf{q} - \frac{\mathbf{k}}{2} \right) a_\beta \left(\mathbf{q} - \mathbf{p} + \frac{\mathbf{k}}{2} \right) a_\gamma(\mathbf{p}) \right\rangle \\ &- 2M^{\alpha\beta\gamma} \left(\mathbf{q} - \frac{\mathbf{k}}{2}, \mathbf{p} - \mathbf{q} + \frac{\mathbf{k}}{2}, \mathbf{p} \right) \left\langle a_\gamma^+(\mathbf{p}) a_\beta \left(\mathbf{p} - \mathbf{q} + \frac{\mathbf{k}}{2} \right) b_\alpha \left(\mathbf{q} + \frac{\mathbf{k}}{2} \right) \right\rangle \\ &- 2M^{\alpha\beta\gamma} \left(\mathbf{q} + \frac{\mathbf{k}}{2}, \mathbf{p} - \mathbf{q} - \frac{\mathbf{k}}{2}, \mathbf{p} \right) \left\langle b_\alpha^+ \left(\mathbf{q} - \frac{\mathbf{k}}{2} \right) a_\beta^+ \left(\mathbf{p} - \mathbf{q} - \frac{\mathbf{k}}{2} \right) a_\gamma(\mathbf{p}) \right\rangle \right]. \end{aligned} \quad (11)$$

In writing (11), it has been taken into consideration that the average of the form $\langle a_\lambda^+(\mathbf{q}) b_\lambda^+(\mathbf{q}') \rangle$ can always be replaced by $\langle b_\lambda^+(\mathbf{q}) b_\lambda^+(\mathbf{q}') \rangle$, as follows from (7) and (8). For the derivation of the kinetic equation it is further necessary to express the average of the products of three Bose operators in (11) in terms of single-particle density matrices and the amplitude of the sound wave. This procedure is analogous to the calculations performed in the derivation of the kinetic equations for the electron-phonon system,^[6,7] and we shall not go into it in detail. We only note the following features. In splitting the Bogolyubov chains of equations to obtain the kinetic equation in the usual form, it is necessary to neglect averages of the type $\langle a_\lambda(\mathbf{q}) a_\lambda^+(\mathbf{q}') \rangle$ and $\langle a_\lambda^+(\mathbf{q}) a_\lambda^+(\mathbf{q}') \rangle$. As Zil'berman has shown,^[7] this can

be done only in the absence of a reflected sound wave in the crystal. The remaining averages can be represented in the form

$$\langle a_\lambda^+(\mathbf{q}) a_\lambda^+(\mathbf{q}') \rangle = \langle b_\lambda^+(\mathbf{q}) b_\lambda^+(\mathbf{q}') \rangle + B_\lambda^*(\mathbf{q}) B_\lambda(\mathbf{q}') \quad (12)$$

and similarly for $\langle a_\lambda(\mathbf{q}) a_\lambda^+(\mathbf{q}') \rangle$. We note that for $|\mathbf{q} - \mathbf{q}'| \lesssim d^{-1}$, where d is the characteristic dimension of the spatial inhomogeneity in the system, the elements of single-particle density matrices that are nondiagonal in the polarization index are quantities of higher order of smallness relative to the diagonal elements. Inasmuch as both the diagonal and the nondiagonal elements of the index are practically equal to zero in the case $|\mathbf{q} - \mathbf{q}'| > d^{-1}$, we can assume that

$$\begin{aligned} \langle b_\lambda^+(\mathbf{q}) b_\lambda^+(\mathbf{q}') \rangle &\approx \langle b_\lambda^+(\mathbf{q}) b_\lambda^+(\mathbf{q}') \rangle \delta_{\lambda\lambda'}, \\ \langle b_\lambda(\mathbf{q}) b_\lambda^+(\mathbf{q}') \rangle &\approx \langle b_\lambda(\mathbf{q}) b_\lambda^+(\mathbf{q}') \rangle \delta_{\lambda\lambda'}. \end{aligned} \quad (13)$$

These same relations are also valid for the average $\langle a_\lambda^+(\mathbf{q}) a_\lambda^+(\mathbf{q}') \rangle$ and $\langle a_\lambda(\mathbf{q}) a_\lambda^+(\mathbf{q}') \rangle$ since the amplitudes $B_\lambda(\mathbf{q})$ and $B_\lambda^*(\mathbf{q}')$ differ from zero only for $\lambda = \lambda' = \sigma$, where σ is the sound polarization index.

By following further the well known research of Bogolyubov and Gurov,^[8] we can immediately obtain the kinetic equation for $n_\alpha(\mathbf{r}, \mathbf{q})$. In the derivation, an assumption is made on the smallness of the mean wavelength of the thermal phonons in comparison with d and the fact that the width of the sound spectrum cannot be less than Γ is also used. Omitting the very cumbersome, but in fact elementary calculations, we obtain:

$$\begin{aligned} \frac{\partial n_\alpha(\mathbf{r}, \mathbf{q})}{\partial t} + \frac{\partial \omega_\alpha(\mathbf{q})}{\partial \mathbf{q}} \frac{\partial n_\alpha(\mathbf{r}, \mathbf{q})}{\partial \mathbf{r}} &= I_N + I_s; \quad (14) \\ I_s &= \frac{\pi\hbar}{V\rho^3} N(\mathbf{r}) \sum_{\beta} \{ [M^{\alpha\beta\sigma}(\mathbf{q}, \mathbf{s} - \mathbf{q}, \mathbf{s})]^2 \delta[\omega_\alpha(\mathbf{q}) + \omega_\beta(\mathbf{s} - \mathbf{q}) - \Omega] \\ &\times [n_\alpha(\mathbf{r}, \mathbf{q}) + n_\beta(\mathbf{r}, \mathbf{s} - \mathbf{q}) + 1] + [M^{\alpha\beta\sigma}(\mathbf{q}, \mathbf{q} + \mathbf{s}, \mathbf{s})]^2 \delta[\omega_\alpha(\mathbf{q}) + \Omega - \omega_\beta(\mathbf{q} + \mathbf{s})] \\ &\times [n_\beta(\mathbf{r}, \mathbf{q} + \mathbf{s}) - n_\alpha(\mathbf{r}, \mathbf{q})] + [M^{\alpha\beta\sigma}(\mathbf{q}, \mathbf{q} - \mathbf{s}, \mathbf{s})]^2 \\ &\times \delta[\omega_\alpha(\mathbf{q}) - \omega_\beta(\mathbf{q} - \mathbf{s}) - \Omega] [n_\beta(\mathbf{r}, \mathbf{q} - \mathbf{s}) - n_\alpha(\mathbf{r}, \mathbf{q})] \}, \end{aligned} \quad (15)$$

where I_N is the Peierls-Boltzmann collision integral,^[9] in which only N-processes are taken into account, \mathbf{s} and \mathbf{q} are the wave vectors of the acoustic and thermal phonons, respectively, and

$$N(\mathbf{r}) = \sum_{\mathbf{p}, \mathbf{k}} e^{i\mathbf{k}\mathbf{r}} B_\sigma^* \left(\mathbf{p} - \frac{\mathbf{k}}{2} \right) B_\sigma \left(\mathbf{p} + \frac{\mathbf{k}}{2} \right) \quad (16)$$

is the total number of acoustic phonons per unit volume.

3. THE CONSERVATION LAWS AND THE HYDRODYNAMIC EQUATIONS

We now add to the kinetic equation (14) the collision integral I_U , which describes the U-processes with participation of thermal phonons only. Then, multiplying (14) by $\hbar\mathbf{q}$ and summing the result over \mathbf{q} and α , we get

$$\begin{aligned} \frac{\partial \mathbf{P}}{\partial t} + \text{div} \hat{\Pi} &= \left(\frac{\partial \mathbf{P}}{\partial t} \right)_v + \left(\frac{\partial \mathbf{P}}{\partial t} \right)_s; \quad (17) \\ \mathbf{P} &= \sum_{\alpha, \mathbf{q}} \hbar \mathbf{q} n_\alpha(\mathbf{r}, \mathbf{q}), \quad \Pi_{ij} = \sum_{\alpha, \mathbf{q}} \hbar q_i \frac{\partial \omega_\alpha(\mathbf{q})}{\partial q_j} n_\alpha(\mathbf{r}, \mathbf{q}), \\ \left(\frac{\partial \mathbf{P}}{\partial t} \right)_v &= \sum_{\alpha, \mathbf{q}} \hbar \mathbf{q} I_v, \quad \left(\frac{\partial \mathbf{P}}{\partial t} \right)_s = \sum_{\alpha, \mathbf{q}} \hbar \mathbf{q} I_s. \end{aligned} \quad (18)$$

Here we have used the well-known property of the integral of normal collisions:

$$\sum_{\alpha\mathbf{q}} \mathbf{q} I_N = 0.$$

$$I_S \ll I_N. \quad (23)$$

The collision term $(\partial \mathbf{P} / \partial t)_S$, with account of the symmetry of the coefficients $M^{\alpha\beta\gamma}(\mathbf{q}, \mathbf{q}', \mathbf{q}'')$ relative to permutations of their arguments can be represented in the form

$$\begin{aligned} \left(\frac{\partial \mathbf{P}}{\partial t}\right)_S &= \hbar s N(\mathbf{r}) \frac{\pi \hbar}{V \rho^3} \sum_{\alpha\beta\mathbf{q}} \{ [M^{\alpha\beta\sigma}(\mathbf{q}, \mathbf{q}-\mathbf{s}, \mathbf{s})]^2 \delta[\omega_\alpha(\mathbf{q}) - \omega_\beta(\mathbf{q}-\mathbf{s}) - \Omega] \\ &\times [n_\beta(\mathbf{r}, \mathbf{q}-\mathbf{s}) - n_\alpha(\mathbf{r}, \mathbf{q})] + 1/2 [M^{\alpha\beta\sigma}(\mathbf{q}, \mathbf{s}-\mathbf{q}, \mathbf{s})]^2 \\ &\times \delta[\Omega - \omega_\alpha(\mathbf{q}) - \omega_\beta(\mathbf{s}-\mathbf{q})] [n_\alpha(\mathbf{r}, \mathbf{q}) + n_\beta(\mathbf{r}, \mathbf{s}-\mathbf{q}) + 1] \}. \end{aligned} \quad (19)$$

The product $\hbar s N(\mathbf{r})$ is the density of the quasimomentum of the sound wave \mathbf{P}_S and the remaining terms in (19) represent the absorption coefficient Γ multiplied by the sound velocity c , as is not difficult to establish. Finally, the law of conservation of the total quasimomentum of the phonon gas will have the form

$$\partial \mathbf{P} / \partial t + \text{div } \hat{\Pi} = (\partial \mathbf{P} / \partial t)_v + c \Gamma \mathbf{P}_S. \quad (20)$$

The energy conservation law for the phonon gas in the presence of heating of the phonons by sound can be obtained in the same way:

$$\partial E / \partial t + \text{div } \mathbf{Q} = c \Gamma E_S, \quad (21)$$

where

$$E = \sum_{\alpha\mathbf{q}} \hbar \omega_\alpha(\mathbf{q}) n_\alpha(\mathbf{r}, \mathbf{q}), \quad \mathbf{Q} = \sum_{\alpha\mathbf{q}} \hbar \omega_\alpha(\mathbf{q}) \frac{\partial \omega_\alpha(\mathbf{q})}{\partial \mathbf{q}} n_\alpha(\mathbf{r}, \mathbf{q}) \quad (22)$$

and E_S the energy density of the sound wave.

The conservation laws (20) and (21) are in fact the desired hydrodynamic equations that describe the motion of the phonon gas in the crystal in the hydrodynamic limit. In this case, the state of the phonon gas is a quasi-equilibrium one and can be completely characterized by the values of two hydrodynamic parameters—the drift velocity and the temperature. As is well known,^[10] in the absence of high-frequency sound, such a state is realized if the normal collisions of thermal phonons take place much more often than collisions with loss of quasimomentum, i.e., $I_N \gg T U$. In the case of interaction of thermal phonons with high-frequency sound, this condition is no longer sufficient, and it is necessary to add a limitation on the value of the collision integral I_S :

The inequality (23) essentially means that the rate of injection of quasimomentum and energy from the sound wave into the gas of thermal phonons should be much less than the rate of thermalization of the transferred energy and quasimomentum. It is clear that only upon satisfaction of the condition (23), together with the condition $I_N \gg I_S$, will the state of the phonon gas be practically in quasiequilibrium. Estimating I_N and I_S , we can show that the inequality (23) reduces to the following:

$$E_S I_N \Gamma \ll E \quad (24)$$

In conclusion, we note that by substituting the Bose-Einstein distribution with drift in (18) and (22), we can obtain the hydrodynamic equations from (20) and (21) for the drift velocity and the temperature, which we shall not write down here, for brevity. In the equations obtained in this fashion, however, viscous terms will be absent. These terms can easily be obtained if we take into account the finiteness of I_N ; they have the same form as in the case of absence of high-frequency sound.^[10,11]

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