

Review article

Heat pulse experiments revisited

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This is a review of heat propagation – theory and experiment – in dielectric solids at low temperatures where the phenomenon of second sound occurs. The review does not merely present a list of the various explanations of the observed phenomena. Rather it views them as special cases of a unified theory which is formulated within the framework of extended thermodynamics of phonos. Field equations are derived by averaging over the phonon-Boltzmann equation and initial and boundary value problems are solved. Thus it became possible to achieve a full explanation of the observations of the heat-pulse experiments in which ballistic phonons, second sound and ordinary heat conduction compete.

1 Introduction

Heat conduction processes in solid bodies at rest may be described by indicating the temperature T in all points of the body as a function of time. The field equation for T relies on the equation of balance of internal energy

$$\frac{\partial e}{\partial t} + \frac{\partial Q_k}{\partial x_k} = 0, \quad (1.1)$$

which has to be supplemented by constitutive equations for the density of energy e and for the heat flux Q_k which depend on the material.

At low temperatures the constitutive relation for the energy density reads

$$e = aT^4 \quad \text{with} \quad a = \text{constant}. \quad (1.2)$$

The constitutive law for the heat flux Q_k is usually assumed to be of the form

$$Q_k = -\kappa(T) \frac{\partial T}{\partial x_k}, \quad (1.3)$$

where κ is the heat conductivity.

Equation (1.3) is called Fourier's law and it leads to a parabolic differential equation for heat conduction, thus implying the paradox of heat conduction: Parts of an initially given local heat pulse will propagate with infinite speed through the body.

For practical purposes the paradox of heat conduction is of no concern, if those parts of a heat pulse that have infinite speed are strongly damped. This is the case in all materials at room temperature.

However, at low temperature damping may become unimportant and the predictions of the parabolic heat conduction equation become measurably false.

A modification of Fourier's law can be derived from a model originally introduced in 1929 by Peierls [1] for the calculation of the heat conductivity. Peierls describes the thermal properties of dielectric solids by the phonon model. As we shall explain in detail in Chapter 2 phonons form a gas of quasi-particles bearing energy and momentum.

Phonons may interact among themselves as well as with lattice imperfections and with boundaries of the crystal. There are two different types of interaction processes:

- i) Normal (N-)processes, where phonon momentum is conserved,
- ii) Resistive (R-)processes, that do not conserve phonon momentum.

Peierls realized that a Fourier heat conduction is due to R-processes and he was able to calculate the heat conductivity in dependence on temperature and on such crystal parameters as the number density of lattice defects.

In fact the heat conductivity is related to the frequency $\frac{1}{\tau_R}$ of R-processes by the equation

$$\kappa = \frac{c^2}{3} c_v \tau_R. \quad (1.4)$$

c is the Debye speed of phonons defined as some mean value of longitudinal and transversal speeds of sound. $c_v = \partial e / \partial T$ denotes the specific heat per unit volume.

A further study of the phonon model shows that Fourier's law (1.3) is not always sufficient for the description of heat conduction in crystals at low temperatures. It gives satisfactory results only for *diffusive processes*, i.e. when there are many more R-processes than N-processes. If, on the other hand, there are only few R-processes and many more N-processes, a wave-like energy transport may occur which is called *second sound*.

In the presence of second sound, Fourier's law must be replaced by the equation

$$\frac{\partial Q_i}{\partial t} + \frac{c^2}{3} c_v \frac{\partial T}{\partial x_i} = - \frac{1}{\tau_R} Q_i. \quad (1.5)$$

Equation (1.5) together with the equation of balance of internal energy forms a hyperbolic system instead of the parabolic equations that follow from Fourier's law. In 1948 Cattaneo [2] proposed a similar system in order to prevent the paradox of heat conduction.

For small values of τ_R , i.e. low heat conductivity (1.5) reduces to Fourier's law.

For large values of τ_R , i.e. high heat conductivity, however, the right hand side of (1.5) may be neglected. In that case (1.5) together with (1.1) and (1.2) provides a wave equation for a temperature disturbance $\tilde{T} = T(x, t) - T_0$ that propagates as second sound,

$$\frac{\partial^2 \tilde{T}}{\partial t^2} - \frac{c^2}{3} \frac{\partial^2 \tilde{T}}{\partial x_i \partial x_i} = 0. \quad (1.6)$$

This equation was first derived by Ward & Wilks in 1951 and it has stimulated experimental research to detect second sound ([3], [4], [5]).

In the beginning those attempts have not been successful, because in addition to second sound and diffusion there is a third mechanism for energy transport which is not included in Cattaneo's modification (1.5) of Fourier's law. This is the energy transport by *ballistic phonons*, i.e. phonons which travel through the crystal without any interaction.

Ballistic phonons may occur at very low temperatures in very pure crystals. Careful investigations, made by Guyer & Krumhansl [6], [7], [8] have lead to the conclusion, that Cattaneo's equation (1.5) must be supplemented by terms including the frequency of momentum conserving N-processes. Pure second sound only appears in very pure crystals and in a small temperature range, see Section 5.1 of this paper. After the studies of Guyer & Krumhansl second sound was detected in crystalline helium He_4 [9], sodium fluorid NaF [10], [11] and bismuth Bi [12].

During the last decade physicists have become interested in hyperbolic systems of partial differential equations for the description of thermodynamic processes, and they have replaced the traditional parabolic field equations of thermodynamics by hyperbolic ones. This approach is called "Extended Thermodynamics". It offers a systematic guideline to non-equilibrium thermodynamics, avoiding some shortcomings of classical irreversible thermodynamics ([13], [14]). Theories within extended thermodynamics usually contain Cattaneo-like equations, similar to (1.5), and since crystals are among the few materials where deviations from Fourier's law are apparent, the study of second sound in crystals has gained new interest.

Extended thermodynamics permits the treatment of non-linear phenomena in crystals, including shock waves or second sound moving into an already disturbed region. The proper description of such phenomena requires a re-examination of the theoretical foundation of heat transport in crystals. The present paper provides such a reexamination in the framework of extended thermodynamics based on the kinetic theory of phonons.

We start this discussion in Chapter 2 with the introduction of the phonon model and of the phonon Boltzmann equation.

Moments of the phase density may be interpreted as thermodynamic quantities for which equations of balance will be derived in Chapter 3.

The collision integrals are approximated by the relaxation time ansatz due to Callaway [15]. The closure problem will be solved by the principle of maximizing entropy ([16], [17]) which leads to a symmetric hyperbolic system of partial differential equations for an arbitrary number N of moments as thermodynamic variables.

In Chapter 4 we shall introduce a typical heat pulse experiment and use the phonon model to interpret the results. This forms the basis for a comparison of several thermodynamic theories in Chapters 5 & 6. We start in Chapter 5 with the hyperbolic system, derived in Chapter 3, and we shall demonstrate that it may serve as a good tool for the description of heat transport in crystals. In particular we shall answer the question of how many variables are needed for a sufficient description of a given experiment.

In Chapter 6 we shall compare thermodynamic theories of other authors with experimental results and with the hyperbolic system of Chapter 3. It will turn out that many of those theories are included here as special cases with a restricted range of applicability.

In the main part of this paper a simplified phonon model is used, describing only phonons that travel with the Debye speed. Actually, however, phonons may travel with the speeds of transversal and longitudinal sound waves. The proper description of heat transport would therefore be a mixture theory of phonons of three types – one longitudinal and two transversal. Such a theory is outlined in Appendix A.

The occurrence of moments of the phase density without a direct physical interpretation raises the question about how to choose their initial and boundary values. In Appendix B we shall introduce a simple approximation that yields a sufficient number of initial values for the simulation of a heat pulse experiment.

Notations

Throughout this paper the tensor index notation is used. A tensor \mathbf{A} of rank n is represented by its components $A_{i_1 \dots i_n}$.

We shall often use the traceless symmetric parts of a tensor \mathbf{A} which are denoted by $A_{\langle i_1 \dots i_n \rangle}$.

The following conditions hold

$$A_{\langle i_1 \dots k \dots l \dots i_n \rangle} = A_{\langle i_1 \dots l \dots k \dots i_n \rangle}$$

$$A_{\langle i_1 \dots k \dots k \dots i_n \rangle} = 0.$$

A traceless symmetric tensor $A_{\langle i_1 \dots i_n \rangle}$ has $2n + 1$ independent components. This holds also for $n = 0$, e.g. a scalar, and for $n = 1$, e.g. a vector.

2 The phonon model

2.1 The simple phonon model

Energy transport processes in dielectric solids can best be described and interpreted by using the phonon model that goes back to Einstein [18], Debye [19] and Peierls [1], [20]. The naive content of the model is shown in Fig. 2.1.

The crystal shown in the left figure is represented here by a simple cubic lattice. The atoms vibrate around their equilibrium positions with temperature dependent amplitudes. The supply of energy to some place will first change

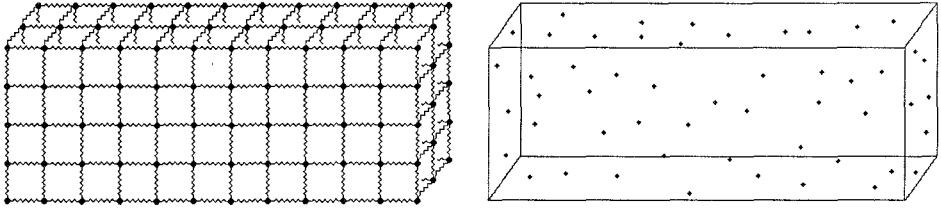


Fig. 2.1. Real crystal and phonon model.

the amplitudes of vibration at that place and then give rise to elastic waves which transport the energy through the crystal.

In the phonon model the actual crystal is replaced by a box, shown in the right figure, containing a gas of phonons. The phonons represent the eigen-vibrations of the atoms such that a vibration of frequency ω with the wave vector \mathbf{k} corresponds to a phonon of energy $\hbar\omega$ and momentum $\hbar\mathbf{k}$. Thus transport processes in crystals may be treated analogously to transport processes in gases. The feasibility of this proposition was proved by Peierls in the afore-mentioned papers.

Despite considerable analogies, there are also important differences between gases of phonons and gases of real particles. Therefore phonons are called quasi-particles. The most important differences are:

- i) Phonons may be created and annihilated. Their number density at some time t and or a given place \mathbf{x} is determined by the local temperature at that time and that place.
- ii) Energy is conserved in phonon interactions whereas generally momentum is not. For this reason phonon momentum is sometimes called quasi-momentum.

Within the phonon gas there are three mechanisms of energy transport, viz.

- i) Energy transport by ballistic phonons.
Phonons may travel through the crystal without any interaction and carry their energy along.
- ii) Energy transport by second sound.
If there is interaction and if the phonons conserve quasi-momentum, one obtains a wave like energy transport. This is similar to a sound wave in ordinary gases which is also transmitted by energy and momentum conserving collisions. Because of this similarity the process is called second sound.
- iii) Energy transport by diffusion.
In most cases phonon interactions do not conserve quasi-momentum. The wave like nature of the energy transport process is then damped after a very short time and there remains a diffusion process, analogous to ordinary heat conduction.

2.2 Extension of the simple phonon model

The concept of phonons originates from the theory of specific heat for dielectric solids. It is well-known that the vibrations of the atoms – assuming harmonic interatomic potentials – can be represented by their eigen-vibrations

or eigen-modes. If there are N atoms then there are $3N$ eigenmodes with frequencies $\omega_s (s = 1, 2, \dots, 3N)$. The possible energies of each eigenmode are given by

$$e_s = \left(n_s + \frac{1}{2} \right) \hbar \omega_s, \quad n_s = 0, 1, 2, 3, \dots \quad (2.1)$$

\hbar denotes Planck's constant and n_s is the number of energy quanta $\hbar \omega_s$ of eigenmode s . In the phonon picture we say that there are n_s phonons with the energy $\hbar \omega_s$. They behave like particles that obey Bose statistics.

This model suffices for the description of thermodynamic equilibrium properties like the specific heat of a crystal. However, the model is not sufficient for the description of non-equilibrium properties, which involve non-uniform fields and require the explicit localization of phonons in space. It was Peierls who made the necessary extension of the theory in 1929 [1].

Peierls considered traveling waves in the crystal using the eigenmode representation. He showed that waves with adjacent wave vectors in the range $[\mathbf{k}, \mathbf{k} + \Delta \mathbf{k}]$ may be combined to form wave packets localized within the space element $[\mathbf{x}, \mathbf{x} + \Delta \mathbf{x}]$, where $\Delta \mathbf{x}$ is determined by $|\Delta \mathbf{k}| \cdot |\Delta \mathbf{x}| = 2\pi$. Each of these wave packets consists of a certain number of phonons with energy $\hbar \omega(\mathbf{k})$.

The function $\omega(\mathbf{k})$ is called the dispersion relation. It follows from the equations of motion for the atoms of the crystal. It is known that wave packets move with the group-velocity $\partial \omega / \partial \mathbf{k}$ and so do the corresponding phonons.

In general $\omega(\mathbf{k})$ is an anisotropic function of the wave vector \mathbf{k} , depending of the crystal structure and on the interatomic interaction. Even for simple lattices, this function is hard to determine. Therefore a simple isotropic dispersion law is often used for explicit calculations, namely

$$\omega_\alpha(k) = c_\alpha k, \quad \alpha = l, t_1, t_2, \quad k = \sqrt{\mathbf{k} \cdot \mathbf{k}} \quad (2.2)$$

where α denotes the three different propagation modes with velocities c_α . There are one longitudinal mode l and two transversal modes t_1, t_2 .

For our purposes it is sufficient to deal with Debye's phonon model which takes into account only one representative mode. Thus we set

$$\omega = ck \quad (2.3)$$

where c is the Debye velocity defined as

$$\frac{3}{c^3} = \sum_{\alpha=1}^3 \frac{1}{c_\alpha^3}. \quad (2.4)$$

The extension to the more general case of three propagation modes will be outlined in Appendix A.

Starting from these considerations Peierls suggested that non-equilibrium properties of a crystal may be described in analogy to the kinetic theory of gases. The state space of phonons is spanned by the momentum $\hbar \mathbf{k}$ and the

position \mathbf{x} and the phase density

$$f(\mathbf{x}, t, \mathbf{k}) d\mathbf{x} d\mathbf{k} \quad (2.5)$$

gives the number of phonons in the vicinity of \mathbf{x} and \mathbf{k} at some time t .

Knowledge of f provides the energy density and its flux by integration, viz.

$$e(\mathbf{x}, t) := \int \hbar\omega f d\mathbf{k} \quad Q_k(\mathbf{x}, t) := \int \hbar\omega \frac{\partial\omega}{\partial k_k} f d\mathbf{k} \quad (2.6)$$

As long as the temperature is low enough for $e = aT^4$ to hold we may take the range of integration to be the whole \mathbf{k} space, see [21]. In a similar manner other thermodynamic quantities of interest can be defined. This will be done in Chapter 3 in a systematic manner.

The temporal development of the phase density f is determined by the phonon Boltzmann equation. In this paper we are only interested in thermal energy transport problems, and for this reason we restrict the attention to rigid bodies, in which case the phonon Boltzmann equations reads

$$\frac{\partial f}{\partial t} + \frac{\partial\omega}{\partial k_k} \frac{\partial f}{\partial x_k} = S(f). \quad (2.7)$$

The production density S includes interactions of phonons among themselves and with lattice imperfections as well as with the boundaries of the crystal.

Peierls [1], [20] showed that, if the atoms of the crystalline lattice interact linearly there is no phonon-phonon interaction at all, and the corresponding production density vanishes. But a non-harmonic cubic term in the interatomic potential implies a production density due to three-phonon interactions: Either one phonon decays into two or two phonons combine to become one. Energy is conserved so that we have

$$\hbar\omega' + \hbar\omega'' = \hbar\omega''' \quad \text{and} \quad \hbar\omega' = \hbar\omega'' + \hbar\omega'''. \quad (2.8)$$

Peierls showed, that there are similar relations for the momenta of the interacting phonons, viz.

$$\hbar\mathbf{k}' + \hbar\mathbf{k}'' = \hbar\mathbf{k}''' + \hbar\mathbf{G} \quad \text{and} \quad \hbar\mathbf{k}' = \hbar\mathbf{k}'' + \hbar\mathbf{k}''' + \hbar\mathbf{G}, \quad (2.9)$$

respectively. Thus momenta are not conserved unless \mathbf{G} equals zero. If it does, we speak of normal phonon scattering or N-processes. The processes with $\mathbf{G} \neq 0$ are called Umklapp processes or U-processes.

The interactions of phonons with lattice imperfections – i.e. dislocations and impurities – and boundaries do not conserve phonon momentum either although both conserve energy*.

Processes where phonon momentum is not conserved are comprehensively called resistive processes or R-processes.

Guided by these considerations we shall formulate the relaxation time approximation of the production density S which was introduced by Callaway [15], see Section 3.4.

* For more details see the excellent textbook “Physics of Phonons” by Reisland [22]

3 Thermodynamics

3.1 General scheme

3.1.1 Variables, equations of balance

The thermodynamic description of transport processes relies on the phonon Boltzmann equation (2.7). We start with the assumption, that a few macroscopic densities

$$u_A(\mathbf{x}, t) = \int \Psi_A(\mathbf{k}) f(\mathbf{x}, t, \mathbf{k}) d\mathbf{k} \quad (A = 1, 2, \dots, N) \quad (3.1)$$

are sufficient to describe the thermodynamic state of a crystal satisfactorily. The number of the densities u_A , viz. the value of N must be determined so as to provide a theory appropriate for the description of experimental results. The determination of N needed for the understanding of the heat-pulse experiment is one of the objectives of this paper.

We choose N densities u_A as thermodynamic variables and proceed by having N arbitrary at first. Thus we obtain a hierarchy of equations of balance for the variables u_A which results from the phonon Boltzmann equation after multiplication by Ψ_A and integration over the \mathbf{k} -space. The generic form of these equations of balance is given by

$$\frac{\partial u_A}{\partial t} + \frac{\partial f_{Ak}}{\partial x_k} = P_A \quad (A = 1, 2, \dots, N). \quad (3.2)$$

The fluxes f_{Ak} and the productions P_A are defined as

$$f_{Ak} = \int \Psi_A \frac{\partial \omega}{\partial k_k} f d\mathbf{k}, \quad P_A = \int \Psi_A S(f) d\mathbf{k}. \quad (3.3)$$

In order to obtain field equations for the variables u_A from the equations of balance (3.2) we have to relate the fluxes and the productions to the variables u_A . Such relations are called constitutive equations. A characteristic property of extended thermodynamics is a system of partial differential equations of first order as field equations. Therefore the constitutive equations for f_{Ak} and P_A are assumed to be of the form

$$f_{Ak} = \tilde{f}_{Ak}(u_B), \quad P_A = \tilde{P}_A(u_B). \quad (3.4)$$

It is important to note that there are no gradients nor rates in the constitutive equations.

A solution of the system of field equations (3.2) and (3.4) for a given initial and boundary value problem is called a thermodynamic process.

If there is no satisfactory agreement between the theory with a given N and experiment we increase the number of variables. This procedure differs from the more common alternative one, in which gradients of u_A are added to the list of variables.

An important task of thermodynamics is the determination of the constitutive functions \tilde{f}_{Ak} and \tilde{P}_A . In principle there are two ways to proceed – phenomenological extended thermodynamics [13] – phonon thermodynamics.

Both are equivalent. We shall describe both methods and start with a brief description of the phenomenological theory.

3.1.2 Constitutive theory, part I: Phenomenological extended thermodynamics

The phenomenological constitutive theory relies on the entropy principle which may be summarized in three parts.

i) The solutions of the field equations (3.2), (3.4) are such that they also satisfy the additional balance law

$$\frac{\partial h}{\partial t} + \frac{\partial \varphi_k}{\partial x_k} = \sigma, \quad (3.5)$$

h is the entropy density, φ_k the entropy flux and σ the entropy production.

ii) h , φ_k and σ are given by constitutive functions that depend only on the variables. Thus we have

$$h = \tilde{h}(u_A), \quad \varphi_k = \tilde{\varphi}_k(u_A), \quad \sigma = \tilde{\sigma}(u_A). \quad (3.6)$$

iii) The entropy density is required to be a maximum in equilibrium, which is defined as a process without any productions. In non-equilibrium the entropy production has to be positive.

$$\frac{\partial^2 h}{\partial u_A \partial u_B} - \text{negative definite}, \quad \sigma \geq 0. \quad (3.7)$$

The evaluation of the entropy principle leads to the conclusions, see [17] for details.

$$u_A = - \frac{\partial h'}{\partial \Lambda_A}, \quad f_{Ak} = - \frac{\partial \varphi'_k}{\partial \Lambda_A}, \quad \sigma = \sum_{A=1}^N \Lambda_A P_A \geq 0, \quad (3.8)$$

where the potentials h' , φ'_k for u_A and f_{Ak} are defined as

$$h' = h - \sum_{A=1}^N \Lambda_A u_A, \quad \varphi'_k = \varphi_k - \sum_{A=1}^N \Lambda_A f_{Ak}. \quad (3.9)$$

The newly introduced quantities Λ_A are called Lagrange multipliers; they may depend on u_A and it is appropriate to use them as variables, instead u_A .

The equations (3.8)_{1,2} imply integrability conditions of the form

$$\frac{\partial u_A}{\partial \Lambda_B} = \frac{\partial u_B}{\partial \Lambda_A}, \quad \frac{\partial f_{Ak}}{\partial \Lambda_B} = \frac{\partial f_{Bk}}{\partial \Lambda_A}. \quad (3.10)$$

The equations (3.10)₁ may serve to eliminate the Lagrange multipliers. The invertibility of the transformation $u_A \leftrightarrow \Lambda_A$ is guaranteed by (3.7)₁ which implies $\frac{\partial u_A}{\partial \Lambda_B}$ – negative definite.

The equations (3.10)₂ are restrictions on the fluxes. Such restrictions are the proper objective of extended thermodynamics. The productions P_A are restricted by (3.8)₃, which however, yields only some inequalities.

We conclude this survey of phenomenological extended thermodynamics with the remark, that if the constitutive functions are determined accordingly, the resulting field equations form a symmetric hyperbolic system. This is a desirable property because it guarantees finite speeds of disturbances and well-posedness for Cauchy problems.

3.1.3 Constitutive theory, part II: Phonon extended thermodynamics and the entropy maximum principle

In the following sections we shall derive the explicit forms of the constitutive equations

$$f_{AK} = \tilde{f}_{AK}(u_B), \quad P_A = \tilde{P}_A(u_B). \quad (3.11)$$

In phenomenological extended thermodynamics we have just seen how these functions are restricted by the *entropy principle*. Now our calculation of the functions (3.15) relies on the knowledge that f_{Ak} and P_A are represented by the integrals

$$f_{Ak} = \int \Psi_A \frac{\partial \omega}{\partial k_k} f d\mathbf{k}, \quad P_A = \int \Psi_A S(f) d\mathbf{k}. \quad (3.12)$$

In order to obtain from (3.12) functions of the form (3.11) we need to know the phase density in the special form

$$f(\mathbf{x}, t, \mathbf{k}) = \tilde{f}(u_A(\mathbf{x}, t), \mathbf{k}), \quad (3.13)$$

which we will derive from the *entropy maximum principle* [16]. Furthermore we shall prove, that this procedure of maximizing entropy leads to the same results as those of phenomenological extended thermodynamics.

We have already mentioned that the phonons are Bose particles. For such particles the entropy density h is defined as

$$h = -k_B \int \left(f \ln \frac{1}{y} f - y \left(1 + \frac{1}{y} f \right) \ln \left(1 + \frac{1}{y} f \right) \right) d\mathbf{k}, \quad (3.14)$$

where Boltzmann's constant is denoted by k_B and $y = 3/8 \pi^3$.

Forming $\partial h / \partial t$ and eliminating $\partial f / \partial t$ by the phonon Boltzmann equation we are led to

$$\frac{\partial h}{\partial t} + \frac{\partial \varphi_k}{\partial x_k} = \sigma, \quad (3.15)$$

a relation which is *derived* here, while in phenomenological thermodynamics it was *postulated*. This procedure permits the identification of the entropy flux and the entropy production as

$$\begin{aligned}\varphi_k &= -k_B \int \frac{\partial \omega}{\partial k_k} \left(f \ln \frac{1}{y} f - y \left(1 + \frac{1}{y} f \right) \ln \left(1 + \frac{1}{y} f \right) \right) d\mathbf{k} \\ \sigma &= k_B \int \left(\ln \left(1 + \frac{1}{y} f \right) - \ln \frac{1}{y} f \right) S(f) d\mathbf{k}\end{aligned}\quad (3.16)$$

The entropy maximum principle states: The phase density $\tilde{f}(u_A(\mathbf{x}, t), \mathbf{k})$ follows by maximizing the entropy density (3.14) with respect to f under the constraint of prescribed values of the variables u_A according to (3.1). We take care of the constraints by introducing Lagrange multipliers Λ_A and obtain by evaluation of the isoperimetric problem

$$f_N = f(u_1, u_2 \dots u_N, \mathbf{k}) = \frac{y}{\exp \Sigma - 1} \quad \text{with } \Sigma = \frac{1}{k_B} \sum_{A=1}^N \Psi_A \Lambda_A. \quad (3.17)$$

as *the* phase density that maximizes the entropy. Next we evaluate the integrals

$$u_A = \int \Psi_A f d\mathbf{k} \quad f_{Ak} = \int \Psi_A \frac{\partial \omega}{\partial k_k} f d\mathbf{k} \quad (3.18)$$

using the special form (3.17) of the phase density. After we have carried out the integrations we use (3.18)₁ to calculate the Lagrange multipliers as functions of the variables. These functions serve to eliminate the Λ_A 's in (3.18)₂. Thus we obtain the desired constitutive functions $f_{Ak} = \tilde{f}_{Ak}(u_B)$.

Although it is difficult to obtain explicit forms it is an easy matter to prove that the phase density (3.17) implies the results of the entropy principle of extended thermodynamics. Indeed, we form $\partial u_A / \partial \Lambda_B$ and $\partial f_{Ak} / \partial \Lambda_B$ and obtain

$$\frac{\partial u_A}{\partial \Lambda_B} = - \frac{1}{k_B} \int \Psi_A \Psi_B \frac{y \exp \Sigma}{(\exp \Sigma - 1)^2} d\mathbf{k} \quad (3.19)$$

$$\frac{\partial f_{Ak}}{\partial \Lambda_B} = - \frac{1}{k_B} \int \frac{\partial \omega}{\partial k_k} \Psi_A \Psi_B \frac{y \Sigma}{(\exp \Sigma - 1)^2} d\mathbf{k}. \quad (3.20)$$

Inspection shows that $\frac{\partial u_A}{\partial \Lambda_B}$ and $\frac{\partial f_{Ak}}{\partial \Lambda_B}$ are symmetric in A and B and that $\frac{\partial u_A}{\partial \Lambda_B}$ is negative definite.

Furthermore we conclude from (3.19) and (3.20) that there exist potentials for u_A and f_{Ak} . Calculation shows that these potentials are given by h' and φ'_k defined as in phenomenological extended thermodynamics, see (3.9).

In Section 3 we shall discuss the form of the production densities implied by the entropy maximum principle.

It will turn out that they are in accordance with the entropy principle of phenomenological thermodynamics.

3.2 Specific forms of balance equations

3.2.1 The 9 moment theory

We proceed with the interpretation of the variables u_A which we shall use in the following. Since we are interested in energy transport processes we start the hierarchy of equations (3.2) with the balance of energy. Therefore our first variable u_1 should be the energy density and the first flux f_{1k} the energy flux, viz.

$$u_1 = e = \int \hbar \omega f \, d\mathbf{k} = c\hbar \int k f \, d\mathbf{k}. \quad (3.21)$$

$$f_{1k} = Q_k = \int \hbar \omega \frac{\partial \omega}{\partial k_k} f \, d\mathbf{k} = c^2 \int \hbar k_k f \, d\mathbf{k}.$$

The last integral is the momentum density of phonons. The hierarchy proceeds with the balance of momentum. We define

$$u_{2,3,4} = p_i = \hbar \int k_i f \, d\mathbf{k} \quad \text{and} \quad (3.22)$$

$$f_{2,3,4,k} = N_{ik} = \hbar c \int \frac{1}{k} k_i k_k f \, d\mathbf{k}.$$

It will prove to be convenient to decompose the momentum flux N_{ik} into an isotropic part, which is related to the energy density and a deviatoric part according to the equation

$$N_{ik} = \frac{e}{3} \delta_{ik} + N_{\langle ik \rangle}. \quad (3.23)$$

If we were to stop here – with the thermodynamic state being given by the four variables e and p_i – ballistic energy transport would not be included at all. Moreover only a few aspects of second sound could be described. We shall discuss this in detail in Chapter 5.

Therefore we continue and consider the deviatoric part of the momentum flux $N_{\langle ij \rangle}$ as the next variable. Thus the next density and its flux are given by

$$u_5, \dots, 9 = N_{\langle ij \rangle} = c\hbar \int \frac{1}{k} k_i k_j f \, d\mathbf{k} \quad (3.24)$$

$$f_{5, \dots, 9, k} = M_{\langle ij \rangle k} = c^2 \hbar \int \frac{1}{k^2} k_i k_j k_k f \, d\mathbf{k}.$$

If we stop now, the situation will turn out as follows: The balance equations read

$$\begin{aligned} \frac{\partial e}{\partial t} + c^2 \frac{\partial p_k}{\partial x_k} &= 0 \\ \frac{\partial p_i}{\partial t} + \frac{1}{3} \frac{\partial e}{\partial x_i} + \frac{\partial N_{\langle ik \rangle}}{\partial x_k} &= P_i \\ \frac{\partial N_{\langle ij \rangle}}{\partial t} + \frac{\partial M_{\langle ij \rangle k}}{\partial x_k} &= P_{\langle ij \rangle}. \end{aligned} \quad (3.25)$$

The vanishing production in (3.25)₁ represents conservation of energy.

The description of diffusion and second sound by the system of equations is in almost perfect qualitative agreement with experiments, in particular the important properties of ballistic energy transport are included. However, there is no quantitative agreement. Therefore we cannot stop here.

3.2.2 The generic equation of balance

We set up the generic equation in our hierarchy by choosing

$$\Psi_A = \left\{ \dots, \hbar \left(\frac{c}{k} \right)^{n-1} k_{\langle i_1} k_{i_2} \dots k_{i_n \rangle}, \dots \right\}^* \quad (3.26)$$

The generic term $\hbar \left(\frac{c}{k} \right)^{n-1} k_{\langle i_1}, k_{i_2} \dots k_{i_n \rangle}$ in this list corresponds to a density and flux as follows

$$u_{\langle i_1 \dots i_n \rangle} = \hbar \int \left(\frac{c}{k} \right)^{n-1} k_{\langle i_1} \dots k_{i_n \rangle} f \, d\mathbf{k},$$

$$f_{\langle i_1 \dots i_n \rangle k} = \hbar \int \left(\frac{c}{k} \right)^n k_{\langle i_1} \dots k_{i_n \rangle} k_k f \, d\mathbf{k}. \quad (3.27)$$

The structure of the flux is such that it reduces to the densities $u_{\langle i_1 \dots i_{n-1} \rangle}$ and $u_{\langle i_1 \dots i_n k \rangle}$ by the recurrence formula

$$f_{\langle i_1 \dots i_n \rangle k} = c^2 \frac{n}{2n+1} u_{\langle i_1 \dots i_{n-1} \rangle} \delta_{i_n \rangle k} + u_{\langle i_1 \dots i_n k \rangle} \quad (3.28)$$

The equation of balance corresponding to (3.27) reads

$$\frac{\partial u_{\langle i_1 \dots i_n \rangle}}{\partial t} + c^2 \frac{n}{2n+1} \frac{\partial u_{\langle i_1 \dots i_{n-1} \rangle}}{\partial x_{i_n \rangle}} + \frac{\partial u_{\langle i_1 \dots i_n k \rangle}}{\partial x_k} = P_{\langle i_1 \dots i_n \rangle},$$

$$n = 0, 1, 2, \dots, M. \quad (3.29)$$

Here M denotes the number of indices in the highest tensor variable. The total number of variables, N , is then given by

$$N \sum_{n=0}^M (2n+1) = (M+1)^2. \quad (3.30)$$

The first 9 equations for $n = 0, 1, 2$ in this set are those of equation (3.25).

Neither the system (3.25) nor the generic system (3.29) is closed. Indeed in (3.25) the last equation of the system contains $M_{\langle ij \rangle k}$, which is not among the variables $e, p_k, N_{\langle ij \rangle}$. Generally in (3.29) it is $u_{\langle i_1 \dots i_M k \rangle}$ in the last equation which is unrelated a priori to the variables $u_{\langle i_1 \dots i_n \rangle}$, $n = 0, 1, \dots, M$. The same is true for all productions.

* This choice of variables follows from the use of the Debye model ($\omega = ck$). The general case is discussed by Larecki & Piekarski [23].

This fact makes it necessary to discuss specific procedures of closure and constitutive equations.

3.3 Specific form of constitutive equations

3.3.1 Equilibrium, definition of temperature

In phenomenological extended thermodynamics equilibrium is defined as a process with vanishing productions. This is equivalent to the statement that the phase density must be an isotropic function of the wave vector \mathbf{k} in equilibrium. It follows from (3.17) with Ψ_A given by (3.26) that the equilibrium phase density assumes the form

$$f_{|E} = \frac{y}{\exp\left(\frac{1}{k_B} \mathcal{A}_{1|E} \hbar c k\right) - 1}. \quad (3.31)$$

Since this should be the well-known Bose distribution, the equilibrium value of the Lagrange multiplier \mathcal{A}_1 is equal to the inverse of the absolute temperature T , and the remaining Lagrange multipliers $\mathcal{A}_2, \dots, \mathcal{A}_N$ vanish in equilibrium.

By insertion of the Bose phase density (3.31) into the integrals (3.1), (3.3)₁ which define the variables and fluxes we obtain in equilibrium

$$u_1 = e = \frac{4}{5} \frac{\pi^5 k_B^4}{c^3 \hbar^3} T^4. \quad (3.32)$$

All other densities and all fluxes vanish in this case.

Equation (3.32) is the Debye law for phonons, and we consider this as the defining equation for temperature, even in non-equilibrium. In other words temperature means energy density of phonons.

3.3.2 Phase density near equilibrium

For the calculation of the constitutive relations we use an approximate form of the phase density. Since all Lagrange multipliers with the exception of

$\mathcal{A}_1 = \frac{1}{T}$ vanish in equilibrium we set

$$\mathcal{A}_A = \frac{1}{T} \delta_{A1} + \lambda_A \quad \text{with} \quad \lambda_{A|E} = 0. \quad (3.33)$$

Linearising f in (3.17) in the λ 's we obtain

$$f = f_{|E} - \frac{T^2}{\hbar c} \sum_{A=1}^N \lambda_A \frac{\partial f_{|E}}{\partial T} \left(\frac{1}{k} \psi_A \right). \quad (3.34)$$

With our choice of ψ_A in (3.26) we obtain from (3.1) for λ_A

$$\lambda = 0$$

$$\lambda_{\langle i_1 \dots i_n \rangle} = \frac{\prod_{j=1}^n (2j+1)}{-4eTc^{2n-4}n!} u_{\langle i_1 \dots i_n \rangle}, \quad (n = 1, 2, \dots, M). \quad (3.35)$$

We recall that closure of the system (3.29) requires the determination of $u_{\langle i_1 \dots i_{M+1} \rangle}$. With the present form (3.34) for f we obtain

$$u_{\langle i_1 \dots i_{M+1} \rangle} = \hbar c \int \frac{1}{k_M} k_{\langle i_1 \dots i_{M+1} \rangle} f dk = 0. \quad (3.36)$$

3.3.2 Linear representation of productions

For the calculation of the productions (3.3)₂

$$P_A = \int \Psi_A S(f) d\mathbf{k} \quad (3.37)$$

we need to know the explicit form of the collision function S , which has been derived for various interaction mechanisms by several authors (see e.g. [1], [20], [22], [24]). However, due to the complexity of S nobody has used the exact representations in theories concerning instationary heat conduction processes. Instead most authors have used an expression for S which is based on relaxation time arguments originally introduced by Callaway in 1958 [15]. The correspondence between Callaway's expression and the exact collision function is discussed by Simons in [25]. Before we motivate the relaxation time ansatz we remind the reader that two different interaction mechanisms contribute to the collision function. Phonons may interact in N-processes and R-processes. While both types of processes conserve energy, only the former conserves momentum as well. The corresponding collision functions are denoted by S_N and S_R and we write

$$S = S_N + S_R. \quad (3.38)$$

S_N and S_R , respectively, must satisfy

$$\int \hbar\omega S_R d\mathbf{k} = 0, \quad \int \hbar\omega S_N d\mathbf{k} = 0, \quad \int \hbar k_i S_N d\mathbf{k} = 0 \quad (3.39)$$

while $\int \hbar k_i S_R d\mathbf{k}$ may not be zero.

We shall now motivate the explicit forms of S_N and S_R . We start with S_N and consider a small volume element of the crystal that is characterized by N variables e, p_i, u_A ($A = 5, \dots, N$). Due to normal processes, which conserve energy and momentum, the state e, p_i, u_A will relax as

$$e, p_i, u_A (A = 5, \dots, N) \xrightarrow{\text{N-processes}} e, p_i, 0. \quad (3.40)$$

In phase space the state on the left hand side is described by the phase density $f_N = f(e, p_i, u_A (A = 5, \dots, N), \mathbf{k})$ while the right hand side is described by $f_4 = f(e, p_i, 0, \mathbf{k})$.

Thus we may write

$$S_N = - \frac{1}{\tau_N(k)} (f - f_4), \quad (3.41)$$

where $1/\tau_N$ is the collision frequency for normal processes of phonons with wave vector \mathbf{k} . $\tau_N(k)$ is called the relaxation time for N-processes.

Due to resistive processes that do not conserve momentum the state e, p_i, u_A ($A = 5, \dots, N$) will relax as

$$e, p_i, u_A \quad (A = 5, \dots, N) \xrightarrow{\text{R-processes}} e, 0, 0. \quad (3.42)$$

In phase space the right hand side is described by the phase density $f_1 = f(e, 0, 0, \mathbf{k})$.

Thus we may write

$$S_R = - \frac{1}{\tau_R(k)} (f - f_1) \quad (3.43)$$

where $\frac{1}{\tau_R(k)}$ is the collision frequency for resistive processes of phonons with wave vector \mathbf{k} and τ_R is the relaxation time for R-processes.

We read off the functions f_4 and f_1 from (3.17) and obtain

$$f_4 = \frac{y}{\exp\left(\frac{\hbar c}{k_B} A_1^{(4)} k + \frac{\hbar}{k_B} A_i^{(4)} k_i\right) - 1}, \quad f_1 = \frac{y}{\exp\left(\frac{\hbar c}{k_B} A_1^{(1)} k\right) - 1}. \quad (3.44)$$

The Lagrange multipliers $A_1^{(4)}$, $A_i^{(4)}$ and $A_1^{(1)}$ must be determined so that the conservation laws are satisfied.

The collision frequencies τ_R and τ_N are functions of temperature T and of the wave vector \mathbf{k} . These functions may be calculated from the properties of the crystal [24], [26–29].

For our purposes it is sufficient to consider τ_R and τ_N as mean relaxation times which depend on the temperature only. Their temperature dependence is obtained from experimental results: τ_R follows from heat-conductivity measurements and τ_N from heat pulse experiments.

Therefore the productions may be written as

$$\begin{aligned} P_{\langle i_1 \dots i_n \rangle} &= - \frac{1}{\tau_R} \int \Psi_{\langle i_1 \dots i_n \rangle} (f - f_1) d\mathbf{k} - \frac{1}{\tau_N} \int \Psi_{\langle i_1 \dots i_n \rangle} (f - f_4) d\mathbf{k}, \\ P_{\langle i_1 \dots i_n \rangle} &= - \frac{1}{\tau_R} (u_{\langle i_1 \dots i_n \rangle} - \int \Psi_{\langle i_1 \dots i_n \rangle} f_1 d\mathbf{k}) - \frac{1}{\tau_N} (u_{\langle i_1 \dots i_n \rangle} - \int \Psi_{\langle i_1 \dots i_n \rangle} f_4 d\mathbf{k}) \\ & \quad n = 0, 1, \dots, M \quad (3.45) \end{aligned}$$

Because of the isotropy of f_1 the integrals $\int \Psi_{\langle i_1 \dots i_n \rangle} f_1 d\mathbf{k}$ vanish for all Ψ 's except when $n = 0$; in that case, by (3.39)₁, we have

$$e = \int \hbar c k f_1 d\mathbf{k}. \quad (3.46)$$

With the definition of temperature (3.32) we conclude from (3.44) that $\Lambda_1^{(1)} = 1/T$ holds, which implies the identity of f_1 with the equilibrium phase density f_E .

The conservation laws (3.39)_{2,3} for N-processes now read

$$e = \int \hbar c k f_4 d\mathbf{k}, \quad p_i = \int \hbar k_i f_4 d\mathbf{k}, \quad (3.47)$$

and therefore the Lagrange multipliers in f_4 are functions of the energy density and the momentum density

$$\Lambda_1^{(4)} = \Lambda_1^{(4)}(e, p_i), \quad \Lambda_i^{(4)} = \Lambda_i^{(4)}(e, p_i). \quad (3.48)$$

Because of the representation theorems of isotropic functions we must then have

$$\int \Psi_{\langle i_1 \dots i_n \rangle} f_4 d\mathbf{k} = A_n(e, p^2) P_{\langle i_1 \dots i_n \rangle} \quad n = 2, \dots, M. \quad (3.49)$$

These contributions to the production densities (3.45) are non-linear in the momentum density and will be neglected in the present linear theory.

In summary we obtain for the productions

$$P = 0; \quad P_i = -\frac{1}{\tau_R} p_i; \quad P_{\langle i_1 \dots i_n \rangle} = -\frac{1}{\tau} u_{\langle i_1 \dots i_n \rangle}, \quad n = 2, \dots, M, \quad (3.50)$$

where we have introduced the total collision frequency

$$\frac{1}{\tau} = \frac{1}{\tau_R} + \frac{1}{\tau_N}. \quad (3.51)$$

We close this section with the proof that Callaway's expression (3.38) with S_N, S_R given by (3.41) and (3.43) leads to a non-negative entropy production in accordance with phenomenological thermodynamics. We prove this statement starting with the representation (3.16)₂ for the entropy production, viz.

$$\sigma = k_B \int \left(\ln \left(1 + \frac{1}{y} f \right) - \ln \frac{1}{y} f \right) S d\mathbf{k}. \quad (3.52)$$

Introducing f from (3.17) into (3.52) we obtain for the bracket in the integrand the expression $\frac{1}{k_B} \Psi_A \Lambda_A$. Therefore, by (3.37), we have $\sigma = \sum_A \Lambda_A P_A$ just like in the phenomenological theory. The inequality $\sigma \geq 0$ may be proved explicitly by insertion of

$$S = S_N + S_R = -\frac{1}{\tau_N} (f - f_4) - \frac{1}{\tau_R} (f - f_1) \quad (3.53)$$

into (3.52). Thus we obtain two contributions to σ called σ_N and σ_R , one due to N-processes and the other one due to R-processes. Both are positive. Indeed we have

$$\sigma_N = k_B \int \frac{f - f_4}{\tau_N} \left(\ln \frac{1}{y} f - \ln \left(1 + \frac{1}{y} f \right) \right) d\mathbf{k}. \quad (3.54)$$

By use of the conservation properties (3.39) this expression may be rearranged to give

$$\sigma_N = k_B \int \frac{f - f_4}{\tau_N} \ln \frac{f - \frac{1}{y} f f_4}{f_4 - \frac{1}{y} f f_4} d\mathbf{k}. \quad (3.55)$$

This is non-negative because inspection shows that the integrand is non-negative; it vanishes for $f = f_4$. An identical calculation leads to $\sigma_R \geq 0$.

3.3.3 Summary of field equations

We summarize the field equations by introducing the productions (3.50) into the equations of balance (3.25) and (3.29). Thus we obtain for the case of 9 fields, i.e. $M = 2$,

$$\begin{aligned} \frac{\partial e}{\partial t} + c^2 \frac{\partial p_k}{\partial x_k} &= 0 \\ \frac{\partial p_i}{\partial t} + \frac{1}{3} \frac{\partial e}{\partial x_i} + \frac{\partial N_{\langle ik \rangle}}{\partial x_k} &= -\frac{1}{\tau_R} p_i \\ \frac{\partial N_{\langle ij \rangle}}{\partial t} + \frac{2}{5} c^2 \frac{\partial p_{\langle i}}{\partial x_{j \rangle}} &= -\frac{1}{\tau} N_{\langle ij \rangle} \end{aligned} \quad (3.56)$$

and for the case of a generic number of fields

$$\frac{\partial u_{\langle i_1 \dots i_n \rangle}}{\partial t} + c^2 \frac{n}{2n+1} \frac{\partial u_{\langle i_1 \dots i_{n-1} \rangle}}{\partial x_{i_n}} + \frac{\partial u_{\langle i_1 \dots i_n k \rangle}}{\partial x_k} = \begin{cases} 0 & \text{for } n = 0 \\ -\frac{1}{\tau_R} p_i & \text{for } n = 1 \\ -\frac{1}{\tau} u_{\langle i_1 \dots i_n \rangle} & \text{for } 1 < n \leq M. \end{cases} \quad (3.57)$$

An important special case of these field equations concerns *one dimensional* heat conduction processes. In that case the equations may be expressed in the form

$$\frac{\partial u_A}{\partial t} + \sum_{B=0}^M \mathbb{C}_{AB} \frac{\partial u_B}{\partial x} = -\frac{1}{\tau_A} u_A, \quad A = 0, 1, \dots, M \quad (3.58)$$

where

$$u_A = \left(\frac{e}{c^2}, p_1, N_{\langle 11 \rangle}, u_{\langle 111 \rangle} \dots \right) \quad \text{and} \quad \frac{1}{\tau_A} = \left(0, \frac{1}{\tau_R}, \frac{1}{\tau}, \frac{1}{\tau} \dots \right). \quad (3.59)$$

out proportional to T^3 and an exponentially descending branch for large temperature. In between the curve reaches a maximum, whose height goes up with increasing purity of the crystal.

The relation between τ_R and κ makes use of the momentum balance appropriate to the stationary case, viz., by (3.56)₂

$$p_i = -\frac{\tau_R}{3} c_v \frac{\partial T}{\partial x_i} - \tau_R \frac{\partial N_{\langle ij \rangle}}{\partial x_j}. \tag{3.61}$$

The easiest way to proceed is by ignoring the last term in this equation. Thus, p_i , or the energy flux $Q_i = c^2 p_i$ is proportional to the gradient of T and the factor of proportionality is the heat conductivity κ . We obtain

$$\kappa = \frac{\tau_R}{3} c^2 c_v. \tag{3.62}$$

This is the desired relation between κ and τ_R which will serve us to determine the temperature dependence of τ_R .

The omission of the last term in (3.61) is not without subtle consequences, because the well-known phonon Poiseuille flow depends on that term [8]. It is possible to show that (3.62) is correct, if the heat conduction is properly one-dimensional.

4 The heat pulse experiment

4.1 The initial and boundary value problem

The heat pulse experiment was introduced into crystal physics by Gutfeld & Nethercot in 1964 to detect second sound which was already predicted in earlier theories by Ward & Wilks [3, 4, 5]. Gutfeld & Nethercot failed to see evidence of second sound; however, they did discover ballistic phonons. In the following years experimental and theoretical examinations culminated in the discovery of second sound in solid helium 1966 [9], [31], sodium fluoride 1969 [10], [11] and bismuth 1972 [12].

The experimental arrangement is shown schematically in Figure 4.1.

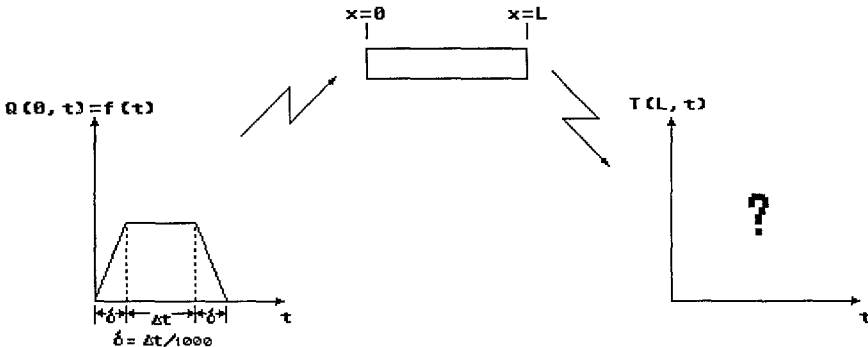


Fig. 4.1. The heat pulse experiment

Two opposite surfaces of the crystal are covered with metal films, which serve as heater and thermometer, respectively. The heat $Q(t)$ supplied to the left hand side of the crystal at $x = 0$ is furnished by an electric current.

The change of the resistance of the metal film at the right hand side of the crystal is taken as a measure for $T(L, t)$.

If we consider the arrangement as a one-dimensional heat conduction problem, the initial and boundary values that can be controlled are

$$u_A(x, 0) = 0 \quad \text{for} \quad A = 0, 1, 2, \dots, M \quad (4.1)$$

$$Q(0, t) = c^2 p(0, t) = f(t) \quad Q(L, t) = c^2 p(L, t) = 0. \quad (4.2)$$

Inspection of the N field equations (3.58) shows that the conditions (4.1), (4.2) provide a unique solution only in the 9 field case.

4.2 Expected phenomena

Before we start to discuss the experimental results we describe the expected phenomena by interpreting the phonon-model. The energy supplied at the heater gives rise to the production of new phonons carrying this energy. The kind of energy transport which follows depends strongly on the collision-frequencies of the various processes. As was explained before in Section 2.1. we distinguish between three main transport mechanism: ballistic phonons, second sound and diffusion. Now, having discussed relaxation times and collision frequencies we may be more specific in identifying those three mechanisms.

- i) Ballistic phonons request low temperature and pure crystals. The frequencies of both N- and R-processes vanish, i.e. $\frac{1}{\tau_N} \rightarrow 0$, $\frac{1}{\tau_R} \rightarrow 0$.
As all phonons travel with the same speed c we expect to detect the heat pulse at the thermometer with a delay $t_B = L/c$.
- ii) Second sound: Temperature is high enough to make phonon-phonon interaction with momentum conservation a frequent event. But still pure crystals are requested to lower the resistance. In terms of the corresponding frequencies this means $\frac{1}{\tau_N} \rightarrow \infty$, $\frac{1}{\tau_R} \rightarrow 0$.
- iii) Diffusion: phonons are frequently scattered on dislocation and impurities.
Thus we have $\frac{1}{\tau_R} \rightarrow \infty$.

4.3 Experimental results

Now we consider experimental data from pure (Fig. 4.2) and very pure (Fig. 4.3) NaF single crystals, reported by Jackson et al. [11] and Jackson & Walker [30].

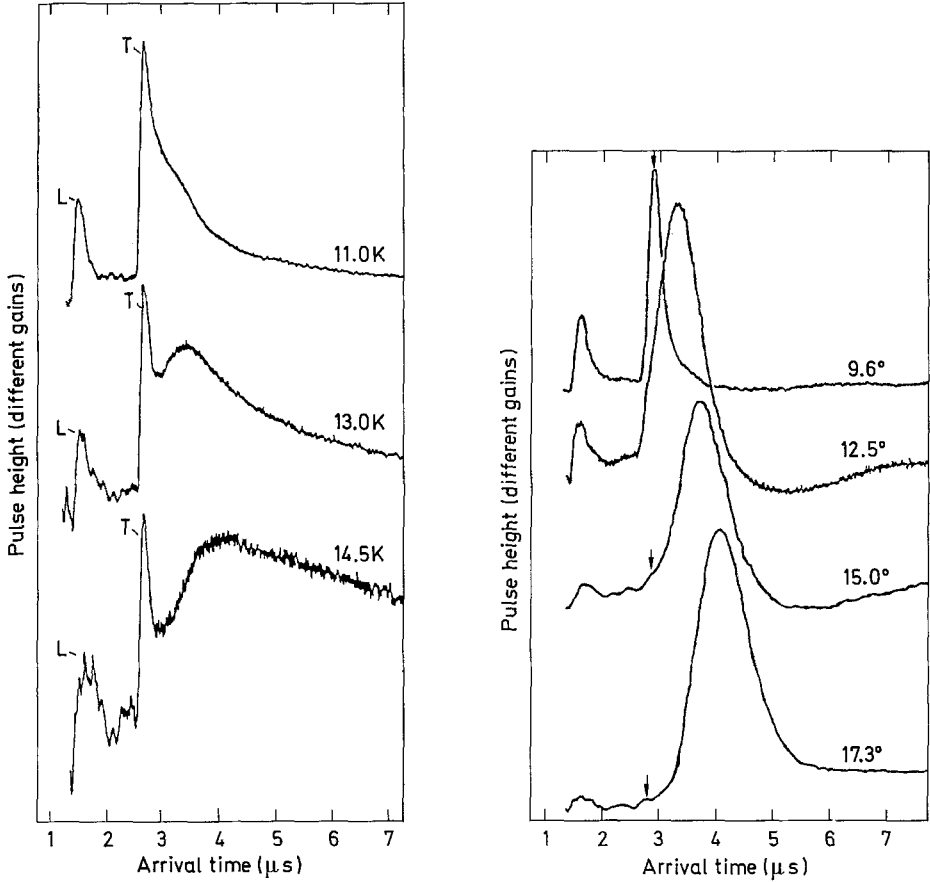


Fig.4.2./4.3. Heat pulses in pure NaF [30] and in very pure NaF [11]

In all curves the temperature $T(L, t)$ at the thermometer is plotted versus time t . It is not clear from the paper [30] which measure of temperature has been used. Anyway the vertical axis is scaled differently for the different curves, so that nothing can be learned from a comparison of the heights of the peaks in the figures.

The fastest peak in all three curves, denoted by L , is induced by ballistic phonons travelling with the speed of a longitudinal sound wave, which is independent of temperature.

The peak which arrives next, denoted by T , is induced by ballistic phonons travelling with the speed of a transversal sound wave, which is also independent of temperature.

The third peak that appears only at 13 K and 14.5 K has been interpreted as partially developed second sound.

The second sound peaks in Figure 4.2 are followed by long tails. These are created by R-processes and represent the diffusive part of the heat pulse.

We proceed to discuss the curves of Figure 4.3 which represent the experimental findings in a crystal of very high purity.

At 9.6 K there are few N-processes and we observe only the two ballistic peaks. At 12.5 K there is only one peak, shifted so far to the right to be due to ballistic phonons. Therefore that peak is due to the propagation of second sound. The transversal ballistic peak is absent.

At still higher temperatures the second sound peak has been shifted to later arrival times proving that the speed of second sound depends on temperature.

5 Theories on heat conduction in crystals

The experimental data have indicated that all three phenomena, namely

- i) ballistic phonons
- ii) second sound
- iii) diffusion

may occur simultaneously. An appropriate theory should therefore be able to describe these phenomena simultaneously as well. We shall present such a theory ignoring, however, the distinction between longitudinal and transversal ballistic phonons.

This chapter is organized as follows: First we compare the reported experimental results with the ‘‘9-field-theory’’ based on the equations (3.56). After having discussed the advantages and shortcomings of that theory we consider the ‘‘N-field case’’. Finally, we discuss previous theories on heat transport processes and compare their predictions with ours.

5.1 The 9-field-theory of extended thermodynamics

5.1.1 Comparison of theory and experiment

The 9-field-theory is the simplest case of the N-field-theory where both relaxation times τ_N and τ_R occur allowing the description of N- and R-processes.

In the one dimensional case the field equations for the variables $e = aT^4$, $p_1 = p$ and $N_{(11)} = N$ read, see (3.58)

$$\frac{\partial e}{\partial t} + c^2 \frac{\partial p}{\partial x} = 0$$

$$\frac{\partial p}{\partial t} + \frac{1}{3} \frac{\partial e}{\partial x} + \frac{\partial N}{\partial x} = - \frac{1}{\tau_R} p$$

$$\frac{\partial N}{\partial t} + \frac{4}{15} c^2 \frac{\partial p}{\partial x} = - \frac{1}{\tau} N. \quad (5.1)$$

The initial and boundary values for the heat pulse experiment are given by (4.1) and (4.2). We have solved the system for $e(x, t) = e_0 + \bar{e}(x, t)$ with $e_0 = aT_0^4$, $\bar{e} = 4aT_0^3 \bar{T}$, $\bar{T} = T - T_0$, using Laplace transforms analytically with a numerical evaluation of the inverse Laplace transformation.

The value for the relaxation time τ_R at the reference temperature T_0 is taken from heat conductivity data corresponding to the crystal of Fig. 4.2 [30] as was explained in Section 3.3.4. The relaxation time τ is adjusted so as to obtain a good fit between the calculation and the experimental $\bar{T}(L, t)$ curves in Fig. 4.2. Figure 5.1. shows the result; it is plotted for

$$\tau_R = (15.4; 10.4; 7.4) \Delta t; \quad \tau = (3.0; 2.1; 2.0) \Delta t.$$

We conclude that there is a good qualitative agreement with the results reported by Jackson & Walker [30] in Figure 4.2.

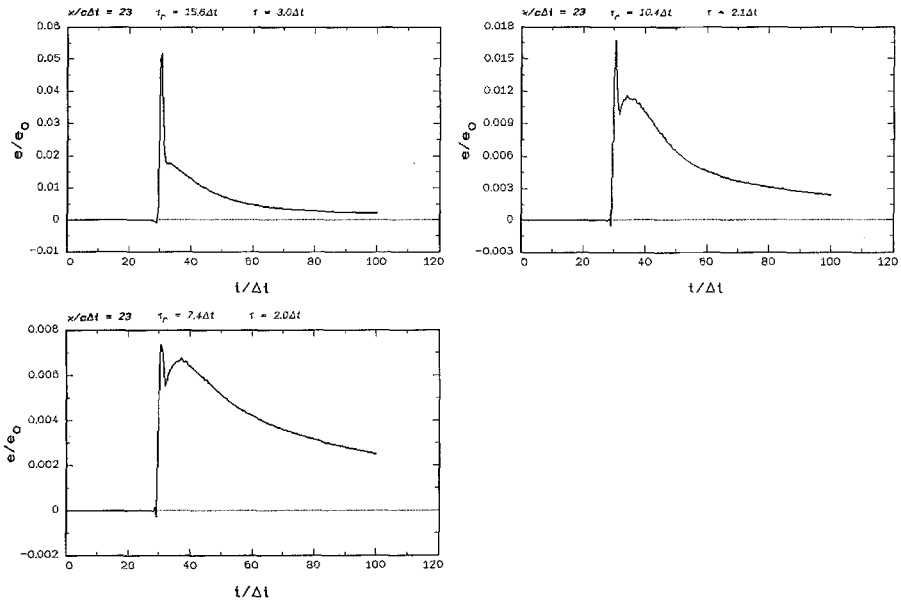


Fig. 5.1. a-c. $T(L, t)$ following the 9-field theory (Pulse duration $\Delta t = 10^{-7}$ s)

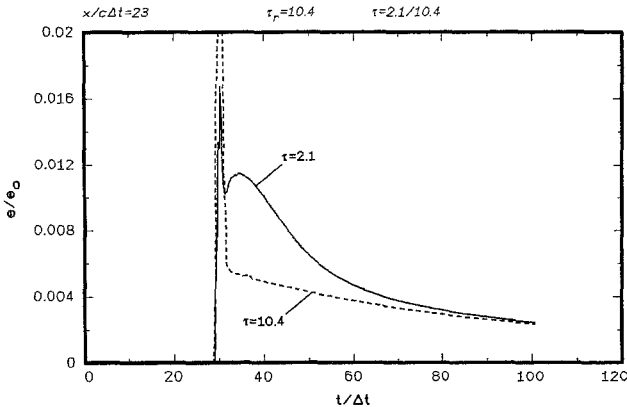


Fig. 5.2. $T(L, t)$ with $\tau_R = 10.4 \Delta t$ and $\tau = 2.1 \Delta t / 10.4 \Delta t$

The second peak which appears in Figures 5.1 b/c has been interpreted as partially developed second sound (see Section 4.3).

This interpretation ought to be checked; it may be checked by testing whether the second peak disappears if the second sound is “switched off” by setting $\tau_N = \infty$, i.e. $\tau = \tau_R$. Indeed it does as is illustrated by Figure 5.2. In that figure the drawn-out line is identical to the one of Figure 5.1. b., it corresponds to $\tau_R = 10.4$, $\tau = 2.1$. The dashed figure corresponds to $\tau_R = \tau = 10.4$, so that no second sound can occur. Accordingly no second peak is observed as we have expected. Note that the dashed curve has a very high ballistic peak. This is understandable from the fact that with no N-processes, the ballistic peak is not as strongly dissipated as with N-processes.

Next we study the influence of the frequency of N-processes on the development of the original pulse. We vary τ_N for fixed large $\tau_R = 30 \Delta t$ appropriate to the properties of the very pure crystal to which the data in Fig. 4.3 refer.

For large values of τ_N ($\tau_N = 4\Delta t$) there is only a ballistic pulse comparable in width to the original pulse. If τ_N is decreased to $2\Delta t$ a second sound pulse appears which absorbs the ballistic pulse completely when we decrease τ_N further. We note that the second sound pulse shows a marked broadening compared to the original pulse; also its position shifts to the right for higher temperature i.e. the second sound speed decreases with temperature. Once again we obtain good qualitative agreement between theory and experiment. Indeed this agreement is evident between the four curves of Figure 4.3 and the curves of Figures 5.3. a, c, d.

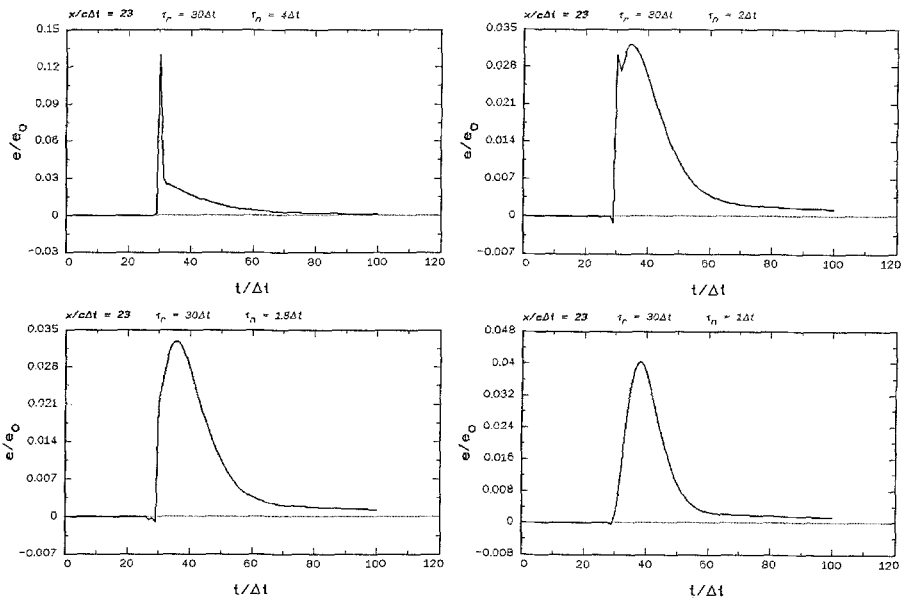


Fig. 5.3. a-d. $T(L, t)$ following the 9-field-theory for various τ_N and a large value of τ_R ($\Delta t = 10^{-7}$ s)

Curves like the one in Figure 5.3. b. which show ballistic and second sound properties have not been recorded among the experimental data of Fig. 4.3. The 9-field-theory implies that such a curve should appear in the range between $T_0 = 9.6$ K and $T_0 = 12.5$ K.

Sofar we have plotted arrival times of pulses, because this is what experimentalists have registered. Now we proceed by discussing a different aspect of this heat transport phenomenon: We plot the temperature field resulting from the pulse for different times as it travels down the crystal. Figure 5.4 shows curves $T(x, t_i)$, $t_i = 5i \Delta t$ ($i = 1 \dots 13$) for a crystal with $\tau_R = 8 \Delta t$, $\tau = 1 \Delta t$, $\Delta t = 10^{-7}$ s.

In the beginning the pulse moves ballistically into the crystal followed by a tail. With increasing time the ballistic peak is damped more and more by N-processes, while a second sound peak develops, see Figures 5.4. b, c, d. At

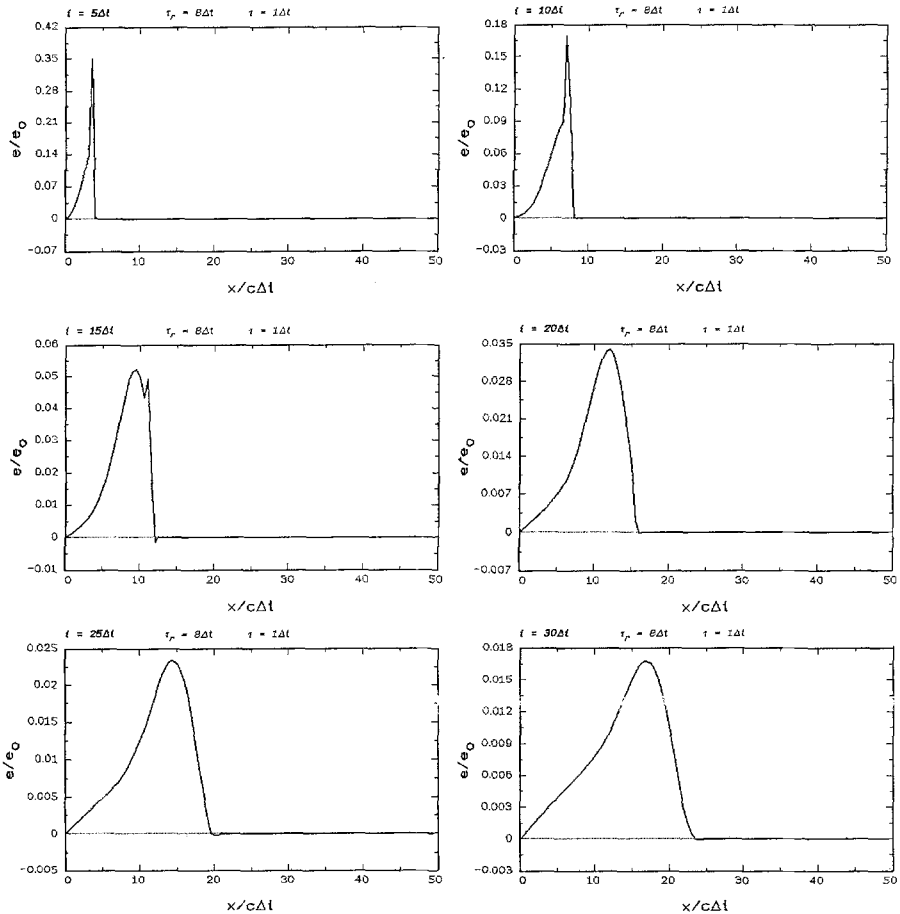


Fig. 5.4a-f. Development of a heat pulse in space for several times

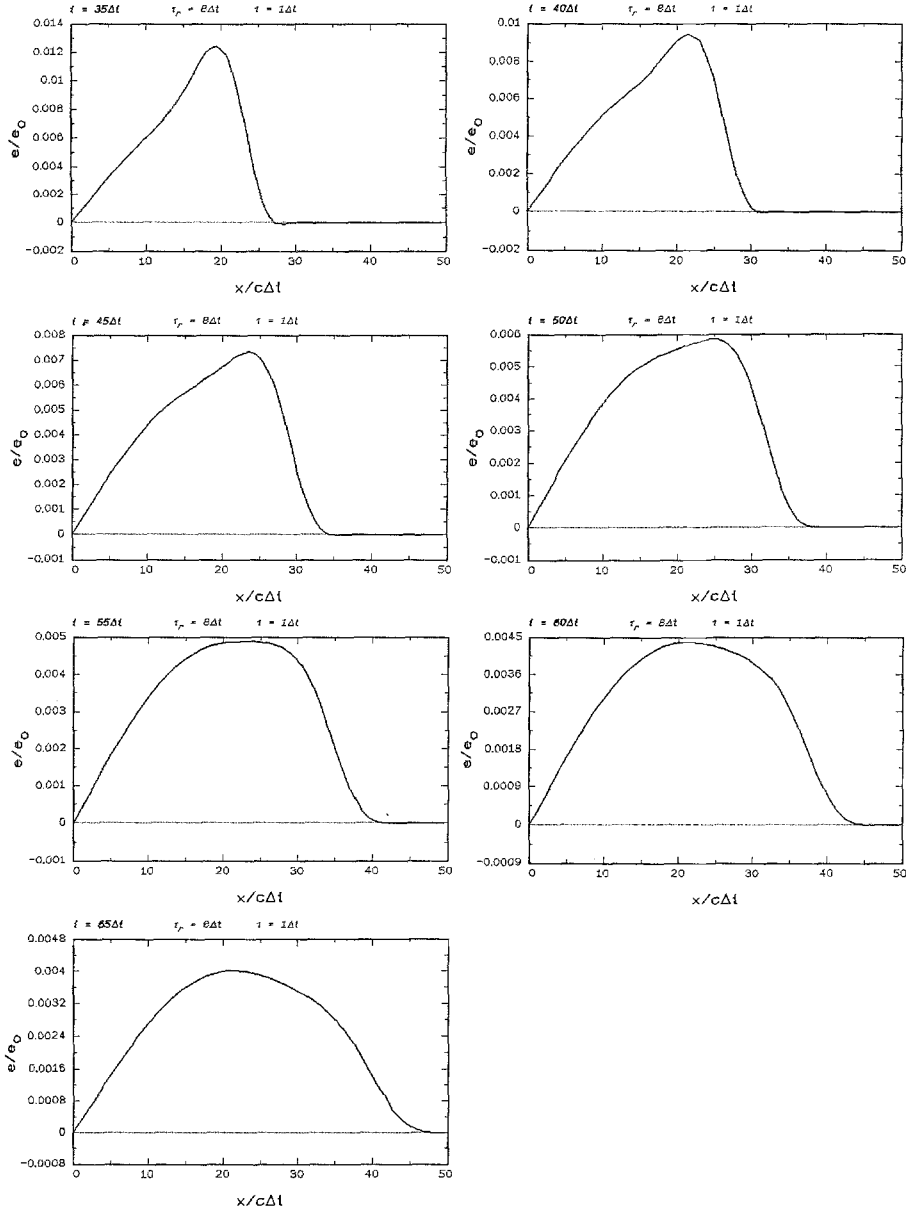


Fig. 5.4g-m. Development of a heat pulse in space for several times

$t = 20 \Delta t$, Figure 5.4.d., the ballistic peak is completely absorbed by the second sound peak. The propagation of this peak can be followed along the crystal in the Figures 5.4.c-i. Starting with $t = 25 \Delta t$, Figure 5.4.g., the back of the second sound peak develops a hump due to resistive processes. This hump becomes more and more pronounced and eventually it absorbs the second sound peak, see Figures 5.4.k, l, m. There remains diffusive spreading of temperature without any noticeable propagation.

The array of Figures 5.4 is particularly instructive – more so than the one of Figure 5.3 – in that it demonstrates the successive development of all three mechanisms ballistic, second sound and diffusive. The ballistic effect dominates the early development, while diffusion dominates the end. In between, during a brief period we observe the propagation of second sound. All this is well-described by the 9-field theory.

5.1.2 Dispersion Relation

For further discussion of the 9-field-theory we shall introduce plane wave solutions of (5.1)

$$e = e_0 + \bar{e} \exp i(\Omega t - qx), \quad p = \bar{p} \exp i(\Omega t - qx), \quad N = \bar{N} \exp i(\Omega t - qx) \quad (5.2)$$

to obtain the dispersion relation

$$q^2 = 3 \frac{\Omega^2}{c^2} \frac{1 + \frac{\tau}{\tau_R} + i \left(\tau \Omega - \frac{1}{\tau_R \Omega} \right)}{1 + \frac{9}{5} i \tau \Omega}. \quad (5.3)$$

Ω and q are frequency and wave number, respectively, and \bar{e} , \bar{p} , \bar{N} denote the complex amplitudes of the fields. The phase velocity v_{ph} and damping coefficient α are defined as

$$v_{ph} = \frac{\Omega}{\text{Re}(q)}, \quad \alpha = -\text{Im}(q). \quad (5.4)$$

We shall now investigate the dispersion relation for several limits of the relaxation times.

i) Ballistic phonons: $\tau_R \rightarrow \infty$, $\tau_N \rightarrow \infty$. In this limit we obtain for the phase speed

$$v_{ph} = \sqrt{\frac{3}{5}} c, \quad (5.5)$$

which has to be identified with the velocity v_{ball} of a ballistic peak. Indeed, careful inspection of the plots 5.3. a–c shows that the ballistic peak propagates with this speed.

The value $v_{ball} = \sqrt{\frac{3}{5}} c$ indicates a shortcoming of the 9 field theory, because ballistic phonons should travel with the Debye velocity c .* We shall later show, see Section 5.2, that this deficiency can be overcome by taking more variables into account.

* Recall that we can only have one ballistic peak here, because transversal and longitudinal speed have been subsumed in one Debye speed.

ii) Second sound: $\tau_R \rightarrow \infty$, $\tau_N \rightarrow 0$. In this limit we obtain the velocity of undamped second sound,

$$v_{II} = \frac{1}{\sqrt{3}} c. \quad (5.6)$$

An undamped second sound with velocity v_{II} given by (5.6) was never observed in experiments. Therefore the requirement $\tau_R \rightarrow \infty$, $\tau_N \rightarrow 0$ is not met in nature. Hence we will discuss the dispersion relation for the weaker requirement

$$\tau_R \Omega \gg 1, \quad \text{i.e.} \quad \tau \Omega = \tau_N \Omega, \quad \text{and} \quad \tau_N \Omega \ll 1. \quad (5.7)$$

The dispersion relation may now be expanded to give

$$q^2 = \frac{3\Omega^2}{c^2} \left(1 - \frac{4}{5} \frac{\tau_N}{\tau_R} - i \left(\frac{1}{\Omega \tau_R} + \frac{4}{5} \tau_N \Omega \right) \right). \quad (5.8)$$

From (5.8) we conclude that the condition

$$\frac{1}{\tau_R} \ll \Omega \ll \frac{1}{\tau_N}, \quad (5.9)$$

which is equivalent to (5.7), guarantees an almost vanishing imaginary part, thus allowing an almost undamped second sound wave with velocity

$$v_{II} = \frac{c}{\sqrt{3}} \left(1 + \frac{2}{5} \frac{\tau_N}{\tau_R} \right). \quad (5.10)$$

The condition (5.9) is called window condition and was first discovered by Guyer & Krumhansl in 1964 [6]. Only after their careful analysis of (5.9) second sound in crystals was observed by Ackermann et al. ([9], [31]). The interpretation of the window condition (5.9) is as follows: The crystal must be of large purity and at low temperature so that there are only few resistive processes. However, the temperature must not be too low, because that would prevent enough normal processes to satisfy $\tau_N \ll \tau_R$. Therefore the condition (5.9) is generally not satisfied. If it is satisfied this can only be in a very small range of temperature. Furthermore, the initial heat pulse must contain the frequencies Ω that satisfy (5.9) for given τ_R and τ_N .

5.2 The N-field-theory of extended thermodynamics

5.2.1 Ballistic phonons

We have seen that – according to the 9-field theory – the ballistic phonons had the wrong speed. All other aspects, i.e. second sound and heat diffusion were satisfactory, even quantitatively, as put in coincidence by the comparison of the Figures 5.1 and 5.2 and by the preceding calculation of the values v_{II} . Therefore we have to modify the 9-field theory so that the ballistic speed

comes out right and the other aspects of heat propagation remain unchanged. This is the subject of the present section.

It will turn out that the N -field theory described in previous chapters satisfies this requirement provided that N is big enough. In particular for large values of N the ballistic speed becomes equal to c . In the ballistic limit ($\tau_R \rightarrow \infty$, $\tau_N \rightarrow \infty$) the one dimensional field equations (3.58) reduce to

$$\frac{\partial u_A}{\partial t} + \sum_B \mathfrak{C}_{AB} \frac{\partial u_B}{\partial x} = 0, \quad A, B = 0, 1, \dots, M, \quad N = M + 1. \quad (5.11)$$

These equations describe undamped waves with phase velocities that are the eigenvalues of the matrix \mathfrak{C}_{AB} given by (3.60). Since the entries in \mathfrak{C}_{AB} are fully specific, we may calculate all of its eigenvalues for any given N , albeit only numerically, the biggest among the eigenvalues is plotted as a function of N in Figure 5.5. Its value represents the ballistic speed ball appropriate to the N -field theory.

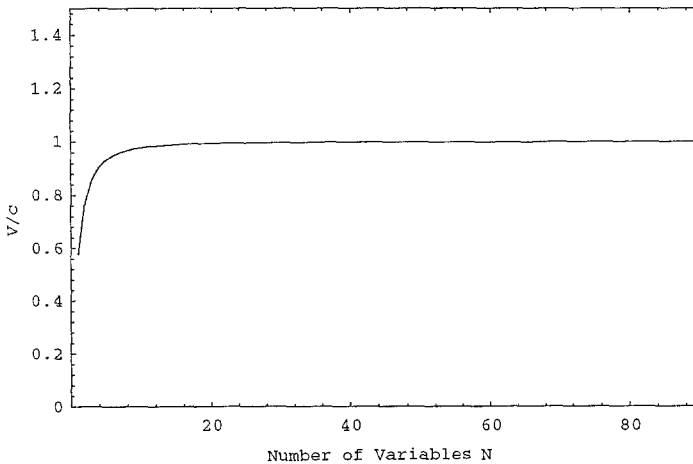


Fig. 5.5. Dependence of the ballistic velocity on the number of variables

We conclude that v_{ball} tends to c with an increasing number of variables. From about 30 one-dimensional variables on we may set $v_{ball} \approx c$. Thus in the one-dimensional case a theory with not less than 30 variables is needed for a proper description of the ballistic peaks.

For the three-dimensional case this means that we need all moments

$$\{e, p_i, u_{\langle i_1 i_2 \rangle}, \dots, u_{\langle i_1 \dots i_n \rangle} \quad \text{for } n = 2, 3, \dots, 30\}$$

for the description of processes where ballistic peaks appear. Unfortunately the variables $u_{\langle i_1 i_2 \rangle}, \dots, u_{\langle i_1 \dots i_M \rangle}$ have no easy physical interpretation and thus their initial and boundary values cannot be controlled in the experiment. This is a serious problem, which however, may be overcome by the assumption that the phonons which are created at the heater travel ballistically into the crystal at first. The resulting ‘ballistic initial values’ will be discussed in Appendix B.

5.2.2 The N -field theory in the limit $\tau_N \rightarrow 0$

While we have seen that the proper description of ballistic phonons requires a many moment theory, we proceed to show that for small values of τ_N , i.e. high frequency of N -processes, the number of variables may be drastically reduced.

For $\tau_N \rightarrow 0$ we have from (3.51)

$$\frac{1}{\tau} = \frac{1}{\tau_N} + \frac{1}{\tau_R} \approx \frac{1}{\tau_N}. \quad (5.12)$$

Therefore we may neglect in the system (3.57) for $n \geq 2$ the time derivatives $\partial u_{\langle i_1 \dots i_n \rangle} / \partial t$ in comparison to the production densities $(-u_{\langle i_1 \dots i_n \rangle} / \tau) \approx (-u_{\langle i_1 \dots i_n \rangle} / \tau_N)$. With the omission of the time derivatives it follows from (3.57) with $n = M$ that we have

$$u_{\langle i_1 \dots i_M \rangle} = -\tau_N c^2 \frac{M}{2M+1} \frac{\partial u_{\langle i_1 \dots i_{M-1} \rangle}}{\partial x_{i_M}}. \quad (5.13)$$

Introduction of (5.13) into (3.57) with $n = M - 1$ and neglecting terms of second order in τ_N yields

$$u_{\langle i_1 \dots i_{M-1} \rangle} = -\tau_N c^2 \frac{M-1}{2(M-1)+1} \frac{\partial u_{\langle i_1 \dots i_{M-2} \rangle}}{\partial x_{i_{M-1}}}.$$

By successive insertion into the next formula we obtain a simple expression for $u_{\langle i_1 \dots i_n \rangle}$ for $n = 2, 3, \dots, M$ in terms of a gradient of the next lower moment, viz.

$$u_{\langle i_1 \dots i_n \rangle} = -\tau_N c^2 \frac{n}{2n+1} \frac{\partial u_{\langle i_1 \dots i_{n-1} \rangle}}{\partial x_{i_n}}, \quad n = 2, 3, \dots, M. \quad (5.14)$$

Thus in the limit $\tau_N \rightarrow 0$ the N -field-system may be reduced to the 9-field-system

$$\begin{aligned} \frac{\partial e}{\partial t} + c^2 \frac{\partial p_i}{\partial x_i} &= 0 \\ \frac{\partial p_i}{\partial t} + \frac{1}{3} \frac{\partial e}{\partial x_i} + \frac{\partial N_{\langle ij \rangle}}{\partial x_j} &= -\frac{1}{\tau_R} p_i \end{aligned} \quad (5.15)$$

$$c^2 \frac{2}{5} \frac{\partial p_{\langle i}}{\partial x_j} = -\frac{1}{\tau_N} N_{\langle ij \rangle}$$

This system must be compared with the 9 field system (5.1) of Section 5.1. The only difference is that here the time derivative of $N_{\langle ij \rangle}$ is missing in the last equation. This is a result of the present approximation.

We conclude from these considerations that the 9-field-theory is sufficient in the case $\tau_N \rightarrow 0$.

5.2.3 The limiting cases $\tau_N \rightarrow 0$ and $\tau_R \rightarrow 0$

If τ_N is in fact *equal* to zero the system (5.15) reduces to the 4-field-theory

$$\begin{aligned} \frac{\partial e}{\partial t} + c^2 \frac{\partial p_i}{\partial x_i} &= 0 \\ \frac{\partial p_i}{\partial t} + \frac{1}{3} \frac{\partial e}{\partial x_i} &= -\frac{1}{\tau_R} p_i. \end{aligned} \tag{5.16}$$

For big values of τ_R the system (5.16) describes a second sound wave with velocity $v_{II} = c/\sqrt{3}$.

We note that such a speed is never observed in experiments and conclude from this that we cannot have $\tau_N = 0$. Thus the 4-field-theory is not sufficient for the description of second sound.

Next we consider the case $\tau_R \rightarrow 0$ which is realized in crystals of high impurity. The system (5.16) is still applicable, irrespective of the value for τ_N . However, we may now neglect the time derivative $\partial p_i/\partial t$ in (5.16)₂ and come

Table 5.1.

	Limits of relaxation times	described phenomena
Fourier: $\frac{\partial e}{\partial t} + c^2 \frac{\partial p_i}{\partial x_i} = 0$ $\frac{1}{3} \frac{\partial e}{\partial x_i} = -\frac{1}{\tau_R} p_i$	$\tau_R \rightarrow 0$	diffusion
4-field: $\frac{\partial e}{\partial t} + c^2 \frac{\partial p_i}{\partial x_i} = 0$ $\frac{\partial p_i}{\partial t} + \frac{1}{3} \frac{\partial e}{\partial x_i} = -\frac{1}{\tau_R} p_i$	$\tau_N \approx 0$ $\tau_R \in (0, \infty)$	diffusion second sound (without taking care for N-processes)
9-field: $\frac{\partial e}{\partial t} + c^2 \frac{\partial p_i}{\partial x_i} = 0$ $\frac{\partial p_i}{\partial t} + \frac{1}{3} \frac{\partial e}{\partial x_i} + \frac{\partial N_{\langle ij \rangle}}{\partial x_j} = -\frac{1}{\tau_R} p_i$ $\frac{\partial N_{\langle ij \rangle}}{\partial t} + c^2 \frac{2}{5} \frac{\partial p_{\langle i}}{\partial x_{j \rangle}} = -\frac{1}{\tau} N_{\langle ij \rangle}$	$\tau_N \rightarrow 0$ $\tau_R \in (0, \infty)$	diffusion second sound (ballistic phonons with wrong velocity)
N-field: $\frac{\partial u_A}{\partial t} + \mathfrak{C}_{AB} \frac{\partial u_B}{\partial x} = -\frac{1}{\tau_A} u_A$ $A, B = 1 \dots N, \quad N > 30$	$\tau_N \in (0, \infty)$ $\tau_R \in (0, \infty)$	diffusion second sound ballistic phonons

up in this special case with Fourier's classical law of heat conduction

$$\frac{\partial e}{\partial t} + c^2 \frac{\partial p_k}{\partial x_k} = 0,$$

$$p_k = -\frac{1}{3} \tau_R \frac{\partial e}{\partial x_k} = -\frac{1}{3} \tau_R \frac{\partial e}{\partial T} \frac{\partial T}{\partial x_k}. \quad (5.17)$$

We close this section with the Table 5.1 which lists the appropriate theories for some limits of the relaxation times.

6 Review of theories of heat conduction in crystals

6.1 Fourier's law

In its early days the phonon picture was used to calculate the heat conductivity κ in Fourier's law

$$Q_i = -\kappa \frac{\partial T}{\partial x_i}. \quad (6.1)$$

Major work on this subject was done by Peierls [1], [20], who had introduced the phonon picture. Among his successors we mention the outstanding work of Callaway [15]. A competent review on this subject was written by Caruthers [29].

As we have seen in Section 5.2.3, Fourier's law is only appropriate in the case $\tau_R \rightarrow 0$. This condition is satisfied in most solids at normal temperature. Therefore Fourier's law is the appropriate tool for most heat conduction problems. The shortcomings of Fourier's law, e.g. the paradox of heat conduction become only apparent in very pure crystals and at low temperature.

6.2 Second Sound

6.2.1 Generic Scheme

Here we shall discuss only theories of second sound which are based on the phonon model. Phenomenological theories of second sound and non-linear theories will be discussed separately in Section 6.4.

Ever since Peierls introduced the phonon model into crystal physics in 1929 many theories of heat transport in crystals have grown out of this model. The most successful theories rely on the phonon Boltzmann equation which is usually combined with the Callaway approximation and Debye's dispersion law $\omega = ck$, viz.

$$\frac{\partial f}{\partial t} + c \frac{k_i}{k} \frac{\partial f}{\partial x_i} = -\frac{1}{\tau_N} (f - f_4) - \frac{1}{\tau_R} (f - f_1). \quad (6.2)$$

While we have used an *arbitrary* number of fields – and accordingly, an arbitrary number of equations of balance – for the description of heat transport processes, other authors choose only *two* fields, viz. temperature T and momentum density p_i . Accordingly they need only two equations of balance, those for energy and momentum.

$$\frac{\partial e}{\partial t} + c^2 \frac{\partial p_i}{\partial x_i} = 0$$

$$\frac{\partial p_i}{\partial t} + \frac{1}{3} \frac{\partial e}{\partial x_i} + \frac{\partial N_{\langle ij \rangle}}{\partial x_j} = P_i. \quad (6.3)$$

We recall that $e, p_i, N_{\langle ij \rangle}$ are moments of the phase density f ,

$$e = \int \hbar c k f d\mathbf{k}, \quad p_i = \int \hbar k_i f d\mathbf{k}, \quad N_{\langle ij \rangle} = \int \hbar c \frac{\partial k_i k_j}{k} f d\mathbf{k} \quad (6.4)$$

and the momentum production is given by

$$P_i = - \int \hbar k_i \frac{1}{\tau_R} (f - f_1) d\mathbf{k}. \quad (6.5)$$

Since the purpose of the theory is the determination of the temperature T and the momentum density p_i , the system (6.3) must be closed by constitutive equations which relate $e, N_{\langle ij \rangle}$ and P_i to T and p_i in a materially dependent manner. The formulation of these equations is dictated by the fact that e through P_i may be derived from the phase density.

From our previous analysis we have concluded that for the proper description of all aspects of heat transport it is imperative to have *two* relaxation times. In the equations (6.3)–(6.5), however, only τ_R occurs explicitly, the relaxation time τ_N will appear as part of the constitutive assumptions.

6.2.1 The work of Ward & Wilks

We merely mention the early work of Tisza [32] and Landau [33] because it refers to second sound in liquid He II rather than in crystals. Whatever motivation for the development of the second sound in solids was drawn from this early work, seems spurious in retrospect.

Nevertheless this work motivated Ward & Wilks [3], [4] in 1951 to formulate a theory of second sound in solids which is compatible with (6.3) provided we set

$$N_{\langle ij \rangle} = 0 \quad \text{and} \quad P_i = 0.$$

The resulting equation by Ward & Wilks are the equations of the 4-field-theory in the limit $\tau_R \rightarrow \infty$, see Section 5.2.3. These equations cannot serve for a proper description of second sound in solids because N-processes are not considered. Also the predicted speed $c/\sqrt{3}$ was never observed.

6.2.2 The work of Sussmann & Thellung

The first authors who took the N-processes into account were Sussmann & Thellung in 1962 [34]. Neglecting the occurrence of R-processes they solved the phonon Boltzmann equation 6.2 by means of the Chapmann-Enskog-method. The resulting constitutive equations read*

$$P_i = 0$$

$$N_{ij} = \frac{1}{3} e \delta_{ij} + N_{\langle ij \rangle} \quad (6.6)$$

with

$$e = aT^4 - \tau_N c^2 \frac{\partial}{\partial x_i} \left(p_i + \frac{4}{3} \tau_N aT^3 \frac{\partial T}{\partial x_i} \right)$$

$$N_{\langle ij \rangle} = - \frac{2}{5} \tau_N c^2 \frac{\partial}{\partial x_{\langle i}} \left(p_{j \rangle} + \frac{4}{3} \tau_N aT^3 \frac{\partial T}{\partial x_{j \rangle}} \right). \quad (6.7)$$

We recognize some distinctions to our system (5.15) which is also appropriate for $\tau_N \rightarrow 0$. Infact we have

$$e = aT^4$$

$$N_{\langle ij \rangle} = - \frac{2}{5} \tau_N c^2 \frac{\partial p_{\langle i}}{\partial x_{j \rangle}}. \quad (6.8)$$

Obviously the differences result from the interpretation of the temperature. While in our definition (6.8)₁ T is a measure for e , by virtue of the relation $e = aT^4$, Sussmann & Thellung consider this relation to be valid only in equilibrium.

Because of the neglect of R-processes the theory of Sussmann & Thellung is not sufficient for the description of second sound.

6.2.3 The work of Guyer & Krumhansl

The most important work on second sound in crystals was the one by Guyer & Krumhansl [6], [7], [8] because it pointed the way to a succesful observation of second sound. The reason is that this was the first theory with both relaxation times.

Guyer & Krumhansl calculated an approximate solution of the phonon Boltzmann equation and obtained – in the limit of small values of τ_N –

* Sussmann & Thellung consider three phonon modes, l , t_1 , t_2 . For simplicity we have introduced the Debye speed in their equations.

the field equations (6.3) with the constitutive equations

$$P_i = -\frac{1}{\tau_R} p_i \quad (6.9)$$

$$N_{ij} = -\frac{1}{3} e \delta_{ij} + N_{\langle ij \rangle} \quad \text{with} \quad (6.10)$$

$$e = aT^4 - \tau_N c^2 \frac{\partial p_n}{\partial x_n}, \quad N_{\langle ij \rangle} = -\frac{2}{5} \tau_N c^2 \frac{\partial p_{\langle i}}{\partial x_{j \rangle}}. \quad (6.11)$$

Thus Guyer & Krumhansl consider e to be equal to aT^4 plus a non-equilibrium contribution, much like Sussmann & Thellung do. However, not all is well, because when e is given by (6.11)₁ in the momentum flux the same expression must be used in the energy balance. This requirement is not reflected in the work of Guyer & Krumhansl. Except for this we recognize a marked similarity of the equations of Guyer & Krumhansl to our system (5.15).

Guyer & Krumhansl were first to derive the window condition (5.9) from their equations. This led to the detection of second sound because it identified the temperature range, where second sound may be observed.

From the discussion in this chapter we conclude that all theories presented here are special cases of the N -field-theory in the approximation valid for small values of τ_N . Discrepancies result only from different interpretations of the temperature.

6.3 Ballistic phonons

Ballistic phonons require large values of τ_N and accordingly equations of transfer of higher order, complete with their time derivatives, see Section 5.2. Therefore ballistic phonons are not covered by the theories discussed in Section 6.2.

The best known theory of ballistic phonons is the theory by Rogers [35]. The important result in Roger's work is his dispersion relation for harmonic waves

$$q^2 = \frac{3\Omega^2}{c^2} \frac{1 + \frac{\tau}{\tau_N} + i\left(\tau\Omega - \frac{1}{\tau_R\Omega}\right)}{1 + 3i\tau\Omega}. \quad (6.12)$$

Roger's dispersion relation is nearly the same one as the one of the 9-field-theory, see (5.3), except for a different factor (3 instead of 9/5) in the denominator. In the limit of undamped second sound ($\tau_N \rightarrow 0$, $\tau_R \rightarrow \infty$) the phase speed comes out as $v_H = c/\sqrt{3}$ whereas in the limit of ballistic phonons ($\tau_R \rightarrow \infty$, $\tau_N \rightarrow \infty$) the correct phase speed $v_{ball} = c$ is obtained. By solving an initial value problem Rogers proved a good agreement between his theory and experiments.

Having said this we feel that a critical remark about Rogers' derivation of the dispersion relation (6.12) is in order. Rogers chose the Navier Stokes equation of hydrodynamics as his field equation for phonon momentum. However he replaced the real bulk viscosity by a frequency-dependent complex quantity. In this way he derives a complex differential equation for the temperature. This is hard to understand. It may reflect ideas about internal relaxation or history dependence which, however, are not made specific.

Beck & Beck [36] solved the phonon Boltzmann equation in Fourier space for an initial value problem. Instead of macroscopic field equations they obtain a dispersion relation, which they discuss in two limits: In the case of ballistic phonons ($\tau_R \rightarrow \infty$, $\tau_N \rightarrow \infty$) they obtain the speeds of longitudinal and transversal phonons as phase speeds. In the limit of second sound ($\tau_N \rightarrow 0$) their dispersion relation agrees with the 9-field-theory, if one introduces the Debye speed.

We prefer the N -field theory of Chapters 1–4 over the theories just discussed. The N -field theory provides a hierarchy of balance equations derived from the phonon Boltzmann equation. Thus it makes explicit – by the time derivatives in the balance equations – whatever history dependence may occur in heat transport phenomena.

6.4 Non-linear theories on heat transport in crystals

In recent years second sound in crystals gained new interest because physicist became interested in non-linear phenomena, for example pulse propagation along temperature gradients [37] or the propagation of shock waves [38], [39]. Of course, these non-linear theories should contain the linear phenomena, for instance the heat pulse experiments.

We proceed to examine some of these non-linear theories with respect to heat pulse propagations.

Using the entropy maximum principle, Larecki derived the following equations from the Phonon-Boltzmann equation [40]

$$\frac{\partial e}{\partial t} + c^2 \frac{\partial p_i}{\partial x_i} = 0$$

$$\frac{\partial p_i}{\partial t} + \frac{1}{3} \frac{\partial e}{\partial x_i} + \frac{\partial}{\partial x_j} \left(\frac{e}{2} (3\chi - 1) \frac{p_{\langle i} p_{j \rangle}}{p^2} \right) = -\frac{1}{\tau_R} p_i, \quad \chi = \frac{5}{3} - \frac{4}{3} \sqrt{1 - \frac{3}{4} \frac{c^2 p^2}{e^2}}. \quad (6.13)$$

Anile, Pennise & Sammartino [41] and Müller & Kremer [42] obtained the same system by phenomenological methods and Dreyer & Seelecke discussed its shock wave solutions [39]. This system is not appropriate for the description of second sound with a temperature dependent speed, because its linear version is equivalent to (5.16); it predicts $v_{II} = c/\sqrt{3}$.

Two further theories concerning second sound were published by Coleman & Newman [37], [43] and Ruggeri et al. [38]. Both theories were developed by

phenomenological considerations. In the linear case they reduce to

$$\frac{\partial e}{\partial t} + \frac{\partial Q_i}{\partial x_i} = 0$$

$$\frac{\partial Q_i}{\partial t} + U_E^2 \frac{\partial e}{\partial x_i} = - U_E^2 \frac{C_v}{\kappa} Q_i. \quad (6.14)$$

Here Q_i is the energy flux, C_v is the specific heat per unit volume, κ is the heat conductivity and $U_E(T)$ is a temperature-dependent speed.

$U_E(T)$ is determined by identifying it with the pulse speed whose value is read off from the Figures 4.3. In this way Coleman & Newman found the analytic expression

$$U_E^{-2} = A + BT^n, \quad n = 3.10, \quad A = 9.09 \cdot 10^{-12} \frac{s^2}{cm^2}, \quad B = 2.22 \cdot 10^{-15} \frac{s^2}{cm^2 K} \quad (6.15)$$

for the temperature dependence of U_E . As far as speeds are concerned this is a good formula. Indeed, in the limit $T=0$ the speed U_E is equal to the speed of transversal ballistic phonons $c_t = 1/\sqrt{A}$ and for higher temperatures it is equal to the speed of second sound.

But the proper value of the speed is not all: We need an explanation for the *broadening* of the peaks in Figure 4.3. This broadening is not described by the equations (6.14). In order to demonstrate this we have calculated the prediction of these equations for the heat pulse experiment at $T = 12.5$ K, using the Coleman & Newman data. The result is shown in Figure 6.1. It shows a peak which is not broadened at all. On the contrary it is just as sharp as the heating signal at $x = 0$. Similar curves appear for all temperatures.

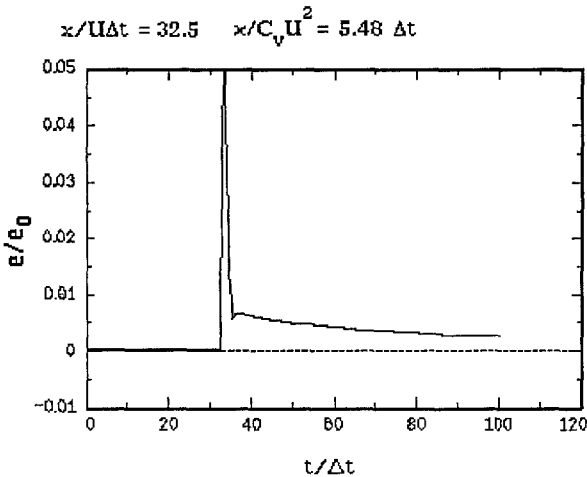


Fig. 6.1. $T(L, t)$ according to [37], [38].

This observation confirms our view that the pulses of Figure 4.3 are of different nature: At low temperature they are due to ballistic phonons and at higher temperatures they are due to second sound. This fact is not reflected in the work of Coleman & Newman. We have shown in Chapter 5 that *both* phenomena may produce their own peak at the same temperature and we have seen that the second sound peak broadens in the way the experiments observe.

7 Conclusion

The irritating complexity of heat propagation in dielectric crystals is due to the fact that over a wide temperature range three mechanisms of propagation are all competing, viz.

ballistic phonons,
second sound and
diffusive heat conduction.

We have shown here that it is possible to treat all three phenomena jointly on the basis of the phonon Boltzmann equation combined with the Callaway ansatz. In this manner the above three mechanisms in their relative importance are controlled by only two relaxation times, τ_N and τ_R . We have

ballistic phonons		$\tau_N \rightarrow \infty$	$\tau_R \rightarrow \infty$
second sound	for	$\tau_N \rightarrow 0$	$\tau_R \rightarrow \infty$
diffusive heat conduction		$\tau_R \rightarrow 0$.	

A difficulty is due to the fact that many moment equations of the phonon Boltzmann equation are needed for a quantitative description of all observed phenomena.

We have shown, however, that the case of $N = 30$ one-dimensional equations can still be handled and that it provides full agreement with experiments.

Equipped with this knowledge we are able to classify the various attempts of previous authors who have all tried to find simpler field equations. We have discussed those previous attempts. All of them are valid in some aspects, but unable to describe the full spectrum of possibilities. Among the theories discussed in Chapter 6 there are those that correctly describe second sound and diffusive heat conduction, or only second sound, or ballistic phonons and second sound. Other theories describe all or some of these phenomena but they exhibit deficiencies – either quantitative or qualitative ones – in certain aspects.

Having seen that the moment equations based on the phonon Boltzmann equation provide a satisfactory description of all three mechanisms of linear heat transport we suggest that the study of non-linear effects be based on the same principles.

Appendix A

Mixture theory of longitudinal and transversal phonons

Up to now we have only considered the simple Debye model $\omega = ck$ where all phonons have the same speed. Now we want to take into account the distinction between longitudinal and transversal phonons. There are one longitudinal mode and two transversal ones. For all three of them we use a simple linear dispersion law, namely

$$\omega_\alpha = c_\alpha k, \quad \alpha = l, t_1, t_2 \quad (\text{A } 1)$$

and assume that the transversal modes are degenerated, meaning that both transversal modes have the same speeds $c_t = c_{t_1} = c_{t_2}$.

The phonon Boltzmann equation for the phase density f^α of mode α reads

$$\frac{\partial f^\alpha}{\partial t} + c_\alpha \frac{k_i}{k} \frac{\partial f^\alpha}{\partial x_i} = S^\alpha, \quad \alpha = l, t_1, t_2. \quad (\text{A } 2)$$

For the collision term S_α we assume the relaxation time approximation (see Section 3.3.2)

$$S^\alpha = S_R^\alpha + S_N^\alpha = -\frac{1}{\tau_R^\alpha} (f^\alpha - f_1^\alpha) - \frac{1}{\tau_N^\alpha} (f^\alpha - f_4^\alpha) \quad (\text{A } 3)$$

with

$$f_R^\alpha = \frac{y}{\exp\left(\frac{\hbar c_\alpha}{k_B} \mathcal{A}_1^{\alpha(1)} k\right) - 1}, \quad f_N^\alpha = \frac{y}{\exp\left(\frac{\hbar c_\alpha}{k_B} \mathcal{A}_1^{\alpha(4)} k + \frac{\hbar}{k_B} \mathcal{A}_i^{\alpha(4)} k_i\right) - 1}. \quad (\text{A } 4)$$

$\frac{1}{\tau_R^\alpha}$ and $\frac{1}{\tau_N^\alpha}$ are the collision frequencies of R- and N-processes for phonons of mode α .

We assume now that the collisions between longitudinal and transversal phonons will lead to equilibrium phase densities f_1^α, f_4^α which are characterized by the same Lagrange multipliers, i.e.

$$\mathcal{A}_1^{(1)} = \mathcal{A}_1^{l(1)} = \mathcal{A}_1^{t(1)}, \quad \mathcal{A}_1^{(4)} = \mathcal{A}_1^{l(4)} = \mathcal{A}_1^{t(4)}, \quad \mathcal{A}_i^{(4)} = \mathcal{A}_i^{l(4)} = \mathcal{A}_i^{t(4)}. \quad (\text{A } 5)$$

Since $\mathcal{A}_1 = \frac{1}{T}$ in the linear theory (A 5) states that both modes will have the same temperature in equilibrium.

The Lagrange multipliers must be determined from the conservation laws for energy in R- and N-processes and for phonon momentum in N-processes, namely

$$\sum_{\alpha=l,t_1,t_2} \int \hbar c_\alpha k S_R^\alpha d\mathbf{k} = 0, \quad \sum_{\alpha=l,t_1,t_2} \int \hbar c_\alpha k S_N^\alpha d\mathbf{k} = 0, \quad \sum_{\alpha=l,t_1,t_2} \int \hbar k_i S_N^\alpha d\mathbf{k} = 0. \quad (\text{A } 6)$$

As variables for the description of the thermodynamic state we choose

$$u_A^\alpha = \int \psi_A^\alpha f^\alpha d\mathbf{k} \quad \text{with} \quad \psi_A^\alpha = \hbar \{c_\alpha k, k_i, \frac{c_\alpha}{k} k_{\langle i} k_{j \rangle}, \dots, \left(\frac{c_\alpha}{k}\right)^{n-1} k_{\langle i_1} k_{i_2} \dots k_{i_n \rangle}, \dots\}. \quad (\text{A } 7)$$

Variables with special physical meaning are

$$\begin{aligned} u_1^\alpha &= e^\alpha && \text{-- energy density of mode } \alpha \\ u_{2,3,4}^\alpha &= p_i^\alpha && \text{-- momentum density of mode } \alpha \\ u_{5,\dots,9}^\alpha &= N_{\langle ij \rangle}^\alpha && \text{-- momentum flux of mode } \alpha. \end{aligned}$$

Using the same methods as in Section 3 of this paper we obtain the following system of linear equations

$$\begin{aligned} \frac{\partial e^l}{\partial t} + c_l^2 \frac{\partial p_i^l}{\partial x_i} &= -2 \left[\frac{1}{\tau_R^l c_l^3 + 2\tau_R^l c_l^3} + \frac{1}{\tau_N^l c_l^3 + 2\tau_N^l c_l^3} \right] (c_l^3 e^l - c_l^3 e^t) \\ \frac{\partial p_i^l}{\partial t} + \frac{1}{3} \frac{\partial e^l}{\partial x_i} + \frac{\partial N_{\langle ij \rangle}^l}{\partial x_j} &= -\frac{1}{\tau_R^l} p_i^l - \frac{2}{\tau_N^l c_l^5 + 2\tau_N^l c_l^5} (c_l^5 p_i^l - c_l^5 p_i^t) \\ \frac{\partial N_{\langle ij \rangle}^l}{\partial t} + \frac{2}{5} c_l^2 \frac{\partial p_{\langle i}^l}{\partial x_{j \rangle}} + \frac{\partial}{\partial x_k} M_{\langle ijk \rangle}^l &= -\left(\frac{1}{\tau_R^l} + \frac{1}{\tau_N^l} \right) N_{\langle ij \rangle}^l \\ &\vdots \\ \frac{\partial u_{\langle i_1 \dots i_n \rangle}^l}{\partial t} + c_l^2 \frac{n}{2n+1} \frac{\partial u_{\langle i_1 \dots i_{n-1} \rangle}^l}{\partial x_{i_n}} + \frac{\partial u_{\langle i_1 \dots i_n k \rangle}^l}{\partial x_k} &= -\left(\frac{1}{\tau_R^l} + \frac{1}{\tau_N^l} \right) u_{\langle i_1 \dots i_n \rangle}^l \\ \\ \frac{\partial e^t}{\partial t} + c_t^2 \frac{\partial p_i^t}{\partial x_i} &= \left[\frac{1}{\tau_R^t + 2\tau_R^t c_t^3} + \frac{1}{\tau_N^t c_t^3 + 2\tau_N^t c_t^3} \right] (c_t^3 e^l - c_t^3 e^t) \\ \frac{\partial p_i^t}{\partial t} + \frac{1}{3} \frac{\partial e^t}{\partial x_i} + \frac{\partial N_{\langle ij \rangle}^t}{\partial x_j} &= -\frac{1}{\tau_R^t} p_i^t + \frac{1}{\tau_N^t c_t^5 + 2\tau_N^t c_t^5} (c_t^5 p_i^l - c_t^5 p_i^t) \\ \frac{\partial N_{\langle ij \rangle}^t}{\partial t} + \frac{2}{5} c_t^2 \frac{\partial p_{\langle i}^t}{\partial x_{j \rangle}} + \frac{\partial}{\partial x_k} M_{\langle ijk \rangle}^t &= -\left(\frac{1}{\tau_R^t} + \frac{1}{\tau_N^t} \right) N_{\langle ij \rangle}^t \\ &\vdots \\ \frac{\partial u_{\langle i_1 \dots i_n \rangle}^t}{\partial t} + c_t^2 \frac{n}{2n-1} \frac{\partial u_{\langle i_1 \dots i_{n-1} \rangle}^t}{\partial x_{i_n}} + \frac{\partial u_{\langle i_1 \dots i_n k \rangle}^t}{\partial x_k} &= -\left(\frac{1}{\tau_R^t} + \frac{1}{\tau_N^t} \right) u_{\langle i_1 \dots i_n \rangle}^t \end{aligned} \quad (\text{A } 8)$$

The total energy $e = e^l + 2e^t$ is conserved, but there is an exchange of energy between the modes unless

$$c_1^3 e_l - c_t^3 e^t = 0 \quad (\text{A } 9)$$

holds. This condition holds in equilibrium, where the phase density f^α is given by the Bose formula $f^\alpha = y / \left\{ \exp\left(\frac{\hbar c_\alpha k}{k_B T}\right) - 1 \right\}$.

Due to N-processes there is an exchange of momentum between the modes unless

$$c_1^5 p_i^l - c_i^5 p_i^t = 0. \quad (\text{A } 10)$$

Remark. Here we treat e^l and e^t as well as p_i^l and p_i^t as independent variables. This demands initial and boundary conditions for energy and momentum in each mode. This presents a problem because we can control the *total* heat flux $Q_i = c_i^2 p_i^l + 2c_i^2 p_i^t$ only. Whereas in equilibrium energy and momentum are distributed among the modes according to (A 9) and (A 10) additional theories must be used to determine the distribution of energy and momentum supplied at the heater. We refer to a paper by Weis [44] where this point is discussed as a question of coupling between heater and crystal. More over the anisotropy of real crystals leads to a focussing of longitudinal and transversal phonons in different propagation directions [45].

We will discuss the system (A 8) in two extreme limits only. In the limit of ballistic phonons, $\tau_R^\alpha \rightarrow \infty$, $\tau_N^\alpha \rightarrow \infty$, (A 8) reduces to two uncoupled systems of differential equations which read in the one-dimensional case

$$\frac{\partial u_A^\alpha}{\partial t} + \sum_B \mathfrak{C}_{AB}^\alpha \frac{\partial u_B^\alpha}{\partial x} = 0, \quad (\text{A } 11)$$

$$\text{with } \mathfrak{C}_{AB}^\alpha = \begin{bmatrix} 0 & 1 & & & & & & & \\ \alpha_1^\alpha & 0 & 1 & & & & & & O \\ & \alpha_2^\alpha & 0 & 1 & & & & & \\ & & \alpha_3^\alpha & 0 & 1 & & & & \\ & & \dots & \dots & \dots & & & & \\ & & & & & \dots & \dots & \dots & \\ & & & & & & & & \\ O & & & & & \alpha_{M-2}^\alpha & 0 & 1 & \\ & & & & & & \alpha_{M-1}^\alpha & 0 & \end{bmatrix} \quad \alpha_i^\alpha = c_\alpha^2 \frac{i^2}{4i^2 - 1}. \quad (\text{A } 11)$$

As discussed in Section 5.2 this system is capable of describing phonons with speed c_α .

We conclude that the system (A 8) describes ballistic phonons with speeds c_l and c_t , respectively.

In the limit of second sound $\tau_R^\alpha \rightarrow \infty$, $\tau_N^\alpha \rightarrow 0$ (A 8) may be reduced considerably. All quantities u_A which occur combined with τ_N in the form u_A / τ_N^α must vanish in order to guarantee finite values of the quotient. It follows

$$u_{\langle i_1 \dots i_n \rangle}^\alpha = 0 \quad \text{for } n = 2, 3 \dots M,$$

$$c_l^3 e^l - c_t^3 e^t = 0$$

$$c_l^5 p_i^l - c_t^5 p_i^t = 0 \quad (\text{A } 12)$$

The only non-vanishing quantities are total energy e and total momentum $p_i = p_i^l + 2p_i^r$ for which we obtain the balance laws

$$\frac{\partial e}{\partial t} + \frac{\zeta_5}{\zeta_3} \frac{\partial p_i}{\partial x_i} = 0$$

$$\frac{\partial p_i}{\partial t} + \frac{1}{3} \frac{\partial e}{\partial x_i} = 0 \quad \text{with} \quad \frac{3}{\zeta_n} = \frac{1}{c_l^n} + \frac{2}{c_r^n}. \quad (\text{A } 13)$$

This system describes waves of undamped second sound with the speed

$$V_{II} = \sqrt{\frac{1}{3} \frac{\zeta_5}{\zeta_3}}. \quad (\text{A } 14)$$

This velocity of second sound was also reported by Sussmann & Thellung [34] and Beck & Beck [36].

Appendix B

Solution of the N -field system with “ballistic initial values”

B.1 Ballistic initial values

The true initial-boundary value problem for the heat pulse experiment is impossible to solve because we cannot control the initial and boundary data of all moments. Therefore we shall now construct and solve an initial value problem which we believe represents an approximative model for the heat pulse experiment.

In the one-dimensional case the N -field system may be written as (3.58)

$$\frac{\partial u_A}{\partial t} + \sum_B \mathfrak{C}_{AB} \frac{\partial u_B}{\partial x} = -\frac{1}{\tau_A} u_A,$$

$$\mathfrak{C}_{AB} = \begin{bmatrix} 0 & 1 & & & & \\ \alpha_1 & 0 & 1 & & & O \\ & \alpha_2 & 0 & 1 & & \\ & & \alpha_3 & 0 & 1 & \\ & & & \dots & \dots & \dots \\ & & & & \dots & \dots & \dots \\ & & & & & \dots & \dots \\ O & & & & & \alpha_{M-2} & 0 & 1 \\ & & & & & & \alpha_{M-1} & 0 \end{bmatrix}, \quad \alpha_i = \frac{i^2}{4i^2 - 1} c^2, \quad A=0, 1, \dots, M$$

$$u_A = \{e/c^2, p_1, N_{(11)}, \dots\}, \quad A = 0, \dots, M, \quad u_{M+1} = 0$$

$$\frac{1}{\tau_A} = \left\{ 0, \frac{1}{\tau_R}, \frac{1}{\tau}, \dots, \frac{1}{\tau} \right\} \quad (\text{B } 1)$$

We ask for the values of the fields $u_A(x, t = 0)$, where $t = 0$ is the time when the heat pulse of duration Δt is just finished. $u_A(x, t = 0)$ will be taken as initial values.

During the time Δt phonons are produced at the heater and travel into the crystal. We assume that these phonons do not interact with other phonons during the heating period. In other words: The new phonons travel ballistically into the crystal for $t \in (-\Delta t, 0)$.

In this case phonon momentum and energy must satisfy

$$p_1 = \frac{V}{c^2} \bar{e} = V u_1 \quad (\text{B } 2)$$

where \bar{e} is the deviation of the energy from its equilibrium value and V is the velocity of ballistic phonons.*

For ballistic propagation we may cancel the production terms $-u_A/\tau_A$ in (B 1)₁ and by introducing this and (B 2) in the field equations (B 1)₁ it follows, that

$$u_A = X_A u_1; \quad X_0 = 1, \quad X_1 = V \quad A = 0 \dots M \quad (\text{B } 3)$$

must hold.

For the field equations we obtain

$$\frac{\partial u_1}{\partial t} + \sum_B \frac{1}{X_A} \mathfrak{C}_{AB} X_B \frac{\partial u_1}{\partial x} = 0 \quad t \in (-\Delta t, 0), \quad A, B = 0, 1, \dots M. \quad (\text{B } 4)$$

These are $M + 1$ equations for the energy density u_1 which must be identically satisfied. Hence follows

$$\sum_B \frac{1}{X_A} \mathfrak{C}_{AB} X_B = A_2 = V \quad \text{or} \quad \sum_B (\mathfrak{C}_{AB} - V \delta_{AB}) X_B = 0. \quad (\text{B } 5)$$

This means that X_B is the right eigenvector of \mathfrak{C} corresponding to the eigenvalue V . Recall that V is the biggest eigenvalue of \mathfrak{C} .

Thus during the heat pulse all fields u_A obey the differential equation

$$\frac{\partial u_A}{\partial t} + V \frac{\partial u_A}{\partial x} = 0. \quad (\text{B } 7)$$

We assume the temperature – or equivalently the energy density – at the heater ($x = 0$) given as shown in Fig. B.1.

Fig. B.2. shows the energy density as function of space at time $t = 0$, which follows from (B 7) with the boundary condition Fig. B.1.

* Naturally $V = c$ should hold ($p_{ph} = \hbar \mathbf{k}$, $e_{ph} = \hbar c k$) but this is only true if the number N of variables reaches infinity (see Fig. 5.5)

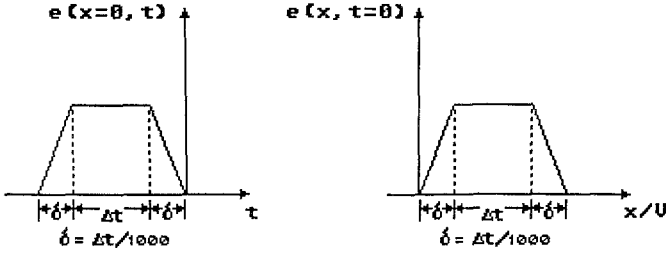


Fig. B.1./B.2. Boundary condition for $u_1 = e$ and energy density at time $t = 0$

The fields $u_A(x, t = 0)$ follow from (B 3) as

$$u_A(x, t = 0) = X_A u_1(x, t = 0) = X_A u^0(x) \quad (\text{B } 8)$$

These functions will be taken as initial values for the initial value problem.

B.2 Solution of initial value problem

Instead of solving the true initial-boundary-value problem for the heat pulse experiment for the finite crystal we consider an infinite crystal with the initial conditions (B 8). We expect solutions of (B 1) in the form of plane waves

$$u_A = C_A \exp i(\Omega t - qx). \quad (\text{B } 9)$$

From (B 9) and (B 1) we obtain

$$\left[\Omega \delta_{AB} - \left(\mathfrak{C}_{AB} q + \frac{i}{\tau_A} \delta_{AB} \right) \right] C_B = 0. \quad (\text{B } 10)$$

(B 10) is the eigenvalue problem of the matrix $\mathfrak{C}_{AB} q = \frac{i}{\tau_A} \delta_{AB}$ with the eigenvalue $\Omega^{(c)}(q)$ and the right eigenvectors $C_B^{(c)}(q)$ ($c = 0, 1, \dots, M$).

(B 9) is a solution of (B 1) for every eigenvalue $\Omega^{(c)}$ and the corresponding eigenvector $C_B^{(c)}$ and for every value of q .

Superposition yields the general solution of (B 1)

$$u_A = \int_{-\infty}^{\infty} \sum_{c=0}^M C_A^{(c)}(q) \exp i(\Omega t - qx) dq. \quad (\text{B } 11)$$

Adapting the ballistic initial conditions we obtain the solution

$$u_B(x, t) = \sum_{c,D} \int_{-\infty}^{\infty} R_B^{(c)}(q) L_D^{(c)}(q) X_0 W(q) \exp i(\Omega t - qx) dq \quad (\text{B } 12)$$

with

$$\begin{cases} R_B^{(c)} & - \text{right eigenvectors} \\ L_B^{(c)} & - \text{left eigenvectors} \\ \Omega^{(c)} & - \text{eigenvalues} \end{cases} \left\{ \text{of } \mathfrak{C}_{AB} q + \frac{i}{\tau_A} \delta_{AB} \right.$$

$$\left(\text{with } \sum_A L_A^{(c)} R_A^{(D)} = \delta_{cD} \right)$$

X_D – right eigenvector corresponding to the biggest eigenvalue of \mathfrak{C}_{AB}

$$W(q) = \frac{1}{2\pi} \int_{-\infty}^{\infty} u^0(x) \exp iqx \, dx \text{ – Fourier-transform of the initial condition}$$

A further analytical reduction of (B.12)₁ is not possible, the evaluation must be done numerically.

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