Physica D 266 (2014) 65–79

Contents lists available at ScienceDirect

Physica D

journal homepage: www.elsevier.com/locate/physd

Influence of nonlinearity of the phonon dispersion relation on wave velocities in the four-moment maximum entropy phonon hydrodynamics

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HIGHLIGHTS

- The four-moment maximum entropy phonon gas hydrodynamics is discussed.
- The weak discontinuity waves propagating into an equilibrium state are considered.
- The nonlinear isotropic approximation of the phonon dispersion relation is assumed.
- It is shown that the wave-front velocity decreases with increasing temperature.
- The comparison with the second-sound experimental data for NaF and Bi is performed.

ARTICLE INFO

Article history:
Received 2 February 2013
Received in revised form
28 August 2013
Accepted 14 October 2013
Available online 22 October 2013
Communicated by V.M. Perez-Garcia

Keywords:
Phonon hydrodynamics
Waves in phonon gas
Genuine nonlinearity
Nonlinear phonon dispersion relation
Second sound

ABSTRACT

This paper analyzes the propagation of the waves of weak discontinuity in a phonon gas described by the four-moment maximum entropy phonon hydrodynamics involving a nonlinear isotropic phonon dispersion relation. For the considered hyperbolic equations of phonon gas hydrodynamics, the eigenvalue problem is analyzed and the condition of genuine nonlinearity is discussed. The speed of the wave front propagating into the region in thermal equilibrium is first determined in terms of the integral formula dependent on the phonon dispersion relation and subsequently explicitly calculated for the Dubey dispersion-relation model: $|\boldsymbol{k}| = \omega c^{-1}(1 + b\omega^2)$. The specification of the parameters c and b for sodium fluoride (NaF) and semimetallic bismuth (Bi) then makes it possible to compare the calculated dependence of the wave-front speed on the sample's temperature with the empirical relations of Coleman and Newman (1988) describing for NaF and Bi the variation of the second-sound speed with temperature. It is demonstrated that the calculated temperature dependence of the wave-front speed resembles the empirical relation and that the parameters c and b obtained from fitting respectively the empirical relation and the original material parameters of Dubey (1973) are of the same order of magnitude, the difference being in the values of the numerical factors. It is also shown that the calculated temperature dependence is in good agreement with the predictions of Hardy and Jaswal's theory (Hardy and Jaswal, 1971) on second-sound propagation. This suggests that the nonlinearity of a phonon dispersion relation should be taken into account in the theories aiming at the description of the wave-type phonon heat transport and that the Dubey nonlinear isotropic dispersion-relation model can be very useful for this purpose.

1. Introduction

In [1], we have studied the four-moment maximum entropy phonon hydrodynamics involving a nonlinear isotropic phonon dispersion relation and a relaxation time for resistive processes. One of the objectives of that study was to verify whether the purely phenomenological theories of wave-type phonon heat transport [2–13] are consistent with the phonon gas hydrodynamics. Contrary to our kinetic-theory approach, the phenomenological modeling of the heat waves does not take into account the microscopic description of a phonon gas. Instead, in order to specify the unknown functions, it makes use of the empirical relations describing the dependence of the second-sound speed on the temperature. These relations were introduced by Coleman and Newman [2], who deduced them from an analysis of the second-sound experimental data for sodium fluoride (NaF) [14–16] and semimetallic bismuth (Bi) [17]. In the phenomenological theories, the heat waves are represented by the wave fronts of either the waves of weak discontinuity [2,8,13] or the waves of strong discontinuity (shocks) [5–7, 10,11] propagating into the region in thermal equilibrium.

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http://dx.doi.org/10.1016/j.physd.2013.10.006

Phonons are quantized lattice vibrations that carry energy $\hbar\omega$ and quasi-momentum $\hbar\boldsymbol{k}$, where $\hbar$ is the Planck constant divided by 2π, ω is the frequency of a phonon, and $\boldsymbol{k}$ is its wave vector. The frequency ω depends on the wave vector $\boldsymbol{k}$. This dependence is defined by the relation between ω and $\boldsymbol{k}$ called the phonon dispersion relation. In the macroscopic (hydrodynamic) description of a phonon gas, the phonon dispersion relation is one of the elements determining the specific constitutive properties of the medium. It is usually assumed that the linear approximation of a phonon dispersion relation can be applied to the description of phonon processes at low temperatures, particularly when discussing the second-sound propagation. Hence, almost all theories of second sound employed this approximation [18–24]. To the best of our knowledge, the theory of Hardy [25] is the only theory which examined the influence of nonlinearity of the phonon dispersion relation on the values of the second-sound speed [26]. Except for this theory, the observed dependence of the second-sound speed on the sample's temperature was attributed to the variation of the two effective phonon relaxation times with temperature [21–23]. In this context, one should also note that any maximum entropy phonon gas hydrodynamics based on the linear isotropic phonon dispersion relation (such as, e.g., the four-moment hydrodynamics [27] and the nine-moment hydrodynamics [28]) predicts that the speeds of the weak-discontinuity waves propagating into the region in thermal equilibrium are the constant quantities independent of the temperature of a phonon gas ahead of the wave fronts. We now see that the nonlinear phonon dispersion relation must be introduced in order to ensure the existence of temperature-dependent wave-front speeds. In the present paper, this fact is demonstrated for the case of the nonlinear four-moment phonon gas hydrodynamics proposed in [1].

Dubey [29] calculated the lattice thermal conductivity of NaF in the temperature range from 2 K to 100 K. Sharma et al. [30] presented the calculation of the phonon conductivity of germanium between temperatures of 2 K and 1000 K. These authors and many other authors [31–34] investigated various theoretical fits to the thermal-conductivity data using Callaway's relaxation-time formalism [35], and they found that at all temperatures the nonlinearity of a phonon dispersion relation played an important role in fitting the data of lattice thermal conductivity. Consequently, assuming isotropic dispersion, a number of nonlinear phonon dispersion models (such as the Sharma–Dubey–Verma model [30], Tiwari–Agrawal model [31], the Brillouin zone boundary condition model [32], etc.) have been proposed and tested. With these observations in mind, the natural question then arises concerning the role of nonlinearity of the phonon dispersion relation in the propagation of heat waves in a phonon gas. Also, the question arises as to whether it is possible to effectively apply the nonlinear isotropic dispersion-relation models to the analysis of wave phenomena.

In this paper, we follow the approach of Dubey [29]. Thus, instead of considering the linear isotropic phonon dispersion relation $\omega = c|\boldsymbol{k}|$, we consider an improved dispersion relation $|\boldsymbol{k}| = \omega c^{-1}(1 + b\omega^2)$, where $\boldsymbol{k}$ is, as before, the phonon wave vector, ω is the angular frequency of the phonon moving with velocity c, and $b > 0$ is a suitably chosen constant parameter. Such a nonlinear isotropic model of the phonon dispersion relation was originally used to calculate the thermal conductivity of NaF [29] and germanium [30,31]. Here, after its appropriate adjustment to the single-branch approximation of phonon excitations, we apply it to the four-moment maximum entropy phonon hydrodynamics [1]. Therefore, we substitute the dispersion relation $|\boldsymbol{k}| = \omega c^{-1}(1 + b\omega^2)$ into the equations of this hydrodynamics. As a consequence, we obtain the system of equations depending on the two parameters c and b. The specification of these parameters for NaF and Bi then makes it possible to compare the calculated wave speeds with both the empirical relations of Coleman and Newman [2] for the second-sound speeds and the predictions of Hardy and Jaswal's linear theory [26] for them. Such comparisons need to be done because our aim is to assess the influence of nonlinearity of the phonon dispersion relation $\omega = \omega(\boldsymbol{k})$, whose nonlinearity with respect to $\boldsymbol{k}$ is modeled by a simple isotropic formula, on the temperature dependence of the propagation speeds of pulses in a phonon gas. For this purpose, we apply a very simple analysis based on the study of the propagation of the weak-discontinuity wave front into the region in thermal equilibrium.

It was proved in [36] that, for a one-dimensional quasi-linear hyperbolic system with dissipation, the velocity of the wave of weak discontinuity propagating into the region in equilibrium – i.e., the equilibrium characteristic velocity – coincides with the high-frequency limit of the phase velocity of the harmonic wave solutions of this hyperbolic system linearized around constant equilibrium states. Therefore, the analysis of plane harmonic waves in the linearized one-dimensional phonon gas hydrodynamics is also presented as an alternative to the discontinuity wave analysis, and the contribution of the nonlinear phonon dispersion relation to the limiting linear dispersion relation for harmonic waves is indicated.

The condition of genuine nonlinearity and the effect of linear degeneracy play an important role in the analysis of the wave-type solutions of the hyperbolic systems of conservation equations [37]. In [6,8], this condition has been analyzed for the case of the equations governing the phenomenological model of phonon heat transport developed in [3,4]. If the condition of genuine nonlinearity holds, then there exists a critical time such that the amplitude of the wave of weak discontinuity becomes unbounded, provided the initial wave amplitude assumes a suitable value. If the linear degeneracy occurs at some isolated points of the state space, henceforth referred to as the critical points, one can prove in turn the existence of different regimes for the wave propagation. In [6,8], it has been found that the loss of genuine nonlinearity takes place in the case of the phenomenological model of phonon heat transport [3,4], and the critical values of the temperature have also been determined. Here, we show that the same effect occurs in the case of the equations of the four-moment phonon gas hydrodynamics derived in [1]. For NaF and Bi, we calculate the critical temperatures predicted by the phonon gas hydrodynamics involving the dispersion relation $|\boldsymbol{k}| = \omega c^{-1}(1 + b\omega^2)$ and compare them with those calculated in [6,8].

The calculated dependence of the wave-front speed on the temperature resembles the empirical relation of Coleman and Newman [2]. Namely, we find that the wave-front speed decreases as the temperature is increased. The coefficients in $|\boldsymbol{k}| = \omega c^{-1}(1 + b\omega^2)$ obtained from fitting respectively the empirical relation and the original phonon dispersion relations of Dubey [29] are of the same order of magnitude, the difference being in the values of the numerical factors. We note that the empirical relation of Coleman and Newman was deduced from measurements of the propagation speed of the peak of the second-sound pulse preceded in the experiment by the ballistic pulse. Thus, it is a rough approximation to assume that the second-sound pulse propagates into the region in thermal equilibrium. This fact is probably one of the reasons of discrepancy between our calculations and the empirical relation. Another reason is that the derivation of the four-moment hydrodynamics rests upon certain simplifying conditions. Therefore, the four-moment hydrodynamics cannot be treated as an accurate theory for describing the second-sound propagation.

To sum up, our analysis suggests that the nonlinearity of a phonon dispersion relation is an important factor that makes the second-sound speed temperature dependent. Consequently, the theories aiming at the description or explanation of the phonon heat transport should take into account this nonlinearity. The Dubey nonlinear isotropic dispersion-relation model [29] seems to be very useful for this purpose.