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ORIGINAL PAPER

ZAMM

Thermal processes in a one-dimensional crystal with regard for the second neighbor interaction

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An influence of the second neighbor interaction on the process of heat propagation in a one-dimensional crystal is studied. Previously developed model of the ballistic nature of the heat transfer is used. It is shown that the initial thermal perturbation evolves into two consecutive thermal wave fronts propagating with finite and different velocities. The velocity of the first front corresponds to the maximum group velocity of the discrete crystalline model. The velocity of the second front is determined by the second group-velocity extremum, which arises at a certain ratio between the stiffnesses of the first and second neighbor interaction in the lattice.

KEYWORDS
lattice, thermal processes, wave

INTRODUCTION

At the macroscopic level, heat propagation in a majority of materials is described by Fourier's law, which assumes a linear relationship between the heat flux and the temperature gradient with a proportionality coefficient, defined as the thermal conductivity coefficient. However, at small temporal and spatial scales, noticeable deviations from the Fourier law are observed.[1,2] An understanding of the heat transfer at the microlevel is essential to get a connection between the microscopic and macroscopic description of solids.

The lattice dynamics is a powerful tool for a joint description of the mechanical processes at the micro- and macrolevel.[4–13] It is known[17–19] that in the simplest discrete systems, such as a one-dimensional harmonic crystal (chain of material points interacting with the linearized in strains forces), the heat propagation does not obey the Fourier law. The main reason is that the ballistic heat transfer dominates at the microlevel, in contrast to the macrolevel where the diffusive (Fourier) heat conduction prevails. The anomalies associated with the ballistic heat transfer are the most noticeable for a harmonic crystal.

At present, the problem of the non-stationary thermal processes at the molecular level has an exact analytical solution only for a limited class of systems. Considerable progress has been achieved for harmonic crystals.[19–21,24,25,27,28] An analytical description of the ballistic heat transfer in harmonic lattices has been developed in [22,23]. For a one-dimensional nonquantum case, it allows us to obtain the macroscopic heat conduction equation and the corresponding anomalous heat conduction law (alternative to the Fourier law). This law predicts the finite velocity of the thermal fronts and the independence of the heat flux on the length of the crystal. Using the correlation analysis, the initial stochastic problem for individual particles is reduced to a deterministic problem for the statistical characteristics of the crystal. The expansion of this approach to the heat propagation in the multi- dimensional systems is obtained in [25,27,28]. The investigation of the solutions of the equation for slow thermal processes at different initial thermal perturbations is carried out in [26].

An influence of non- neighboring particles on the processes in discrete media is an important issue. The dynamic features of the discrete systems with the additional non-neighboring interactions are studied in [14–16]. The detailed influence of the

particles of the second neighbor interaction on the heat propagation has not been studied previously. In the presented paper, the concept of a non-local temperature (a generalization of the kinetic temperature for two separate particles) is used to obtain a closed system of equations for a description of the heat transfer in the one-dimensional harmonic crystal with taking into account the interaction with the second coordination sphere. An analysis of the discrete crystalline model is performed to obtain the dispersion relation and the group velocities which are further used in the framework of previously developed ballistic heat transfer model. We consider the initial thermal perturbations in the form of the Heaviside function and a rectangular pulse to obtain numerical solutions describing arising of two waves due to an influence of non-neighboring interactions in the lattice.

1 | STATEMENT OF THE PROBLEM

Consider thermal processes in a one-dimensional crystal consisting of identical masses m taking into account the interaction with the second neighbors. It was shown in Ref. [25] that the evolution of an initial temperature field $T_0(x)$ in an arbitrary one-dimensional infinite scalar lattice is

$$T(x,t) = \frac{1}{4\pi}\int_0^{\pi} \big(T_0\big(x - c_{gr}(ak)t\big) + T_0\big(x + c_{gr}(ak)t\big)\big)\mathrm{d}(ak), \tag{1}$$

where $c_{gr}(ak)$ is the group velocity function, k is the wave number, a is the lattice constant. Equation 1 results after using the correlation analysis to reduce the initial stochastic problem to a deterministic one for the statistical characteristics of the crystal, it reflects the ballistic nature of the heat transfer. Implementation of Equation 1 requires knowledge of the group velocity. To obtain the group velocity, we consider the discrete equation of motion of the one-dimensional crystalline lattice with non-neighboring interactions,

$$m\ddot{u}_n = C_1\big(u_{n+1} - 2u_n + u_{n-1}\big) + C_2\big(u_{n+2} - 2u_n + u_{n-2}\big), \tag{2}$$

where u_n is the displacement of the n-th particle, C_1 is the stiffness of the coupling between neighboring particles, C_2 is the stiffness of the second neighbor interaction.

We use the following notation for the stiffnesses,

$$C_0 \overset{\text{def}}{=} C_1 + 4C_2\,, \tag{3}$$

which allows us to rewrite the equation of motion in the form

$$4m\ddot{u}_n = C_0\big(u_{n+2} - 2u_n + u_{n-2}\big) - C_1\big(u_{n+2} - 4u_{n+1} + 6u_n - 4u_{n-1} + u_{n-2}\big). \tag{4}$$

This emphasizes the second order difference for the particles of only the second neighbor interaction.

When only the stiffness of the connection between the nearest neighbors is considered, $C_2 = 0$, then $C_0 = C_1$, and equation of motion (4) is

$$m\ddot{u}_n = C_1\big(u_{n+1} - 2u_n + u_{n-1}\big). \tag{5}$$

If we take into account only the stiffness of the connection between the second neighbors, $C_1 = 0$, then $C_0 = 4C_2$, and equation (4) is

$$m\ddot{u}_n = C_2\big(u_{n+2} - 2u_n + u_{n-2}\big). \tag{6}$$

Equation (6) is similar to Equation (5) with the duplicated distance between the particles. Note that the stiffness C_2 can take both positive and negative values. For a critical negative value $C_2 = -\frac{1}{4}C_1$, we obtain $C_0 = 0$, and Equation (4) contains a finite difference of the fourth order,

$$4m\ddot{u}_n = C_1\big(u_{n+2} - 4u_{n+1} + 6u_n - 4u_{n-1} + u_{n-2}\big). \tag{7}$$

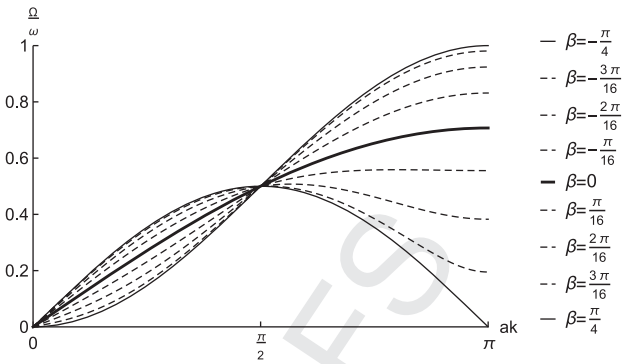

FIGURE 1 Dispersion characteristic of the waves at different values of the parameter β

2 | DISPERSION RELATION

Substitution of the solution in the form $u_n = Ae^{i(akn-\Omega t)}$ into Equation (4) gives rise to the dispersion relation,

$$\Omega^2 = 4\sin^2\frac{ak}{2}\left(\omega_0^2\cos^2\frac{ak}{2} + \omega_1^2\sin^2\left(\frac{ak}{2}\right)\right), \tag{8}$$

where Ω is the wave frequency,

$$\omega_0 \overset{\text{def}}{=} \sqrt{\frac{C_1+4C_2}{m}}, \qquad \omega_1 \overset{\text{def}}{=} \sqrt{\frac{C_1}{m}}. \tag{9}$$

The constants ω_0^2 and ω_1^2 should be positive for real values of the wave frequencies, then

$$C_1 > 0, \qquad C_1 \geq -4C_2. \tag{10}$$

Since the rigidity C_2 can be of either sign it is convenient to introduce the parameters ω and β,

$$\omega_0^2 \overset{\text{def}}{=} \omega^2\sin^2\left(\beta+\frac{\pi}{4}\right), \qquad \omega_1^2 \overset{\text{def}}{=} \omega^2\cos^2\left(\beta+\frac{\pi}{4}\right). \tag{11}$$

Then the parameter β is expressed through the ratio of the stiffnesses,

$$\tan\left(\beta+\frac{\pi}{4}\right) = \frac{\omega_0}{\omega_1} = \sqrt{\frac{C_1+4C_2}{C_1}}. \tag{12}$$

The parameter ω plays the role of a scalar factor in the dispersion relation and doesn't change the behavior of the system. Important variations are described by the parameter β. For negative values of C_2, the parameter β is also negative. Then dispersion relation (8) is expressed through the parameters ω and β,

$$\Omega^2 = \frac{\omega^2}{2}(1+\sin 2\beta\cos a\,k)(1-\cos a\,k), \tag{13}$$

Figure 1 shows a family of dispersion curves corresponding to the different values of the parameter β, which varies within the finite interval $(-\pi/4,\ \pi/4)$. For $\beta = 0$, there is no connection with the second neighbors, and the system is described by Equation (5). For $\beta = \pi/4$, the connection between the second neighbors plays the main role. In fact, the lattice is considered, in which the particles are located at the double distance from each other in comparison to the original one. This is described by Equation (6). The value $\beta = -\pi/4$ corresponds to the limiting value of the negative stiffness $C_2 = -C_1/4$, when the lattice is described by Equation (7).

The group velocity is

$$c_{gr} = \frac{d\Omega}{dk} = \frac{a\omega\sin ak(1+(2\cos ak-1)\sin 2\beta)}{4\sqrt{(1-\cos ak)(1+\cos ak\sin 2\beta)}}, \tag{14}$$

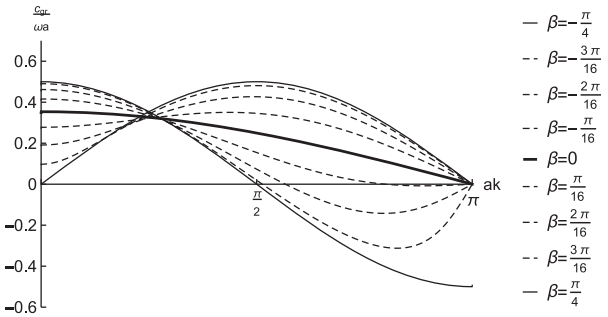

FIGURE 2 Group velocity at different values of the parameter β

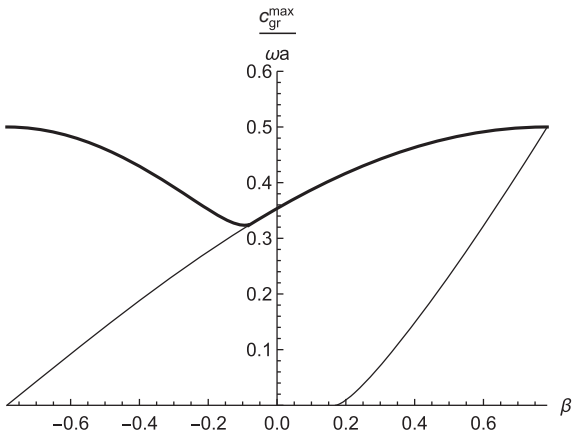

FIGURE 3 Maximum group velocity at different values of the parameter β

TABLE 1

β	$-\frac{\pi}{4}$	0	$\frac{\pi}{4}$
Equation of motion	$\ddot{u} = -c^4 u''''$	$\ddot{u} = c^2 u''$	$\ddot{u} = c^2 u''$
Dispersion relation	$\Omega^2 = \omega^2 \sin^4 \frac{ak}{2}$	$\Omega^2 = \frac{\omega^2}{2} \sin^2 \frac{ak}{2}$	$\Omega^2 = \frac{\omega^2}{4} \sin^2 ak$
Group velocity	$\frac{a\omega}{2} \sin ak$	$\frac{\sqrt{2}a\omega}{4} \cos \frac{ak}{2}$	$\frac{a\omega}{2} \cos ak$

Its dependence on the parameter β is shown in Figure 2. The maximum value of the group velocity determines the maximum speed of the energy propagation in the system. For $\beta \geq 0$, the maximum group velocity is $c_{gr}^{max} = \frac{\sqrt{2}}{4}\sqrt{1+\sin 2\beta}$. For $\beta < 0$ it is not possible to obtain a similar expression for the maximum group velocity. It should be noted that the maximum values of the group velocity coincide when $\beta = \frac{\pi}{4}$ and $\beta = -\frac{\pi}{4}$. There is an interval of the values of β when the curve of the group velocity has two extrema in Figure 2. Shown in Figure 3 is the difference in the group-velocities corresponding to the different extrema. The thick line accounts for the fastest thermal wave while the thin line corresponds to the propagation velocity of the second heat wave. The deviation in the velocities doesn't exist without non-neighboring interactions in the lattice model.

Table 1 contains the continuum equations of motion, dispersion relations and group velocities that correspond to the different values of the parameter β. The continuum equations are obtained as a first order approximation of discrete equations (5), (6), (7), the parameter c is the propagation velocity of the long waves in the crystal. To obtain the dispersion relations and expressions for the group velocities, Equations (13), (14) have been used.

3 | NUMERICAL STUDY OF HEAT PROPAGATION

The evolution of an initial temperature perturbation, $T_0(x)$, numerical simulation of Equation (1) is performed with the group velocity c_{gr} defined by Equation (14). The initial thermal perturbation is chosen in the form of Heaviside's function,

$$T_0(x) = T_0 H(x), \quad \dot{T} = 0. \tag{15}$$

where T_0 is the constant amplitude.

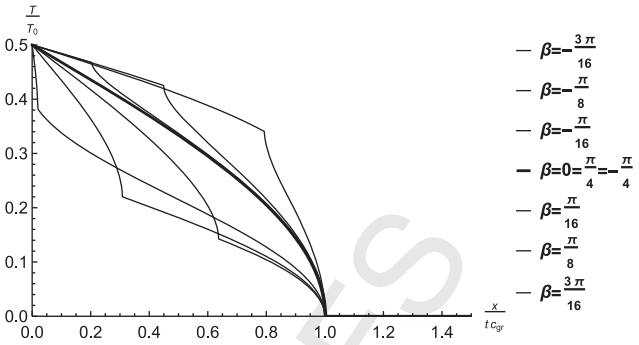

FIGURE 4 Evolution of the initial thermal perturbation (15) at different values of the parameter β

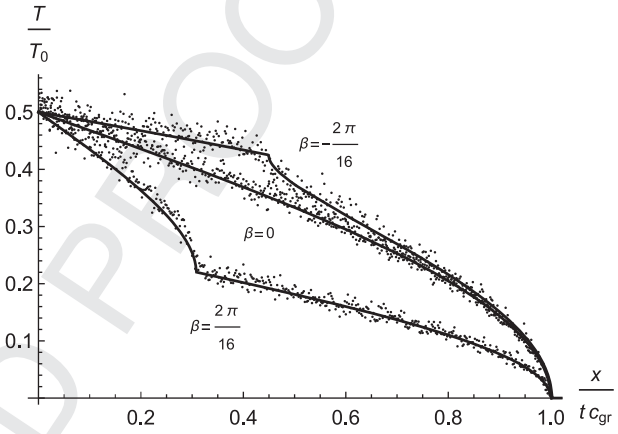

FIGURE 5 Comparison of the heat propagation with the initial perturbation in the form of the Heaviside function for different values of the parameter β (solid lines) with the results of the numerical simulation by the particle dynamics method (points)

Numerical integration of the equation (1) for various values of the parameter β is shown in Figure 4. It should be noted that the curves for $\beta = \pi/4$, $\beta = -\pi/4$ and $\beta = 0$ are the same. There exist the values of β when the curves are not smooth and the group velocity has two extrema (see Figure 2).

To verify the evolution of the temperature field described by Equation(1), the particle dynamics method has been employed. A sample of 1000 particles is considered, for which the equation (2) is solved with the mirror boundary conditions and the initial conditions,

$$u_n\,|_{t=0} = 0, \quad \dot{u}_n\,|_{t=0} = \sigma^2(x)\varrho_n, \tag{16}$$

where $\dot{u}_n$ — velocity of the n-th particle, ϱ_n are independent random variables with zero expectation and unit variance; σ^2 is variance of the initial velocities of the particles.

The kinetic temperature for a harmonic crystal with identical masses, m, is introduced as:

$$k_B T = m\langle \dot{u}_k \rangle^2, \tag{17}$$

where $\langle .. \rangle$ is the operator of averaging over implementations, k_B is Boltzmann's constant. A comparison of the dependencies obtained by Equation (1) with the results of the numerical simulation for the parameter values $\beta = 0$, $\beta = \frac{\pi}{8}$ and $\beta = -\frac{\pi}{8}$ is shown in Figure 5. It can be seen that the points showing the values of the kinetic temperature are located near the numerical solution obtained by the particle dynamics method.

Consider the initial thermal perturbation in the form of a rectangular pulse,

$$T_0(x) = T_0(H(x + l) - H(x - l)), \quad \dot{T} = 0. \tag{18}$$

These initial conditions correspond to a temperature perturbation produced by a laser pulse.[29] In classical thermal conductivity, the maximum is observed at the point x = 0, which decays exponentially. In the case of anomalous thermal conductivity, the solution attenuates faster near zero, forming four fronts, which pairwise propagate in the opposite directions with the constant velocities. Figures 6 and 7 describe the evolution of the temperature profile in a one-dimensional crystal ((1) under the initial conditions (18)) over the time interval ($t_0 < t_1 < t_2 < t_3$) for $\beta = \frac{\pi}{8}$ and $\beta = -\frac{\pi}{8}$, respectively. The choice of the value of β is

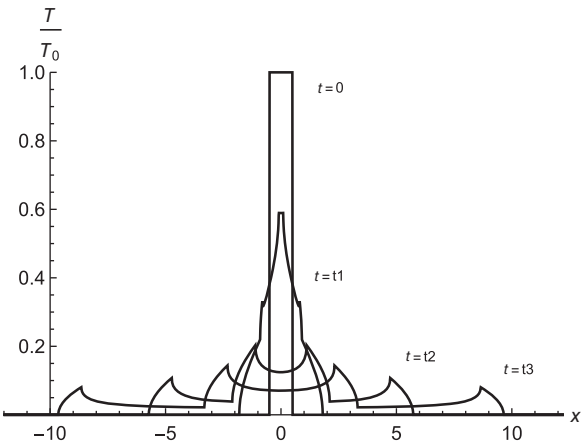

FIGURE 6 Heat propagation with the initial perturbation in the form of a rectangular temperature distribution at $\beta = \frac{\pi}{8}$

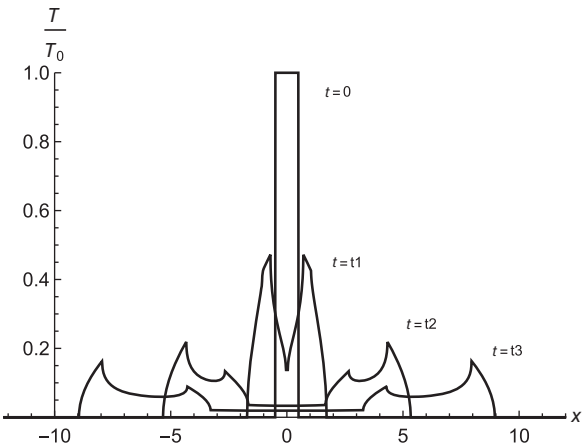

FIGURE 7 Heat propagation with the initial perturbation in the form of a rectangular temperature distribution at $\beta = -\frac{\pi}{8}$

motivated by our analysis of the dispersion relation revealing two extrema for the group velocities in Figures 2, 3. Two pairs of waves propagate symmetrically in the opposite directions. The velocity of the first wave is equal to the maximum group velocity (14). The velocity of the second wave corresponds to the second extremal group velocity shown by thin lime in Figure 3.

4 | CONCLUSION

The paper deals with the process of heat propagation in the model of the one-dimensional harmonic crystal taking into account the influence of the second neighbor interactions. An equation describing the evolution of the temperature field is studied. The temperature field is represented as a superposition of the waves having a shape of an initial temperature distribution and traveling with the group velocity. It is shown, that the presence of non-neighboring interactions leads to the formation of two thermal waves. The maximum value of the group velocity determines the maximum speed of the energy propagation in the system. The first wave propagates with the maximum group velocity. The velocity of the second wave is determined by the second extremum of the curve of the group velocity, which exists at certain ratio between the stiffness of the first and second neighbor interactions. In addition, in the case of the stiffnesses of different signs, the second wave has a profile opposite to that of the first wave. Comparison of the analytical results with the numerical simulations confirms the validity of the developed theory.

The presence of the second heat wave has some analogies with the phenomenon of the second sound. The existence of the second sound was predicted theoretically in the superfluid liquid helium by L.D. Landau.[30] It was shown that along with the usual sound in helium, sound can propagate when, on the whole, the mass does not move, and the oscillations of the normal and superfluid parts occur relative each other. The heat containing part of the helium oscillates relative to the rest of the helium. Later, the second sound was experimentally detected in liquid and solid helium.[31,32] Although the nature of the second sound is somewhat different than that of the processes considered in this paper, in both cases we observe two waves that propagate at different speeds. It is possible that further research will reveal a closer relationship between these two phenomena.

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