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Heat Propagation in a One-Dimensional Harmonic Crystal on an Elastic Foundation

A. M. Krivtsov[1,2]*, M. B. Babenkov[1,2], and D. V. Tsvetkov[1]

[1] *Peter the Great St. Petersburg Polytechnic University, St. Petersburg, 195251 Russia*
[2] *Institute for Problems in Mechanical Engineering, Russian Academy of Sciences, St. Petersburg, 199178 Russia*
* *e-mail: akrivtsov@mail.ru*

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Abstract—A closed system of differential equations has been derived to describe thermal processes in a one-dimensional harmonic crystal on an elastic foundation. It is shown that the evolution of thermal perturbation in such a crystal is described by a discrete unsteady-state equation, a special case of which is the hyperbolic equation of ballistic heat conduction. This equation remains valid with negative stiffness of bonds between particles of the crystal in its entire stability range. The thermal perturbation front propagates with the maximum group velocity of mechanical waves. The propagation of a short-term thermal perturbation in the crystal on the elastic foundation is determined by the equation of ballistic thermal conductivity of the same type as in the crystal without an elastic foundation. The only parameter of this equation is the maximum group velocity (in absolute value), i.e., the maximum rate of energy propagation in the crystal on the elastic foundation. This quantity is proportional to the absolute value of the half-difference of the upper and lower cutoff frequencies. The rate of heat wave propagation in the crystal on the elastic foundation with positive stiffness is always lower than that in the crystal without an elastic foundation. The obtained equation is found to be valid both for positive stiffness values and for negative ones, for which the chain stability condition is satisfied. As an example, a dynamic problem of heat distribution is solved exactly for a parabolic initial temperature profile to model heating of a one-dimensional crystal on a foundation by a short laser pulse. Due to the dispersion of mechanical waves in the chain on the foundation, their group velocity depends on the wave number and the ratio of bond stiffnesses in the chain and the elastic foundation. The thermal front propagates with the maximum possible group velocity in the system, which depends only on this ratio.

Keywords: one-dimensional crystal, thermal conductivity, elastic foundation, negative stiffness coefficient, group velocity, covariance

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1. INTRODUCTION

Modern technologies give specimens of a one-dimensional carbon crystal (carbyne), with more than 6 thousand carbon atoms assembled inside a double-wall carbon nanotube [1]. One-dimensional crystals consisting of atoms of various substances (the so-called "ionic crystals") can be grown inside carbon nanotubes providing their stability [2]. The development of technologies producing one-dimensional structures raises the question of physical properties of the synthesized objects. The theoretical prediction [3] points to their excellent heat conductivity and applicability, for example, to contact heat removal in MEMS/NEMS and in molecular electronics when natural convection and radiation cooling is difficult or impossible.

To synthesize stable one-dimensional structures, which are highly chemically active, it is necessary to use a molecular "thermostat", the role of which is played by a double-wall carbon nanotube [2]. The system of the carbon nanotube and the one-dimensional crystal can be modeled, in linear approximation, as a one-dimensional chain of masses with a harmonic potential of interaction of particles with each other and with the rigid foundation. During linearization of the complex interaction potential between material particles located in the field of the foundation potential, the interatomic bond stiffness may be negative [4] and, in some cases, asymmetric [5]. The heat transfer

equation obtained in this work is applicable to both positive and negative bond stiffnesses provided that the system is stable.

The discreteness of the atomic structure of matter significantly affects wave processes in it [6, 7], introducing dispersion into the wave propagation law. The presence of free electrons of thermal conduction in the conductor lattice gives rise to a photoacoustic effect that influences the propagation of mechanical waves [8]. Mechanical waves propagating in a system with the foundation potential demonstrate the filtering law of dispersion characterized by the lower and upper cutoff frequencies. Similar effects arise in nanostructures, in particular, in the array of parallel nanosized oscillators. Eremeev et al. [9, 10] found that the law of wave dispersion for such an array presents a discontinuous function of frequency. Among the features of thermomechanical processes in discrete systems are negative thermal expansion [11, 12] and the possibility of structural transitions [13, 14]. Such a variety of thermal phenomena adds complexity to the description of heat transfer in discrete media.

The recent experimental studies [15–17] show that the Fourier law of thermal conductivity is violated in low-dimensional nanostructures. The indicated anomalies are most pronounced in the simplest lattice models, in particular, in one-dimensional harmonic crystals [18–20]. The analytical and computer investigations [21–24] point to significant deviations from the classical Fourier thermal conductivity in an ideal single crystal. These deviations can be reduced or even completely eliminated using special laws of interaction [25–28] or rather complex structures [29, 30].

Compared to the generally accepted models of wave transfer of heat at the nano- and microscale levels in continuous media [31–35], thermal processes in discrete media occur in a significantly different way. In particular, a thermal shock initiates high-frequency oscillations in a discrete system [36], associated with the equilibration of the potential and kinetic energies according to the virial theorem [37]. The exact solution was obtained to describe such a process in a harmonic crystal [38, 39]. Guzeev and Dmitriev [40, 41] deduced a fundamental solution using Chebyshev polynomials and Bessel functions and studied the temperature distribution inside a one-dimensional harmonic crystal with regard to correlations in particle positions. A solution was derived for high-frequency energy oscillations in a harmonic crystal on the elastic foundation, with the construction of its asymptotics for the hard and soft foundations [42]. High-frequency thermal processes were investigated in vector lattices [43]. A general solution was obtained for the problem of heat propagation in the 1D and 2D cases for scalar lattices, with emphasis on slow and fast oscillations and measurement of the heat pulse front velocity [44].

In this paper, we study the slow process of heat propagation in a crystal, after the fast transient process decays [42, 45, 46]. The crystal is taken as a stochastic system, in which randomness is introduced through initial conditions, and deterministic dynamic equations are obtained for covariances of particle velocities and displacements. The approach described in this paper is based on the previous works [38, 45, 47, 48] and provides a rather simple dynamic equation of heat transfer in partial derivatives, which contains information on dispersion and the pattern of heat wave decay in a one-dimensional crystal on the elastic foundation.

2. DYNAMIC EQUATIONS OF CHAIN OF MASSES

Provided that at the initial moment particles of a one-dimensional chain rest on the elastic foundation and their velocities are set randomly, a process of conversion of kinetic energy into potential energy of spring deformation begins in the lattice. High-frequency oscillations of the kinetic and potential energies characteristic of discrete media arise [36]. This process will proceed until the energy is distributed, according to the virial theorem [37], equally between the kinetic and deformation degrees of freedom. The transient process of equalization of potential and kinetic energies is of a high-frequency nature and decays for several tens of periods; the stiffer the foundation, the slower the decay [42]. At the end of the transient process in the crystal, the temperature of the discrete system can be associated with the kinetic energy [38].

Let us consider a chain consisting of equal masses m connected by springs with stiffness C_0. The chain is on an elastic foundation of stiffness C_1. Then the dynamic equation of chain particles has the form

$$\ddot{u}_n = \omega_0^2(u_{n-1} - 2u_n + u_{n+1}) - \omega_1^2 u_n, \quad \omega_0 = \sqrt{C_0/m}, \omega_1 = \sqrt{C_1/m}, \tag{1}$$

where u_n is the displacement of the nth particle, n is the subscript taking arbitrary integer values, C_0 is the stiffness of bonds between masses, and C_1 is the stiffness of bonds between masses and the foundation.

The chain can be stable at negative stiffness values subject to the condition [49] $C_0 > -C_1/4$. In the case,

an alternative form of Eq. (1) is convenient, which has real coefficients in the allowed range of stiffnesses C_0 and C_1:

$$\ddot{u}_n = \frac{1}{4}\omega_2^2(u_{n-1} - 2u_n + u_{n+1}) - \frac{1}{4}\omega_1^2(u_{n-1} + 2u_n + u_{n+1}), \quad (2)$$

$$\omega_2 = \sqrt{\frac{C_1 + 4C_0}{m}},$$

where the quantities $\omega_1 < \omega_2$ are the lower and upper cutoff frequencies (for more detail see Section 4), which are related to partial frequency ω_0 as $4\omega_0^2 = \omega_2^2 - \omega_1^2$.

Let us assume the periodicity condition $u_{k+N} + u_k$, where $N \gg 1$ is the number of independent particles. With the second-order difference operator Δ_n^2 defined as

$$\Delta_n^2 f_n \stackrel{\text{def}}{=} f_{n-1} - 2f_n + f_{n+1}, \quad (3)$$

Eq. (1) can be written as

$$\ddot{u}_n = (\omega_0^2\Delta_n^2 - \omega_1^2)u_n. \quad (4)$$

The initial conditions correspond to instantaneous thermal perturbation resulted from the exposure of the crystal to an ultrashort laser pulse:

$$u_n|_{t=0} = 0, \ \dot{u}_n|_{t=0} = \sigma(x)\rho_n, \quad (5)$$

where ρ_n is the independent random values with zero mathematical expectation and unit variance, and $\sigma(x)$ is the deterministic deviation of initial velocities. Of practical interest is the case when $\sigma(x)$ is a slowly varying function of x.

3. DEDUCTION OF EQUATIONS FOR COVARIANCE TEMPERATURE

To deduce heat transfer equations, we use an approach based on correlation analysis [38, 45, 46, 48]. By introducing linear operator L, we rewrite motion Eq. (1) as

$$\ddot{u}_n = L_n u_n, \ L_n \stackrel{\text{def}}{=} \omega_0^2\Delta_n^2 - \omega_1^2. \quad (6)$$

Obviously, the particle velocity $v_n \stackrel{\text{def}}{=} \dot{u}_n$ satisfies the same equation.

We assume that the initial displacements and velocities are random quantities that have zero mathematical expectation. Let us consider displacement and velocity covariances of chain particles:

$$\xi_{pq} \stackrel{\text{def}}{=} \langle u_p u_q \rangle, \ \eta_{pq} \stackrel{\text{def}}{=} \langle v_p v_q \rangle, \quad (7)$$

where angle brackets stand for mathematical expectation. Direct differentiation of relations (7) gives

$$\ddot{\xi}_{pq} = (L_p + L_q)\xi_{pq} + 2\eta_{pq}, \quad \ddot{\eta}_{pq} = (L_p + L_q)\eta_{pq} + 2L_pL_q\xi_{pq}. \quad (8)$$

Elimination of η_{pq} from the system results in the fourth-order equation:

$$\partial_t^4\xi_{pq} - 2(L_p + L_q)\partial_t^2\xi_{pq} + (L_p - L_q)^2\xi_{pq} = 0. \quad (9)$$

Velocity covariances η_{pq} satisfy the same equation. For the operators L_p and L_q, the following relations are valid:

$$L_p + L_q = \omega_0^2(\Delta_p^2 + \Delta_q^2) - 2\omega_1^2, \quad L_p - L_q = \omega_0^2(\Delta_p^2 - \Delta_q^2). \quad (10)$$

To turn to long-wave approximation, we introduce a spatial coordinate x and covariance subscript n:

$$x \stackrel{\text{def}}{=} \frac{p+q}{2}a, \ n \stackrel{\text{def}}{=} q - p, \quad (11)$$

where a is the crystal lattice distance. We assume covariances (7) to be functions of x and n:

$$\xi_{pq} = \xi_n(x), \ \eta_{pq} = \eta_n(x), \quad (12)$$

and the dependence on the spatial coordinate to be rather smooth so that the functions allow for Taylor series expansion. We have

$$\Delta_p^2\xi_{pq} = \xi_{n-1}\left(x + \frac{a}{2}\right) - 2\xi_n(x) + \xi_{n+1}\left(x - \frac{a}{2}\right), \quad \Delta_q^2\xi_{pq} = \xi_{n+1}\left(x + \frac{a}{2}\right) - 2\xi_n(x) + \xi_{n-1}\left(x - \frac{a}{2}\right). \quad (13)$$

An expansion of the covariances in a series in a up to the second-order terms gives

$$\Delta_p^2\xi_{pq} = \Delta_n^2\xi_n + \frac{a}{2}(\xi_{n-1} - \xi_{n+1})' + \frac{a^2}{8}(\xi_{n-1} + \xi_{n+1})'', \quad \Delta_q^2\xi_{pq} = \Delta_n^2\xi_n + \frac{a}{2}(\xi_{n+1} - \xi_{n-1})' + \frac{a^2}{8}(\xi_{n+1} + \xi_{n-1})'', \quad (14)$$

where the stroke designates the derivative with respect to x. By summing and subtracting these relations, we derive

$$\Delta_p^2 + \Delta_q^2 = 2\Delta_n^2 + \frac{a^2}{4}(\Delta_n^2 + 2)\partial_x^2, \quad \Delta_p^2 - \Delta_q^2 = -a(\Delta_n\Sigma_n)\partial_x, \quad (15)$$

with the use of

$$(\Delta_n^2 + 2)\xi_n = \xi_{n+1} + \xi_{n-1}, \ (\Delta_n\Sigma_n)\xi_n = \xi_{n+1} - \xi_{n-1}. \quad (16)$$

The first relation is an apparent identity, and the second one can be considered as a designation for simplicity. As a result, operators (10) take the form

$$L_p + L_q = 2(\omega_0^2\Delta_n^2 - \omega_1^2) + \frac{1}{4}c^2(\Delta_n^2 + 2)\partial_x^2, \quad L_p - L_q = -\omega_0 c(\Delta_n\Sigma_n)\partial_x, \tag{17}$$

where $c \overset{\text{def}}{=} \omega_0 a$ is the sound velocity. A substitution of (17) into (9) yields a continuum equation for covariances:

$$\partial_t^4\xi_n - 4(\omega_0^2\Delta_n^2 - \omega_1^2)\partial_t^2\xi_n - \frac{1}{2}c^2(\Delta_n^2 + 2)\partial_t^2\xi_n'' + \omega_0^2c^2(\Delta_n\Sigma_n)^2\xi_n'' = 0, \tag{18}$$

where strokes symbolize partial time derivative t. Use is also made of the operator representation of Eq. (18) $\Lambda\xi_n = 0$, where the differential difference operator λ is defined as follows:

$$\Lambda \overset{\text{def}}{=} \partial_t^4 - 4(\omega_0^2\Delta_n^2 - \omega_1^2)\partial_t^2 - \frac{1}{2}c^2(\Delta_n^2 + 2)\partial_t^2\partial_x^2 + \omega_0^2c^2(\Delta_n\Sigma_n)^2\partial_x^2. \tag{19}$$

The derived equation is difficult to analyze as it includes the fourth time derivative, the second coordinate derivative, and difference operator $\Delta_n{}^2$. According to the previous investigation [36], two types of dynamic processes are observed in lattice structures: rapidly decaying oscillations without energy transfer along coordinate x, that arise immediately after the heat application, and heat wave propagation as such. The wave front is assumed to form during decaying of fast oscillatory processes, necessary for redistribution of potential and kinetic energies in the crystal [42]. Keeping the same-order terms in operator (19) enables a division of (18) into equations for slow and fast motions.

3.1. Fast Motion

For fast motion, the order relation is valid for differential operators $\partial_t \sim \omega$, $c\partial_x \sim \Omega$, where $\Omega \ll \omega \sim \omega_0 \sim \omega_1$. By keeping only the highest terms of order ω^4 in the operator (19), we derive

$$\Lambda \approx \partial_t^4 - 4(\omega_0^2\Delta_n^2 - \omega_1^2)\partial_t^2, \tag{20}$$

which gives the following equation for ξ_n:

$$\ddot{\xi}_n - 4(\omega_0^2\Delta_n^2 - \omega_1^2)\xi_n = A_1 + A_2t. \tag{21}$$

Note that the derived equation has no derivatives with respect to x, i.e. fast motion occurs without spatial transfer. If the integration constants A_1 and A_2 are zero, Eq. (21) coincides with the earlier derived one for energy oscillations for a one-dimensional harmonic crystal on the elastic foundation [42].

3.2. Slow Motion

For slow motion, $\partial_t \sim c\partial_x \sim \Omega$, where $\Omega \ll \omega \sim \omega_0 \sim \omega_1$. By keeping only the highest terms of order $\omega^2\Omega^2$ in operator (19), we derive

$$\Lambda \approx -4(\omega_0^2\Delta_n^2 - \omega_1^2)\partial_t^2 + \omega_0^2c^2(\Delta_n\Sigma_n)^2\partial_x^2, \tag{22}$$

which gives the following equation for ξ_n:

$$4(\omega_0^2\Delta_n^2 - \omega_1^2)\ddot{\xi}_n = \omega_0^2c^2(\Delta_n\Sigma_n)^2\xi_n''. \tag{23}$$

In the absence of elastic foundation ($\omega_1 = 0$), Eq. (23) acquires the form

$$\ddot{\xi}_n - \frac{1}{4}c^2\Sigma^2\xi_n'' = B_1 + B_2n. \tag{24}$$

If the integration constants B_1 and B_2 are zero, Eq. (21) coincides with the covariance dynamics equation derived earlier for a one-dimensional harmonic crystal on the elastic foundation [48]. With the designation $\lambda \overset{\text{def}}{=} \omega_1^2/\omega_0^2 + 2$, the derived equation of slow motion (23) is explicitly written for velocity covariance η_n. As noted above, it has the same form as the equation for displacement covariances ξ_n:

$$(\eta_{n+1} - \lambda\eta_n + \eta_{n-1})^{\cdot\cdot} = \frac{1}{4}c^2(\eta_{n+2} - 2\eta_n + \eta_{n-2})''. \tag{25}$$

This equation describes completely the macroscopic process of heat propagation in a one-dimensional harmonic crystal on the elastic foundation. The equation has two parameters: sound velocity c and dimensionless parameter λ defined by the stiffness ratio $\lambda = C_1/C_0 + 2$, where C_1 is the stiffness of the elastic foundation, C_0 is the stiffness of bond between crystal particles. A substitution $k_B(-1)^n\theta_n \overset{\text{def}}{=} m\eta_n$ [49] gives the equation for covariance temperature θ_n:

$$(\theta_{n+1} + \lambda\theta_n + \theta_{n-1})^{\cdot\cdot} = -\frac{1}{4}c^2(\theta_{n+2} - 2\theta_n + \theta_{n-2})''. \tag{26}$$

In the allowed ranges of stiffness $-C_1/4 \le C_0 < \infty$ and $0 \le C_1 < \infty$, the parameter λ acquires values from the intervals $-\infty < \lambda < -2$ and $2 < \lambda < +\infty$. The initial conditions for covariance temperature has the form

$$\theta_n(x,t)|_{t=0} = \begin{cases} T_0(x), & n = 0, \\ 0, & 0 < n < N, \end{cases} \quad \dot{\theta}_n(x,t)|_{t=0} = 0. \tag{27}$$

The solution of problem (26) and (27) derived under the Fourier transform [50, 51] in terms of covari-

ance coordinate n and positional coordinate x is given in the (n, k, t) representation:

$$\hat{\theta}_n(k,t) = \hat{T}_0(k)\frac{1}{\pi} \times\int_0^{\pi}\cos\left(\frac{aC_0kt\sin\delta}{\sqrt{am(1+4C_0/C_1\cos^2(\delta/2))}}\right)\cos(\delta n)\mathrm{d}\delta, \quad (28)$$

where δ is the integration variable. The condition of the real-number root in formula (28) imposes a restriction on an allowed range of stiffness $C_0 \geq -C_1/4$ of a stable chain [49].

Considering uncorrelated oscillation alone, let us assume that $n = 0$. Then integral (28) can be represented via Bessel functions (this statement is proved in Appendix A):

$$\hat{\theta}_0(k,t) = \hat{T}_0(k)J_0c_*kt, \quad (29)$$

where $c_* = a/2|\omega_2 - \omega_1|$ is the maximum group velocity of mechanical waves in the chain on the foundation.

If the foundation stiffness is much higher than the chain stiffness and positive ($C_1 \gg C_0$), then $c_* \approx c \times \sqrt{C_0/C_1}$, and conversely if $C_1 \ll C_0$, then $c_* \approx c$. For equal stiffnesses $C_1 = C_0$, the velocity $c_* = c/2\,(\sqrt{5} - 1) \approx 0.62c$. At $C_1 = 0$, the solution goes over into the earlier derived one [45]. At negative stiffness C_0, the heat wave velocity c_* remains real as long as the condition $C_0 \geq -C_1/4$ is valid.

From representation (29) and the Bessel function properties it follows that the distribution of kinetic temperature $\hat{T}(k,t) = \hat{\theta}_0(k,t)$ in the chain on the foundation satisfies the following problem:

$$\ddot{\hat{T}} + \frac{1}{t}\dot{\hat{T}} = -c_*^2k^2\hat{T},\ \hat{T}|_{t=0} = T_0(x),\ \dot{\hat{T}}|_{t=0} = 0. \quad (30)$$

Fourier transform inverse to (30) with respect to k gives the equations [45, 52]

$$\ddot{T} + \frac{1}{t}\dot{T} = c_*^2T'',\ T|_{t=0} = T_0(x),\ \dot{T}|_{t=0} = 0, \quad (31)$$

where t is the physical time counted from the instant of exposure of the chain to a short heat pulse. The heat front velocity in the chain c_* is equal to the maximum (in absolute value) group velocity of mechanical waves in the considered system (see Appendix A). A conclusion on the heat front velocity can be inferred also by analyzing the Green function expansion for the chain (formula (26) in [51]) plotted by the stationary-phase method.

Note that Eq. (31) is similar to the Darboux equation [53, 54]

$$\frac{\partial^2T(x,r)}{\partial r^2} + \frac{\alpha-1}{r}\frac{\partial T(x,r)}{\partial r} = \Delta_xT(x,r), \quad (32)$$

describing the spherical mean solution of the wave equation in the space of dimension $\alpha + 1$ in averaging with respect to a sphere of radius r.

The solution of initial problem (31) can be represented [53–55] both as a convolution

$$T(x,t) = \frac{1}{\pi}\int_{-\infty}^{\infty}T_0(x-c_*\tau)\frac{H(t^2-\tau^2)}{\sqrt{t^2-\tau^2}}\mathrm{d}\tau = \frac{1}{\pi}\int_{-t}^{t}\frac{T_0(x-c_*\tau)}{\sqrt{t^2-\tau^2}}\mathrm{d}\tau, \quad (33)$$

and as a sum of direct and reverse waves

$$T(x,t) = \frac{1}{2\pi}\int_0^{\pi}\left[T_0\left(x-c_*t\sin\frac{\delta}{2}\right) + T_0\left(x+c_*t\sin\frac{\delta}{2}\right)\right]\mathrm{d}\delta = \frac{1}{2\pi}\int_{-\pi}^{\pi}T_0\left(x+t\sin\frac{\delta}{2}\right)\mathrm{d}\delta. \quad (34)$$

A similar expression was previously deduced [44]. The substitution $\tau = t\sin(\delta/2)$ in the last expression can lead to the form (34). For illustration of the solution of heat transfer problem (30), we assume that an infinite one-dimensional crystal at the initial time instant is heated by a short laser pulse whose intensity decreases with distance from the spot center. Let us assume that the initial temperature distribution is parabolic:

$$T|_{t=0} = T_0(l^2 - x^2)H(x^2 - l^2), \quad (35)$$

where T_0 is the temperature in the laser spot center, l is the laser beam radius, and H is the Heaviside function. Then, a substitution of (35) into (33) yields a function describing the time evolution of the temperature profile in a one-dimensional crystal (Fig. 1, solid lines).

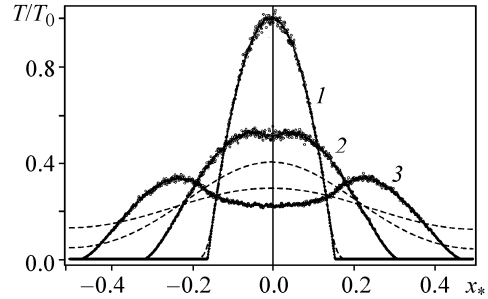

Fig. 1. Temperature distribution in an infinite one-dimensional crystal: solid lines show the solution of the initial Cauchy problem derived by formula (33) and under initial conditions (35), dashed lines correspond to the solution plotted within the classical Fourier heat conductivity model. Dots stand for the numerical solution. Curves *1–3* illustrate temperature distribution at the time instants $t_1 < t_2 < t_3$.

The solution for $T(x, t)$ is represented in Appendix B. The solution of problem (30) under other initial conditions is analyzed elsewhere [55]. The problems on heat input into the bulk were studied by Gavrilov et al. [56].

The system of discrete dynamics equations (1) for the chain with stochastic initial conditions (5), where

$$\sigma(x) = T_0(l^2 - x^2)H(x^2 - l^2),$$

is solved numerically by the central-difference method at the integration step $5\times10^{-4}\tau_0$, where $\tau_0 = 2\pi/\omega_0$. The numerical solution is shown by dots in Fig. 1. Initial velocities are set by a uniformly distributed random number generator. The mathematical expectation is an average value over the crystal. To derive a numerical solution of adequate accuracy, the use is made of a chain with 50 realizations of 10 000 particles each.

As the only constant in the heat transfer equation is group velocity, of interest is its dependence on system parameters (1). To do this, the next section is devoted to the analysis of dispersion relations, including in the negative region of stiffness C_0.

4. DISPERSION RELATIONS

The dispersion relation for waves propagating in the chain on the foundation (1) has the form

$$\Omega^2(k) = (\omega_2^2 - \omega_1^2)\sin^2\left(\frac{ak}{2}\right) + \omega_1^2, \qquad \omega_2^2 = 4\omega_0^2 + \omega_1^2. \tag{36}$$

Dispersion relation (36) includes two cutoff frequencies $\omega_1 < \omega_2$, thus the chain on the foundation presents a band-pass filter. Waves with frequencies out of the band pass are called exponential (zigzag-like) and do not propagate [57]. To analyze dispersion dependences both at positive and negative stiffnesses C_0, it is convenient to turn to the parameters ω and β, which are set so that

$$\omega_1^2 \overset{\text{def}}{=} \omega\cos\left(\beta + \frac{\pi}{4}\right),\ \omega_2^2 \overset{\text{def}}{=} \omega\sin\left(\beta + \frac{\pi}{4}\right), \qquad \omega^2 = \omega_1^2 + \omega_2^2. \tag{37}$$

The introduced parameter β depends on the foundation stiffness and the stiffness of bond between chain particles in the following way:

$$\tan\left(\beta + \frac{\pi}{4}\right) \overset{\text{def}}{=} \frac{\omega_2}{\omega_1} = \sqrt{\frac{C_1 + 4C_0}{C_1}}. \tag{38}$$

At negative stiffness values C_0, the parameter β is likewise negative. Values of β from the interval $-\pi/4 \le \beta \le \pi/4$ correspond to frequencies ω_1 and ω_2 varying in the interval $(0, \omega)$ or stiffnesses C_1 and C_2 in the intervals $-C_1/4 \le C_0 < \infty$ and $0 \le C_1 < \infty$. These values are listed in the table. The use of parameter β gives symmetrical curves of quantities describing wave propagation in system (1) at any allowed stiffness values C_0 and C_1. In so doing, the parameter β remains real and does not go into infinity in the entire range.

Consistency of parameters β and ω to parameters ω_1, ω_2, ω_0, c_* and factors C_0, C_1. The quantity ω enters dispersion relations as a factor

β	$-\pi/4$	0	$\pi/4$
ω_1	ω	$\sqrt{2}/2\,\omega$	0
ω_2	0	$\sqrt{2}/2\,\omega$	ω
ω_0	$-i/2\,\omega$	0	$i/2\,\omega$
c_*	$a/2\,\omega$	0	$a/2\,\omega$
C_0	$-C_1/4$	0	∞
C_1	$-4C_0$	–	0

The dispersion characteristic of waves in the chain on the elastic foundation (36) is expressed via parameters ω and β in the following way:

$$\Omega(k) = \omega/\sqrt{2}\,\sqrt{1 - \sin(2\beta)\cos(ak)}. \tag{39}$$

Figure 2 plots a family of dispersion curves at different values of parameter β. At negative and posi-

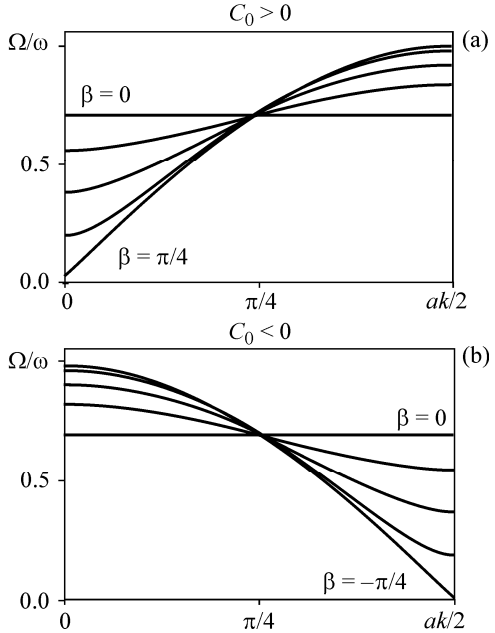

Fig. 2. Dispersion characteristic of waves in the chain on the elastic foundation at the parameter β varying from 0 to π/4 with the step π/16, for positive $C_0 > 0$ (a) and negative $C_0 < 0$ stiffnesses (b).

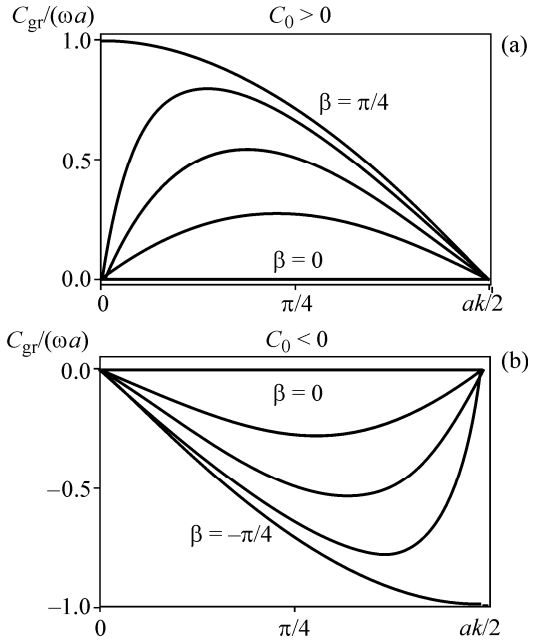

Fig. 3. Wave group velocity in the chain on the elastic foundation at the parameter β varying from 0 to π/4 with the step π/16, for positive $C_0 > 0$ (a) and negative $C_0 < 0$ stiffnesses (b).

tive β, the diagrams are seen to be symmetrical. Thus, owing to the parameterization method, a clear analogy is seen in the behavior of system (1) at negative $-C_1/4 \le C_0 < 0$ and positive $0 \le C_0 < \infty$ stiffnesses of the chain. At β = π/4 the foundation is absent, and at β = 0 the stiffness vanishes $C_0 = 0$, which corresponds to the system of uncorrelated oscillators. The value β = –π/4 corresponds to the ultimate negative stiffness $C_0 = -C_1/4$, at which the chain on the foundation retains stability. All dispersion curves in Fig. 2 are bounded by the upper and lower cuttoff frequencies:

$$\omega_1 = \omega\sin\left(\beta+\frac{\pi}{4}\right),\ \omega_2 = \omega\cos\left(\beta+\frac{\pi}{4}\right). \qquad (40)$$

The dependence of the group velocity on the wave number has the form

$$C_{gr} \overset{\text{def}}{=} \frac{d\Omega}{dk} = \frac{a\omega\sin(2\beta)\sin(ak)}{2\sqrt{2}\sqrt{1-\sin(2\beta)\cos(ak)}}. \qquad (41)$$

The wave group velocity in the chain on foundation is always lower than that in the chain without foundation, which is plotted at β = π/4 in Fig. 3a. At positive and negative stiffnesses, the group velocity curves are antisymmetrical. At $C_0 > 0$ the group velocity is positive, and at $C_0 < 0$ it is negative and is opposed to the phase one. The maximum (in absolute value) group velocity in the chain on the foundation

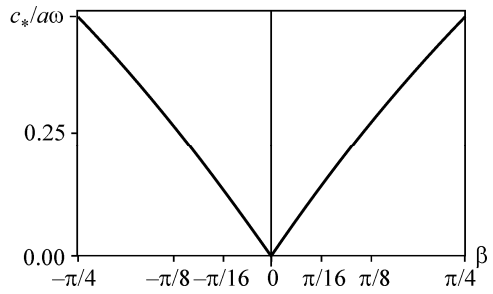

Fig. 4. Maximum (in absolute value) group velocity as a function of parameter β.

determines the maximum velocity of energy propagation in the system, which amounts to $c_* = a/2|\omega_2 - \omega_1|$.

The value of c_* is proportional to the difference between the upper and lower cuttoff frequencies. Going to the parameters β and ω, the velocity can be expressed as

$$c_* = a\omega/\sqrt{2}\,|\sin\beta|\,. \qquad (42)$$

In the case of no foundation at $\omega_1 = 0$ and consequently β = π/4, the velocity c_* takes on the value $c = a\omega_0$.

The parameter ω at the allowed stiffness values $-C_1/4 \le C_0 < \infty$ and $0 \le C_1 < \infty$ varies within $-14C_1/m \le \omega < \infty$ and enters the expressions for dispersion (39), group velocity (41), and maximum (in absolute value) wave group velocity (42) merely as the scale factor. Thus, our concern is solely with the dependence of the mentioned quantities on the parameter β.

Figure 4 plots the dependence of the maximum (in absolute value) group velocity (42) on the parameter β. At negative parameter $-\pi/4 \le \beta \le 0$ corresponding to negative stiffness $-C_1/4 \le C_0 < 0$, the curve behaves symmetrically to that in the interval $0 \le \beta \le \pi/4$ corresponding to positive stiffness $0 \le C_0 < \infty$. It is seen that at the end points of the diagram β = –π/4, π/4 (i.e. at $C_0 = -C_1/4$ and $C_0/C_1 \to \infty$, respectively) the velocity c_* takes on the maximum value equal to the long-wave velocity in the chain without foundation $c = a\omega_0$. In the case β = 0 corresponding to $c_0 = 0$, no waves propagate in the chain $c_* = 0$.

The used method of parameterization of dispersion relations distinguishes two quantities: ω entering the dispersion relations as a multiplier and presenting a scale factor, and β determining the qualitative behavior of the diagrams $\Omega(k, \beta)$, $C_{gr}(k, \beta)$, and $c_*(\beta)$. Both quantities are uniquely determined from model parameters (1), maintaining consistency with each other and with the rest designations (see the table).

5. CONCLUSIONS

The work discloses that the propagation of a short-term thermal perturbation in the crystal on the elastic foundation is determined by the ballistic heat conductivity equation of the same form as in the crystal without elastic foundation [45]:

$$\ddot{T} + 1/t\,\dot{T} = c_*^2 T'', \; T|_{t=0} = T_0(x), \; \dot{T}|_{t=0} = 0.$$

The only parameter in the equation is the maximum (in absolute value) group velocity $c_* = a|\omega_1 - \omega_2|/2$, i.e. the maximum velocity of energy propagation in the crystal on the elastic foundation. This quantity is proportional to the absolute value of the semidifference of the upper ω_2 and lower ω_1 cuttoff frequencies. If the foundation stiffness is much higher than the chain stiffness ($C_1 \gg C_0$), then $c_* \approx c\sqrt{C_0/C_1}$, and conversely if $C_1 \ll C_0$, then $c_* \approx c$. The heat wave velocity c_* in the crystal on the elastic foundation with positive stiffness C_0 is always lower than the heat wave velocity c in the crystal without foundation $c_* < c$.

It is found that Eq. (31) is valid both for positive chain stiffness and for negative one subject to $C_0 > -C_1/4$. If the chain stiffness is negative and the condition $C_0 > -C_1/4$ is satisfied, the heat wave velocity remains real and can be expressed by formula (42).

For illustration an exact solution of Eq. (31) is derived for a parabolic initial temperature profile, which models short-pulse laser heating of a one-dimensional crystal on the foundation.

Due to dispersion of mechanical waves in the chain on the foundation, their group velocity depends on the wave number k and the chain-to-foundation stiffness ratio β. The heat front propagates with the maximum possible group velocity in the system, which depends only on β. Thus, heat and acoustic waves can have different velocities at the fixed β. The heat transfer velocity can exceed the acoustic wave velocity if the mass bond stiffness in the chain is positive $C_0 > 0$, and conversely it can be less than the acoustic wave velocity at $C_0 < 0$ (Fig. 3).

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APPENDIX A. SOLUTION OF THE KINETIC ENERGY TRANSFER EQUATION VIA BESSEL FUNCTIONS

Let us prove that the following equality is valid:

$$\frac{1}{\pi}\int_0^\pi \cos\left(\frac{aC_0 kt\sin\delta}{\sqrt{am(1+4C_0/C_1\cos^2\delta/2)}}\right)\mathrm{d}\delta = J_0(c_* kt). \quad \text{(A1)}$$

Using an integral representation of the Bessel function [58], we transform the right-hand side:

$$\int_0^\pi \cos\left(\frac{aC_0 kt\sin\delta}{\sqrt{am(1+4C_0/C_1\cos^2(\delta/2))}}\right)\mathrm{d}\delta = \int_0^\pi \cos(c_* kt\sin(\delta/2))\mathrm{d}\delta. \quad \text{(A2)}$$

The Laplace integral transform of the right- and left-hand sides of equality (A2) is applied with respect to time $t \to \omega$

$$\int_0^\pi \left(\frac{a(C_0 k\sin\delta)^2}{m\omega(1+4C_0/C_1\cos^2(\delta/2))}\right)^{-1}\mathrm{d}\delta = \int_0^\pi \frac{\omega}{c_*^2 k^2\sin^2(\delta/2)+\omega^2}\mathrm{d}\delta. \quad \text{(A3)}$$

A definite integral over δ is found for the left- and right-hand sides of (A3). Under the assumption that $c_* = a/2|\omega_2 - \omega_1|$, the derived expression is reduced to an algebraic identity, which is transformed to the simple form:

$$\sqrt{\mu + 2\omega^2 - 2\sqrt{c^4k^4 + \mu\omega^2 + \omega^4}} + \sqrt{2(\mu+2\omega^2) - 2c^2k^2\sqrt{\lambda^2-4}} = \sqrt{\mu + 2\omega^2 + 2\sqrt{c^4k^4 + \mu\omega^2 + \omega^4}}, \quad \text{(A4)}$$

$$\mu = c^2k^2\lambda.$$

At positive stiffness $C_0 > 0$ and the parameters c, k, $\omega > 0$, $\lambda > 2$, the validity of this statement is proved by successive identity transformations. At negative stiffness $-C_1/4 < C_0 < 0$ and the parameter $-\infty < \lambda \le -2$, the proof is the same. At $C_0 = 0$ or, what is the same, at $\lambda = 2$, heat and acoustic disturbances do not propagate in system (1). Thus, the left- and right-hand sides of equality (A1) have the same Laplace image, and consequently their originals also coincide, as was to be proved.

APPENDIX B. SOLUTION OF THE PROBLEM OF EVOLUTION OF A HEAT PULSE WITH THE INITIAL PARABOLIC PROFILE

We introduce dimensionless variables x_* and t_*, such that

$$x = c_*\tau x_*,\ t = \tau t_*, \tag{B1}$$

where c_* is the maximum (in absolute value) group velocity, and τ is the scale along the time axis. With the new variables and under initial conditions (35), problem (31) takes the form

$$\ddot{T} + 1/t_*\dot{T} = T'',\ T|_{t_*=0} = T_0(l_*^2 - x_*^2)H(x_*^2 - l_*^2),$$
$$\dot{T}|_{t_*=0} = 0, \tag{B2}$$

where $l_* = l/(c_*\tau)$. An integration of (33) gives the following expression for temperature (for brevity, the subscripts are omitted in the notation)

$$T(x,t) = T_1(x,t) + T_1(-x,t) + T_2(x,t) + T_3(x,t), \tag{B3}$$

where the quantities T_1, T_2, and T_3 are set by the expressions

$$T_1(x,t) = \frac{1}{4\pi}\left(p(x)\left(2\arcsin\frac{l+x}{t} + \pi \right) + 2q(x) \right) \times H(l^2 - (t+x)^2),$$

$$T_2(x,t) = \frac{1}{2\pi}\left(p(x)\left(2\arcsin\frac{l-x}{t} + \arcsin\frac{l+x}{t} \right) + q(-x) + q(x) \right) H((t-l)^2 - x^2),$$

$$T_3(x,t) = \frac{1}{2}p(x)H((t-l)^2 - x^2)H(l-t),$$

$$q(x) = (l-3x)\sqrt{t^2 - (l+x)^2},\ \ p(x) = 2l^2 - t^2 - 2x^2.$$

The solution exhibits wave diffusion: there is only a leading front and no trailing front. The functions $T_2(x, t)$ and $T_3(x, t)$ determine the internal part of a propagating wave at different time periods; $T_1(x, t)$ and $T_1(-x, t)$ determine its external part at any time values.

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