===== **MECHANICS** =====

Heat Transfer in Infinite Harmonic One-Dimensional Crystals[1]

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Abstract—A closed system of differential-difference equations describing thermal processes in one-dimensional harmonic crystals is obtained in the paper. An equation connecting the heat flow and the kinetic temperature is obtained as a solution of the system. The obtained law of heat conduction is different from Fourier's law and results in an equation that combines properties of the standard heat equation and the wave equation. The resulting equation is an analytic consequence from the dynamical equations for the particles in the crystal. Unlike equations of hyperbolic heat conduction, this equation is time-reversible and has only one independent parameter. A general analytical solution of this differential equations is obtained, and the analytical results are confirmed by computer simulations.

Heat conduction at macroscopic scale level in most materials is described by Fourier's law. According to this law the heat flux is proportional to the temperature gradient. Being a convenient mathematical model, Fourier's law however leads to a number of physical paradoxes, such as an instantaneous heat propagation. Significant deviations from Fourier's law are also observed at small spatial and temporal scales [1, 2]. Furthermore, it is known that in the simplest discrete systems, such as a one-dimensional harmonic crystal (a chain of particles connected by linear springs) the heat distribution can not be described by Fourier's law [3−5]. At the present time the question about the heat propagation in a perfect crystalline systems remains open. However, this issue is of particular relevance, as with the development of nanotechnologies the creation of ideal defect-free crystals becomes possible, which opens opportunities for application of their unique thermal properties. In addition, the rational description of the heat transfer processes is necessary to close the mechanical equations of discrete media [6−8] and for description of thermomechanics of solids at the nanoscale level [9, 10].

This work is an extension of the work [11] for the case of non-equilibrium processes: the equations con-

necting the heat flux and the kinetic temperature are analytically derived for one-dimensional harmonic crystals. Closed equations for the heat propagation are obtained and their analytical solution is constructed, which is confirmed by computer simulations. The obtained results are based on the combination of two approaches—the correlation analysis and the long-wave approximation. The main idea of the correlation analysis is to use co-variances[2] of velocities of different particles in the crystal [3, 12]. The covariances allow to close the system of equations, and the variance determines the kinetic temperature [4, 11]. The long-wave approximation is based on the principle that the averaged values change little at the ranges comparable with the distances between the particles [6, 13].

Let us consider an infinite one-dimensional harmonic crystal: a chain of equal particles with a mass m connected by linear springs with a stiffness C. The corresponding dynamics equations have the form

$$\ddot{u}_k = \omega_0^2(u_{k-1} - 2u_k + u_{k+1}), \quad \omega_0 \stackrel{\text{def}}{=} \sqrt{\frac{C}{m}}, \quad (1)$$

where u_k is the displacement of kth particle; k is taking arbitrary integer values. The following initial conditions will be used

$$u_k|_{t=0} = 0, \quad \dot{u}_k|_{t=0} = \sigma(x)\rho_k, \quad (2)$$

where ρ_k are independent random variables with zero expectation and unit variance; σ is variance of the initial particle velocity. The variance is a slowly changing function of the spatial coordinates $x = ka$, where a is

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[2] The mathematical expectation (average) of the product of two centered random variables.

the initial distance between neighboring particles. The chosen initial conditions can be interpreted as a result of an ultrashort laser impulse, acting on the crystal [2].

Let us rewrite the equations of motion (1) in the form

$$\dot{v}_k = \omega_0^2 \Delta \varepsilon_k, \quad \dot{\varepsilon}_k = \Delta v_k, \tag{3}$$

where the particle velocity v_k, the bond strain ε_k, and the central difference operator Δ are determined by the formulas

$$v_k \stackrel{\text{def}}{=} \dot{u}_k, \quad \varepsilon_k \stackrel{\text{def}}{=} \Delta u_k, \quad \Delta f_k \stackrel{\text{def}}{=} f_{k+1/2} - f_{k-1/2}. \tag{4}$$

Here and below, integer values of k-index are used for displacements and velocities; half-integer values are used for strains.

Let us introduce a covariance energy $\mathcal{E}$ and a heat flux $\mathcal{H}$ as

$$\mathcal{E}_{pq} \stackrel{\text{def}}{=} \frac{m}{2} \langle v_p v_q \rangle + \frac{C}{2} \langle \varepsilon_p \varepsilon_q \rangle,$$

$$\mathcal{H}_{pq} \stackrel{\text{def}}{=} -\frac{1}{2} C \langle \varepsilon_p v_q + v_p \varepsilon_q \rangle, \tag{5}$$

where $\langle \ldots \rangle$ is a spatial averaging operator, defined by

$$\langle f_{pq} \rangle \stackrel{\text{def}}{=} \frac{1}{\Lambda} \sum_{s=-\Lambda/2}^{\Lambda/2} f_{\tilde{p}+s, \tilde{q}+s}, \quad 1 \ll \Lambda \ll \frac{\lambda}{a}, \tag{6}$$

where Λ is the averaging interval, λ is the characteristic length for macroscopic waves in the crystal. Indexes $\tilde{p}$, $\tilde{q}$ are chosen equal to p, q or $p + \frac{1}{2}, q + \frac{1}{2}$ depending whether integer or half-integer values of the indices are used.

Time-differentiation of the expression (5) with the use of (3) gives

$$\dot{\mathcal{E}}_{pq} = -(\Delta_p + \Delta_q)\mathcal{H}_{pq}, \quad \dot{\mathcal{H}}_{pq} = -\omega_0^2(\Delta_p + \Delta_q)\mathcal{E}_{pq}, \tag{7}$$

where Δ_p and Δ_q are the central difference operators (4) with respect to indexes p and q. Elimination of the covariance heat flux from this system gives a closed equation for the covariance energy, and vice versa.

Let us represent the quantities (5) as functions of the spatial coordinate $x = \frac{p+q}{2} a$ and correlational index $n = q - p$, so as $\mathcal{E}_{pq} = \mathcal{E}_n(x)$, $\mathcal{H}_{pq} = \mathcal{H}_n(x)$. Let us denote

$$\rho \stackrel{\text{def}}{=} \frac{1}{a}, \quad h_n \stackrel{\text{def}}{=} \frac{1}{2}(\mathcal{H}_{n-1/2} + \mathcal{H}_{n+1/2}), \tag{8}$$

where ρ is the density (the number of particles per unit volume), h_n is an alternative representation of the heat flux. Quantity h_n is more convenient then H_n for the forthcoming transfer to continuum equations. In par-

ticular, $h_0 = -\frac{1}{2} C \langle (\varepsilon_{k-1/2} + \varepsilon_{k+1/2}) v_k \rangle$ is a well-known expression for the heat flux in one-dimensional crystals [4, 6].

Assuming that the considered quantities are slowly changing functions of x, we can use the decomposition

$$f(x+a) = f(x) + af'(x) + \frac{1}{2}a^2 f''(x) + \ldots. \tag{9}$$

Then Eqs. (7) in a first approximation take the form

$$\rho \dot{\mathcal{E}}_n = -h_n', \quad \dot{h}_n = -\frac{1}{4}\rho c^2 (\mathcal{E}_{n+1} + 2\mathcal{E}_n + \mathcal{E}_{n-1})', \tag{10}$$

where $c \stackrel{\text{def}}{=} a\omega_0$ is the speed of sound in the one-dimensional crystal, the dash stands for x-derivative. The first equation from Eqs. (10) expresses balance of the covariance energy, the second one is an analogue of the Fourier law for the covariational heat flow, together they provide a closed system of differential-difference equations. The initial conditions for these equations, according to (2), are of the form

$$\mathcal{E}_n|_{t=0} = E_0(x)\delta_n, \quad h_n|_{t=0} = 0, \tag{11}$$

where $E_0(x) \stackrel{\text{def}}{=} \frac{m}{2}\sigma^2(x)$ is the initial distribution of the thermal energy in the crystal; the symbol δ_n is equal to 1 when $n = 0$ and it is equal to 0 otherwise. Elimination of the covariational heat flux h_n from the system (10) gives the closed equation for the covariance energy:

$$\ddot{\mathcal{E}}_n = \frac{1}{4}c^2(\mathcal{E}_{n+1} + 2\mathcal{E}_n + \mathcal{E}_{n-1})'', \quad \mathcal{E}_n|_{t=0} = E_0(x)\delta_n, \tag{12}$$

$$\dot{\mathcal{E}}_n|_{t=0} = 0.$$

Solution of the initial problem (10), (11) gives uniquely the covariances $\mathcal{E}_n(t, x)$ and $h_n(t, x)$. For $n = 0$ we obtain the usual (variance) energy $E(t, x)$ and the usual heat flux $h(t, x)$. The kinetic temperature can be found only after attenuation of the fast transients leading to equalization of the kinetic and potential energies [11] according to the virial theorem. In paper [11] it is shown that Lagrangian (the difference between kinetic and potential energy of the crystal[3] satisfies Bessel's differential equation[4] and it can be expressed through the Bessel function of the 1st kind $J_0(z)$:

$$\ddot{L} + \frac{1}{t}\dot{L} + 16\omega_0^2 L = 0, \quad L(t, x) = E_0(x)J_0(4\omega_0 t). \tag{13}$$

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[3] In the work [11] an averaging over the whole crystal was used, however, the results of the paper can be easily transferred to the averaging (6) applied to Λ-neighborhood of x.

[4] There is a misprint in the Eq. (10) of paper [11]—the coefficient at $\dot{L}$ instead of $1/t$ is mistakenly written as $16\omega_0^2\frac{1}{t}$, which, however, do not affect the other the results of the paper.

According to (13), Lagrangian L performs attenuating oscillations and tends to zero at times much greater then $\tau_0 = \dfrac{2\pi}{\omega_0}$. The characteristic times for Eqs. (10) are of the order of $\dfrac{\lambda}{c} \gg \tau_0$. Therefore, after attenuation of the high frequency processes the kinetic energy K become equal to a half of the total energy E. This gives for the kinetic temperature of the one-dimensional crystal the expression $\dfrac{1}{2}kT = K = \dfrac{1}{2}E$, where k is the Boltzmann constant. Thus, after the system (10) is solved the temperature T and heat flow h can be found as

$$kT(t, x) = \mathscr{E}_0(t, x), \quad h(t, x) = h_0(t, x), \quad (14)$$

which gives a complete description of the thermal processes in the crystal.

Solution of the initial problems (10)–(12) can be obtained using an integral Fourier transform. According to (10)–(12) the initial problems similar to the one considered in [11] are realized for the Fourier images of the covariances. This allows to construct solutions of (10)–(12) in the terms of Bessel functions of the 1st kind with even indexes: $J_{2n}(z)$. Application of the inverse Fourier transform allows obtaining the explicit formulas for the unknown functions:

$$\mathscr{E}_n(t, x) = \frac{(-1)^n}{2\pi} \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} E_0(y) J_{2n}(\kappa ct) e^{i\kappa(x-y)} d\kappa dy, \quad (15)$$

$$h_n(t, x)$$

$$= (-1)^n \frac{i\rho c}{2\pi} \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} E_0(y) J'_{2n}(\kappa ct) e^{i\kappa(x-y)} d\kappa dy. \quad (16)$$

Calculation of the integrals with respect to κ for $n = 0$ gives an explicit representation for the kinetic temperature and heat flux

$$T(t, x) = \frac{1}{\pi} \int_{-t}^{t} \frac{T_0(x - c\tau)}{\sqrt{t^2 - \tau^2}} d\tau,$$

$$h(t, x) = \frac{k\rho c}{\pi t} \int_{-t}^{t} \frac{T_0(x - c\tau)}{\sqrt{t^2 - \tau^2}} \tau d\tau, \quad (17)$$

where $kT_0(x) = E_0(x)$ is the initial temperature distribution.[5] Direct differentiation of the expressions (15), (16) with the use of Bessel's differential equation and the identity $J_1(z) = -J'_0(z)$ [14] gives for $n = 0$ the

modified Fourier's law, which connects the temperature and heat flux (14) as

$$\dot{h} + \frac{1}{t}h = -k\rho c^2 T'. \quad (18)$$

Differentiation of this relation with respect to x using law of energy-balance $\rho\dot{E} = -h'$ gives closed initial problem for the temperature T:

$$\ddot{T} + \frac{1}{t}\dot{T} = c^2 T'', \quad T|_{t=0} = T_0(x), \quad \dot{T}|_{t=0} = 0. \quad (19)$$

Using the formula (17) let us obtain an evolution of the temperature and heat flux for the following two variants of the initial temperature distribution.

(1) Sinusoidal distribution: $T_0(x) = A\sin\kappa x + B$. The solution is

$$T(t, x) = AJ_0(\kappa ct)\sin\kappa x + B,$$
$$h(t, x) = -k\rho cAJ_1(\kappa ct)\cos\kappa x \quad (20)$$

—according to properties of Bessel's functions [14] the temperature and heat flux perform oscillations with an amplitude proportional to $\dfrac{1}{\sqrt{t}}$. For comparison: the heat equation in this case gives an exponential decay (without oscillations), the wave equation gives harmonic oscillations without decay.

(2) Step distribution: $T_0(x) = A$ for $x < 0$, otherwise $T_0(x) = 0$. The solution for $|x| \leq ct$ is

$$|x| \leq ct: T(t, x) = \frac{A}{\pi}\arccos\frac{x}{ct},$$
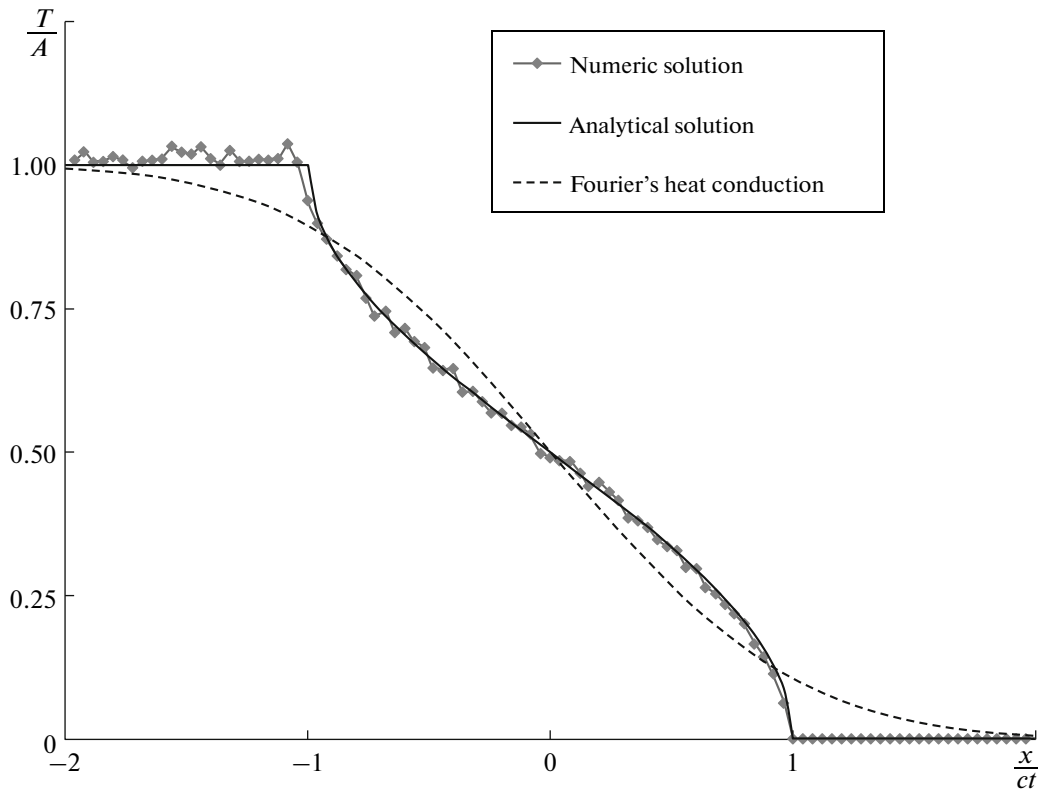$$h(t, x) = \frac{k\rho A}{\pi t}\sqrt{c^2 t^2 - x^2}; \quad (21)$$

for $|x| > ct$ the initial temperature distribution is preserved and $h \equiv 0$. The obtained solution shows two fundamental differences from the thermal conductivity on the basis of Fourier's law: (1) the perturbation front propagates with finite speed c, (2) there is a constant heat flux $h|_{x=0} = \dfrac{k\rho cA}{\pi}$ from the hot region to the cold one (according to Fourier's law at $t = 0$ the heat flux is infinite, and for $t > 0$ it decreases as $1/\sqrt{t}$). The figure shows comparison of the analytical solution (21) and the numerical solution of the initial problem (1), (2), where a chain containing one million particles is used for the computations. From figure it is clear that the solutions coincide apart from small thermal oscillations.

Thus, in the paper a closed system of differential-difference equations (10) is obtained. The system describes thermal processes in one-dimensional harmonic crystals. Solution of the system in the case of instantaneous thermal perturbation leads to the ther-

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[5] Here the thermal energy is taken to be equally distributed between the kinetic and potential ones. This virial equality is a result of the quick transition process [11] described by the formula (13).

Comparison of analytical solution (21) with the numerical solution of Eq. (1) (chain containing 10^6 particles; each point is an average over an interval containing 10^4 particles; integration by central differences method with the step of $\frac{1}{40}\tau_0$; mirror boundary conditions). The dashed line corresponds to the solution of the similar problem with Fourier's law of heat conduction.

mal law, which is different from Fourier's law. Below one can see a comparison of Fourier's law (a), the empirical law of heat conduction by Maxwell−Cattaneo−Vernotte (b) [1, 15], and the obtained law (c):

$$\text{(a) } h = -\kappa T', \quad \text{(b) } \dot{h} + \frac{1}{\tau}h = -\frac{\kappa}{\tau}T',$$
$$\text{(c) } \dot{h} + \frac{1}{t}h = -k\rho c^2 T', \tag{22}$$

where κ is the coefficient of thermal conductivity, τ is the relaxation time, k is Boltzmann's constant, ρ is the density, c is the speed of sound. In the Eq. (c) the constant τ is replaced by the physical time t. Therefore, when t is close to relaxation time τ, the laws (b) and (c) give similar results, but for small and large times these laws are significantly different. Law (c) gives the modified heat equation (19): $\ddot{T} + \frac{1}{t}\dot{T} = c^2 T''$, which contains the only one parameter—the speed of sound c. Note that this equation is an analytical consequence of the dynamics equations for the particles that form the crystal. Equation (19) combines the properties of the classical heat equation and the wave equation, but it is time-reversible (it does not change when t is replaced by $-t$). It is likely that the processes described by the law (18) and Eq. (19) play an important role in non-equilibrium thermodynamics of ideal defect-free crystals, which are expected to be widely used in the nearest future due to the fast development of nanotechnologies.

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