

An Analytical Description of Transient Thermal Processes in Harmonic Crystals¹

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Abstract— We consider two transient thermal processes in uniformly heated harmonic crystals: (i) equalization of kinetic and potential energies and (ii) redistribution of the kinetic energy among the spatial directions. Equations describing these two processes in two-dimensional and three-dimensional crystals are derived. Analytical solutions of these equations for the square and triangular lattices are obtained. It is shown that the characteristic time of the transient processes is of the order of ten periods of atomic vibrations. The difference between the kinetic and potential energies oscillates in time. For the triangular lattice, amplitude of the oscillations decays inversely proportional to time, while for the square lattice it decays inversely proportional to the square root of time. In general, there is no equipartition of the kinetic energy among spatial directions, i.e. the kinetic temperature demonstrates tensor properties. In addition, the covariance of velocities of different particles is nonzero even at the steady state. The analytical results are supported by numerical simulations. It is also shown that the obtained solutions accurately describe the transient thermal processes in weakly nonlinear crystals at short times.

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1. INTRODUCTION

A quantitative description of nonequilibrium thermal processes in crystals is one of the challenging problems in modern physics. The problem is topical due to the recent development of nanotechnologies [1–3]. In particular, the processes of transition towards the thermodynamic equilibrium state in solids are of a great interest [4, 5]. A nonequilibrium state is caused, for example, by shock waves [6–9] or by a short laser impulse [10–14]. In such cases, the kinetic energies of the thermal motion in different spatial directions may differ significantly [7–9]. In other words, the kinetic temperature exhibits tensor properties.² In addition, the kinetic and potential energies of the thermal motion may be different.

Computer simulations [15] show that transition towards the equilibrium state is accompanied by two processes, namely: (i) equalization of the kinetic and potential energies and (ii) redistribution of the kinetic

energy among the spatial directions.³ This paper focuses on analytical description of the transient thermal processes in harmonic crystals.

The harmonic crystal is a lattice composed of material points interacting via linearized (harmonic)⁴ forces. This mathematical model is often used in literature to describe the thermal processes in solids [16–21, 23, 24]. In principle, equations of motion for a harmonic crystal can be solved analytically. However, due to random⁵ initial conditions, this approach leads to stochastic solutions.

Modeling of thermal processes is usually focused on the behavior of statistical characteristics, such as the kinetic temperature or its generalization, the tensor temperature [7, 9] rather than the random motion of individual particles. The problem in terms of the statistical characteristics is formulated using correlation analysis [16–19]. In the framework of this approach, a closed system of equations is derived for the covariances (mathematical expectations of the

¹ The article was translated by the authors.

² In particular, at the front of a shock wave propagating along the x direction, the following relation applies: $T_{xx} > T_{yy}$, where $k_B T_{xx} = m\langle v_x^2 \rangle$, $k_B T_{yy} = m\langle v_y^2 \rangle$, and k_B is the Boltzmann constant

³ Exchange between energies corresponding to motion of particles in different spacial directions is considered. There is no energy exchange between the normal modes.

⁴ Force is linearly dependent on particle displacement.

⁵ As a rule, particles are given random initial velocities in thermal problems.

products) of the particle displacements and velocities. The initial conditions for the covariances are deterministic. A solution of the system describes the evolution of the kinetic temperature. No assumptions about velocity distribution function are made in the derivation. The behavior of the distribution function during the transition towards equilibrium and its convergence to Gaussian distribution are discussed, for example, in papers [20–22].

Correlation analysis is used to describe thermal processes in harmonic crystals in papers [16–19]. In particular, the heat transfer is investigated. An analytical solution of the stationary heat transfer problem in a harmonic chain is obtained in the pioneering work of Rieder et al. [16]. The solution shows that heat propagation is not described by the Fourier law. This anomaly in harmonic and anharmonic crystals is investigated, for example, in papers [19, 24–27]. In particular, an equation describing the propagation of heat in the one-dimensional harmonic crystal is obtained in paper [19].

Correlation analysis also describes transient processes in uniformly heated crystals [17, 28]. In paper [17], harmonic chain with random initial velocities and zero initial displacements is considered. Initially, the total energy of the system is equal to the kinetic energy, and the potential energy is zero. It is shown that the kinetic and potential energies equilibrate in time, while their difference (Lagrangian) undergoes decaying oscillations described by the Bessel function of the first kind. The generalization to the case of a chain on an elastic foundation is given in paper [28].

In the present paper, we consider an analytical description of transient thermal processes in two- and three-dimensional uniformly heated harmonic crystals. Initially, the particles have random velocities and displacements. Using correlation analysis, we derive deterministic equations describing two transient processes: (i) equilibration of the kinetic and potential energies and (ii) redistribution of the kinetic energy among the spatial directions. We obtain exact analytical solutions of these equations for the square and triangular lattices. Numerical integration of the lattice dynamic equations provide a check for the analytical results. The influence of weak nonlinearity is investigated. The results obtained in the present paper provide an estimate of the time-scale of transient thermal processes in harmonic crystals, as well as the conditions under which the temperature demonstrates tensor properties.

2. LATTICE DYNAMICS EQUATIONS (STOCHASTIC PROBLEM)

Consider an infinite simple lattice consisting of identical particles connected by linear springs. Particles are identified by their radius vectors in the unde-

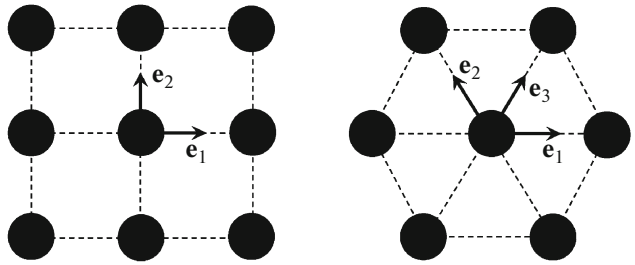


Fig. 1. Vectors \mathbf{e}_α for square and triangular lattices.

formed state. The equation of motion of a particle with radius vector \mathbf{r} has the form

$$\dot{\mathbf{v}}(\mathbf{r}) = \omega_*^2 \sum_{\alpha} \mathbf{e}_\alpha \mathbf{e}_\alpha \cdot (\mathbf{u}(\mathbf{r} + \mathbf{a}_\alpha) - 2\mathbf{u}(\mathbf{r}) + \mathbf{u}(\mathbf{r} - \mathbf{a}_\alpha)), \quad (1)$$

where $\mathbf{u}(\mathbf{r})$, $\mathbf{v}(\mathbf{r})$ are the displacement and velocity of a particle with radius vector \mathbf{r} ; \mathbf{a}_α is a vector connecting two neighboring particles; $\mathbf{e}_\alpha = \mathbf{a}_\alpha / |\mathbf{a}_\alpha|$; $\omega_* = \sqrt{C/m}$; C is the bond stiffness; m is particle mass. Summation is carried out over non-collinear directions of the bonds α . For the square lattice $\alpha = 1, 2$, and for the triangular lattice $\alpha = 1, 2, 3$ (see Fig. 1).

The following operator form of the equations of motion is used:

$$\dot{\mathbf{v}}(\mathbf{r}) = \mathcal{D} \cdot \mathbf{u}(\mathbf{r}), \quad \mathcal{D} = \omega_*^2 \sum_{\alpha} \mathbf{e}_\alpha \mathbf{e}_\alpha \Delta_{\alpha}^2, \quad (2)$$

$$\Delta_{\alpha}^2 \mathbf{u}(\mathbf{r}) = \mathbf{u}(\mathbf{r} + \mathbf{a}_\alpha) - 2\mathbf{u}(\mathbf{r}) + \mathbf{u}(\mathbf{r} - \mathbf{a}_\alpha).$$

Here \mathcal{D} is the tensor difference operator of the second order.⁶ The following initial conditions for equation (2) are considered:

$$\mathbf{u}(\mathbf{r}) = \mathbf{u}_0(\mathbf{r}), \quad \mathbf{v}(\mathbf{r}) = \mathbf{v}_0(\mathbf{r}), \quad (3)$$

where \mathbf{u}_0 , \mathbf{v}_0 are independent random vectors with zero mean. Hereinafter, the initial conditions are denoted by index “0.”

Equation (2) with initial conditions (3) completely determine the dynamics of the crystal. This problem can be solved analytically. The resulting displacements and velocities of the particles are random quantities. Analysis of motion of individual particles is important, for example, in problems of fracture [29, 30]. Description of the thermal processes usually focuses on the behavior of statistical characteristics, such as covariances (mathematical expectations of the product) of velocities and displacements of the particles. The initial conditions for the covariances are deterministic. A closed system of equations describing the dynamics of the covariances is derived in the following section.

⁶ It follows that the motion of particles is governed by a differential-difference equation.

3. THE DYNAMICS EQUATIONS FOR THE COVARIANCES (A DETERMINISTIC PROBLEM)

We consider an infinite number of realizations of the same crystal. The realizations differ by random velocities and displacements of the particles (see Eq. (3)). We introduce the covariances of displacements and velocities for all pairs of particles. For particles i, j the covariances are given by the following formulae:

$$\begin{aligned}\xi(\mathbf{r}_i, \mathbf{r}_j) &= \langle \mathbf{u}_i \mathbf{u}_j \rangle, & \kappa(\mathbf{r}_i, \mathbf{r}_j) &= \langle \mathbf{v}_i \mathbf{v}_j \rangle, \\ \mathbf{v}(\mathbf{r}_i, \mathbf{r}_j) &= \langle \mathbf{u}_i \mathbf{v}_j \rangle,\end{aligned}\quad (4)$$

where $\mathbf{r}_i, \mathbf{r}_j$ are radius vectors of corresponding particles; $\mathbf{u}_i = \mathbf{u}(\mathbf{r}_i)$; $\mathbf{v}_i = \mathbf{v}(\mathbf{r}_i)$. Hereinafter, the angular brackets denote the mathematical expectation. It is also assumed that the displacements and velocities are centered random variables, i.e., $\langle \mathbf{u}_i \rangle = 0$, $\langle \mathbf{v}_i \rangle = 0$.

We consider thermal processes in a uniformly heated crystal. In this case,

$$\begin{aligned}\xi(\mathbf{r}_i, \mathbf{r}_j) &= \xi(\mathbf{r}_i - \mathbf{r}_j), & \kappa(\mathbf{r}_i, \mathbf{r}_j) &= \kappa(\mathbf{r}_i - \mathbf{r}_j), \\ \mathbf{v}(\mathbf{r}_i, \mathbf{r}_j) &= \mathbf{v}(\mathbf{r}_i - \mathbf{r}_j).\end{aligned}\quad (5)$$

The argument $\mathbf{r}_i - \mathbf{r}_j$ is omitted for brevity. Note that a set of points defined by vectors $\mathbf{r}_i - \mathbf{r}_j$ forms the same lattice as the particles. Therefore, problems formulated for the covariances are solved “on the same lattice” as the equations of motion (2).

Differentiating covariances (4) with respect to time and taking into account equations of motion (2) and relations (5), yields

a system of the first-order differential equations:

$$\begin{aligned}\dot{\xi} &= \mathbf{v} + \mathbf{v}^*, & \dot{\kappa} &= \mathcal{D} \cdot \mathbf{v} + \mathbf{v}^* \cdot \mathcal{D}, & \dot{\mathbf{v}} &= \kappa + \xi \cdot \mathcal{D}, \\ (\mathbf{v}(\mathbf{r}_i - \mathbf{r}_j))^* &= \mathbf{v}^T(\mathbf{r}_j - \mathbf{r}_i);\end{aligned}\quad (6)$$

a system of the second-order differential equation for ξ and κ :

$$\begin{aligned}\ddot{\xi} &= \mathcal{D} \cdot \dot{\xi} + \dot{\xi} \cdot \mathcal{D} + 2\kappa, \\ \ddot{\kappa} &= \mathcal{D} \cdot \dot{\kappa} + \dot{\kappa} \cdot \mathcal{D} + 2\mathcal{D} \cdot \xi \cdot \mathcal{D};\end{aligned}\quad (7)$$

a system of the second-order differential equation for \mathbf{v} :

$$\begin{aligned}\dot{\mathbf{v}} &= \mathcal{D} \cdot \mathbf{v} + (\mathbf{v} + 2\mathbf{v}^*) \cdot \mathcal{D}, \\ \dot{\mathbf{v}}^* &= \mathcal{D} \cdot (\mathbf{v}^* + 2\mathbf{v}) + \mathbf{v}^* \cdot \mathcal{D};\end{aligned}\quad (8)$$

the fourth-order equation

$$\begin{aligned}\ddot{\ddot{\kappa}} - 2(\mathcal{D} \cdot \ddot{\kappa} + \ddot{\kappa} \cdot \mathcal{D}) \\ + \mathcal{D}^2 \cdot \kappa - 2\mathcal{D} \cdot \kappa \cdot \mathcal{D} + \kappa \cdot \mathcal{D}^2 = 0.\end{aligned}\quad (9)$$

Here $\mathcal{D}^2 = \mathcal{D} \cdot \mathcal{D}$; \mathbf{v}^T is the transpose of tensor \mathbf{v} . Note that displacements covariance ξ also satisfies equation (9). Equations (6)–(9) allow one to calculate all covariances at any moment of time.

We show that covariances of velocities and displacements \mathbf{v} satisfy conservation laws. It follows from (6) that

$$\dot{\mathbf{v}} - \dot{\mathbf{v}}^* = \xi \cdot \mathcal{D} - \mathcal{D} \cdot \xi. \quad (10)$$

Multiplying both parts of equation (10) by \mathcal{D}^n , yields⁷

$$\mathcal{D}^n \cdot (\mathbf{v} - \mathbf{v}^*) = \text{const}, \quad n = 0, 1, 2, \dots \quad (11)$$

Hereinafter $\mathcal{D}^0 = \mathcal{I}$, where \mathcal{I} is the unit tensor. It follows from the Cayley–Hamilton theorem that the number of independent conservation laws (11) is equal to the number of space dimensions.

The initial conditions for equations (6)–(9) are uniquely determined by the initial displacements and velocities of the particles. In particular, initial conditions for equations (6) have the form

$$\xi = \langle \mathbf{u}_i^0 \mathbf{u}_j^0 \rangle, \quad \kappa = \langle \mathbf{v}_i^0 \mathbf{v}_j^0 \rangle, \quad \mathbf{v} = \langle \mathbf{u}_i^0 \mathbf{v}_j^0 \rangle, \quad (12)$$

where $\mathbf{u}_i^0, \mathbf{v}_i^0$ are initial velocities and displacements. Note that in contrast to initial conditions (3) for the displacements, initial conditions (12) for the covariances are deterministic.

Thus, the lattice dynamics problem with random initial conditions (3) is reduced to equations (6)–(8) or (9) for covariances with deterministic initial conditions (12).

4. GENERALIZED ENERGIES

One of the central quantities in the description of thermal processes is the kinetic temperature T [31] or its generalization, the tensor temperature \mathcal{T} [7, 9]⁸

$$\frac{k_B}{2} \mathcal{T}(\mathbf{r}_i) = \frac{m}{2} \langle \mathbf{v}_i \mathbf{v}_i \rangle = \frac{m}{2} \kappa_{i=j}, \quad T = \frac{1}{d} \text{tr} \mathcal{T}, \quad (13)$$

where k_B is the Boltzmann constant, and d is the space dimensionality.

In the previous section, it is shown that the kinetic temperature is insufficient for derivation of a closed system of equations. Hence, consideration of velocity covariances is required (see Eq. (9)). In papers [17, 19, 32] it is proposed to consider generalized energies (linear combinations of covariances). We introduce the generalized (two-particle) kinetic \mathcal{H} and potential \mathcal{U} energies [19] for a pair of particles i, j :

$$\mathcal{H}(\mathbf{r}_i - \mathbf{r}_j) = \frac{m}{2} \kappa, \quad (14)$$

$$\mathcal{U}(\mathbf{r}_i - \mathbf{r}_j) = -\frac{m}{4} (\mathcal{D} \cdot \xi + \xi \cdot \mathcal{D}).$$

In the case $i = j$, traces of tensors \mathcal{H} and \mathcal{U} correspond to the conventional potential and kinetic energies per

⁷ A double dot symbol stands for the double scalar product, e.g., $\mathbf{ab} \cdot \cdot \mathbf{cd} = (\mathbf{b} \cdot \mathbf{c})(\mathbf{a} \cdot \mathbf{d})$

⁸ In papers [7, 9], molecular dynamics simulations of shock waves in liquids is investigated.

particle. The argument of generalized energies $\mathbf{r}_i - \mathbf{r}_j$ is further omitted for brevity. We also introduce a generalized total energy \mathcal{H} and a generalized Lagrangian \mathcal{L} :

$$\mathcal{H} = \mathcal{K} + \mathcal{U}, \quad \mathcal{L} = \mathcal{K} - \mathcal{U}. \quad (15)$$

In the previous section, it is shown that covariances ξ and κ satisfy equation (9). Therefore, generalized energies \mathcal{K} , \mathcal{U} , \mathcal{L} , \mathcal{H} also satisfy equation (9). For brevity, we write this equation in operator form

$$\mathcal{L}\mathcal{G} = 0, \quad (16)$$

$$\mathcal{G} = \{\xi, \kappa, \mathcal{K}, \mathcal{U}, \mathcal{L}, \mathcal{H}\},$$

$$\begin{aligned} \mathcal{L}\mathcal{G} = & \ddot{\mathcal{G}} - 2(\mathcal{D} \cdot \dot{\mathcal{G}} + \dot{\mathcal{G}} \cdot \mathcal{D}) + \mathcal{D}^2 \cdot \mathcal{G} \\ & - 2\mathcal{D} \cdot \mathcal{G} \cdot \mathcal{D} + \mathcal{G} \cdot \mathcal{D}^2, \end{aligned}$$

where \mathcal{L} is a linear differential-difference operator. Note that the symmetric and antisymmetric parts of tensors ξ , κ , \mathcal{K} , \mathcal{U} , \mathcal{L} , \mathcal{H} satisfy equation (16).⁹

As a result, covariances and generalized energies satisfy equation (16). Initial conditions for equation (16) are uniquely determined by the initial displacements and velocities of the particles (3).

The generalized total energy satisfies several conservation laws. From the system of equations (6), it follows that

$$\dot{\mathcal{H}} = \frac{m}{4} (\mathcal{D} \cdot (\mathbf{v} - \mathbf{v}^*) - (\mathbf{v} - \mathbf{v}^*) \cdot \mathcal{D}). \quad (17)$$

Multiplying equation (17) by \mathcal{D}^n , we obtain the conservation laws

$$\mathcal{D}^n \cdot \mathcal{H} = \text{const}, \quad n = 0, 1, 2, \dots \quad (18)$$

In the case $n = 0$, $i = j$, formula (18) coincides with the conventional law of energy conservation. From the Cayley–Hamilton theorem it follows that the number of independent conservation laws (18) is equal to the number of space dimensions.

Thus, the dynamics of the generalized energies is described by equation (16) with deterministic initial conditions. Solution of this equation determines the behavior of the tensor temperature (13). Note that the generalized total energy satisfies conservation laws (18). In the next section, we use the conservation laws to calculate the generalized energies in a steady state.

5. STEADY STATE

Numerical simulations show that after a rapid transitory period, the crystal reaches an almost stationary state. The steady state is defined as the state of the crystal in which the second time derivatives of the covariances are equal to zero. In this section, we obtain a relation between the generalized energies in the steady state and the initial conditions. Canceling

out the time derivatives in equation (16) for \mathcal{H} , and using conservation laws (18), we obtain a closed system of equations for the steady state:

$$\begin{aligned} \text{tr}\mathcal{H} &= \text{tr}\mathcal{H}_0, \quad \mathcal{D} \cdot \mathcal{H} = \mathcal{D} \cdot \mathcal{H}_0, \\ \mathcal{D}^2 \cdot \mathcal{H} &= \mathcal{D}^2 \cdot \mathcal{H}_0, \end{aligned} \quad (19)$$

$$\mathcal{D}^2 \cdot \mathcal{H} - 2\mathcal{D} \cdot \mathcal{H} \cdot \mathcal{D} + \mathcal{H} \cdot \mathcal{D}^2 = 0,$$

where \mathcal{H}_0 is the initial value of the generalized total energy. The first equation of (19) represents the spherical part of the generalized total energy, while the remaining equations give the deviatoric part. These equations can be solved analytically, for example, by using a discrete Fourier transform (see Subsection 8.2).

Consider the ratio between the generalized kinetic and potential energies \mathcal{K} and \mathcal{U} in the steady state. Rewriting the first equation of (7) in the form

$$\frac{m\xi}{4} = \mathcal{L} \quad (20)$$

and canceling out the time derivative, we obtain

$$\mathcal{L} = 0, \quad \mathcal{K} = \mathcal{U} = \frac{1}{2}\mathcal{H} \quad (21)$$

in the steady state. From formulae (21), it follows that the generalized kinetic and potential energies are equal in the steady state. The first equation of system (19) and equation (21) specify the traces of the generalized energies,

$$\text{tr}\mathcal{K} = \text{tr}\mathcal{U} = \frac{1}{2}\text{tr}\mathcal{H}_0. \quad (22)$$

In the case $i = j$, formula (22) shows that conventional kinetic and potential energies are equal in the steady state. This fact also follows from the virial theorem [33]. However, in contrast to the approach used in this study, the virial theorem does not describe the transition to the steady state.

Deviators of the generalized energies are calculated using system (19). Note that system (19) is valid both for two-dimensional¹⁰ and three-dimensional cases.

Thus, in the steady state, the generalized kinetic energy is equal to the generalized potential energy. The relation between energies in the steady state and the initial conditions is given by equations (19), (21), and (22). Solutions of these equations for square and triangular lattices are obtained below. In Subsection 8.2, it is shown that the temperature tensor (13) in general is not isotropic, even in the steady state.

6. TRANSITION TO THE STEADY STATE

Transition towards the steady state is accompanied by two simultaneous processes. Firstly, the kinetic and potential energies equilibrate. This process is described by equation (16). Secondly, the energy is

⁹ Consequently, the symmetric and antisymmetric part of generalized energies can be considered independently.

¹⁰ In the two-dimensional case, the third equation of the system (19) follows from the first two.

redistributed among the spatial directions. The redistribution takes place, for example, in the case when initial kinetic energies corresponding to motions in different directions are not the same ($\langle v_x^2 \rangle \neq \langle v_y^2 \rangle$). In this section, we consider the dynamics of this transient process.

Difference between energies corresponding to different spatial directions is characterized by $\text{dev}\mathcal{H}$.¹¹ It is shown above that tensor \mathcal{H} satisfies equation (16). From conservation law (18) it follows that trace \mathcal{H} does not depend on time. Then deviator \mathcal{H} also satisfies equation (16):

$$\mathcal{L}(\text{dev}\mathcal{H}) = 0. \quad (23)$$

If the initial velocities and displacements of the particles are uncorrelated ($\mathbf{v} = 0$), then initial conditions for equation (23) have the form

$$\begin{aligned} \text{dev}\mathcal{H} &= \text{dev}\mathcal{H}_0, & \text{dev}\dot{\mathcal{H}} &= 0, & \text{dev}\ddot{\mathcal{H}} &= 0, \\ & & \text{dev}\dot{\mathcal{H}} & & & \\ & & \text{dev}\ddot{\mathcal{H}} & & & \end{aligned} \quad (24)$$

$$= -\frac{m}{4}(\mathcal{D}^2 \cdot \text{dev}\xi_0 - 2\mathcal{D} \cdot \text{dev}\xi_0 \cdot \mathcal{D} + \text{dev}\xi_0 \cdot \mathcal{D}^2),$$

where ξ_0 is the initial value of the displacements covariance and \mathcal{H}_0 is the initial generalized total energy. Formula (24) shows that independent quantities $\text{dev}\mathcal{H}_0$ and $\text{dev}\xi_0$ influence the redistribution of energy among the spatial direction. However, in the steady state, the value of $\text{dev}\mathcal{H}$ is affected only by $\text{dev}\mathcal{H}_0$ (see Eq. (19)).

Thus, the transition to the steady state is accompanied by two simultaneous processes: (i) equilibration of the kinetic and potential energies and (ii) redistribution of energy among the spatial directions. These processes are described by the same equation (16) formulated for \mathcal{L} and $\text{dev}\mathcal{H}$, respectively. Solutions of the equation for the square and triangular lattices are obtained below. In particular, for the triangular lattice it is shown that at large times the solution of equation (16) for $\text{dev}\mathcal{H}$ tends to the solution of system (19), describing the steady state.

7. THE SQUARE LATTICE

We consider an infinite square lattice with basis vectors $\mathbf{e}_1, \mathbf{e}_2$ (see. Fig. 1). The particles oscillate in the plane of the lattice.¹² This lattice is used as an example to illustrate the presented ideas. Initially, particles have independent random velocities and zero displacements. Under these initial conditions tensors \mathcal{H}

¹¹ $\text{dev}\mathcal{H} = \mathcal{H} - \frac{1}{d}\text{tr}(\mathcal{H})\mathcal{I}$, where d is the dimensionality of space and \mathcal{I} is the unit tensor

¹²Note that in literature, the out-of-plane vibrations are often considered (see, e.g., [34]).

and \mathcal{L} are symmetrical.¹³ We consider the redistribution of energy among the spatial directions and the equilibration of kinetic and potential energies.

It is previously shown that the generalized energies depend on vectors $\mathbf{r}_i - \mathbf{r}_j$ connecting the particles. Points defined by these vectors form the square lattice. We use the following representation for $\mathbf{r}_i - \mathbf{r}_j$:

$$\mathbf{r}_i - \mathbf{r}_j = a(k\mathbf{e}_1 + n\mathbf{e}_2), \quad (25)$$

where k, n are integer numbers and a is an equilibrium distance.

Consider the dynamics of generalized total energy \mathcal{H} . We restrict ourselves to the case when the components of the initial particle velocities in directions $\mathbf{e}_1, \mathbf{e}_2$ are independent. Then, the initial conditions for \mathcal{H} have the form

$$\begin{aligned} \mathcal{H} &= \mathcal{H}_0 = (K_1^0\mathbf{e}_1\mathbf{e}_1 + K_2^0\mathbf{e}_2\mathbf{e}_2)\delta_k\delta_n, \\ \dot{\mathcal{H}} &= 0, & \ddot{\mathcal{H}} &= 0, & \ddot{\mathcal{H}} &= 0, \end{aligned} \quad (26)$$

where δ_n is the function equal to 1 for $n = 0$ and equal to 0 in all the other cases. The change in \mathcal{H} during the transition to the steady state is described by equation (9), where operator \mathcal{D} has the form

$$\mathcal{D} = \omega_*^2(\Delta_1^2\mathbf{e}_1\mathbf{e}_2 + \Delta_2^2\mathbf{e}_2\mathbf{e}_2). \quad (27)$$

Taking into account (27), equation (9) decomposes into independent scalar equations for $H_{ij} = \mathbf{e}_i \cdot \mathcal{H} \cdot \mathbf{e}_j$:

$$\begin{aligned} \ddot{H}_{11} - 4\omega_*^2\Delta_1^2\dot{H}_{11} &= 0, & \ddot{H}_{22} - 4\omega_*^2\Delta_2^2\dot{H}_{22} &= 0, \\ \ddot{H}_{12} - 2\omega_*^2(\Delta_1^2 + \Delta_2^2)\dot{H}_{12} + \omega_*^4(\Delta_1^2 + \Delta_2^2)^2 H_{12} &= 0. \end{aligned} \quad (28)$$

Therefore, there is no energy redistribution among the spatial directions in a square lattice. In particular, under initial conditions (26) equation (28) has the solution $\mathcal{H} = \mathcal{H}_0$, i.e., the generalized total energy is conserved.

Consider the equilibration of the kinetic and potential energies. The initial conditions for the generalized Lagrangian \mathcal{L} have the form

$$\begin{aligned} \mathcal{L} &= \mathcal{H}_0, & \dot{\mathcal{L}} &= 0, \\ \ddot{\mathcal{L}} &= 2(\mathcal{D} \cdot \mathcal{H}_0 + \mathcal{H}_0 \cdot \mathcal{D}), & \ddot{\mathcal{L}} &= 0. \end{aligned} \quad (29)$$

It can be shown that components $L_{ij} = \mathbf{e}_i \cdot \mathcal{L} \cdot \mathbf{e}_j$ of the generalized Lagrangian satisfy equations (28). The equation for L_{12} with initial conditions (29) has a trivial solution. The equations for L_{11} and L_{22} are rewritten as follows:

$$\ddot{L}_{11} - 4\omega_*^2\Delta_1^2L_{11} = 0, \quad \ddot{L}_{22} - 4\omega_*^2\Delta_2^2L_{22} = 0. \quad (30)$$

Equations (30) are similar to the equation for the dynamics of Lagrangian in the harmonic one-dimensional chain, obtained in paper [17]. The solu-

¹³It was noted earlier that the antisymmetric part of tensors \mathcal{H} and \mathcal{L} satisfy equation (16). In this case, the initial conditions for the anti-symmetric parts are zero.

tion of equation (30) with initial conditions (29) has the form [17]

$$\mathcal{L} = K_1^0 J_{2k}(4\omega_* t) \delta_n \mathbf{e}_1 \mathbf{e}_1 + K_2^0 J_{2n}(4\omega_* t) \delta_k \mathbf{e}_2 \mathbf{e}_2, \quad (31)$$

where J is the Bessel function of the first kind. Using the asymptotic formulae for the Bessel functions, we show that the generalized Lagrangian oscillates with an amplitude inversely proportional to the square root of time. Taking into account the conservation law of generalized total energy $\mathcal{H} = \mathcal{H}_0$, in the steady state we have

$$\mathcal{H} = \mathcal{U} = \frac{1}{2} \mathcal{H}_0. \quad (32)$$

It follows from formulas (13) and (32) that the tensor temperature in a stationary state is isotropic only if the initial velocities are uniformly distributed among spatial directions (tensor \mathcal{H}_0 is isotropic).

Thus in a square lattice, the potential and kinetic energies corresponding to the same spatial direction equilibrate. The equilibration is governed by the same law as in a one-dimensional chain [17]. There is no redistribution of energy among the spatial directions. In general, the tensor temperature (13) is not isotropic.

8. THE TRIANGULAR LATTICE

8.1. General Relations

In this section, we discuss transient thermal processes in a triangular lattice (see Fig. 1). As already mentioned, the generalized energies depend on vectors $\mathbf{r}_i - \mathbf{r}_j$. The set of points, defined by vectors $\mathbf{r}_i - \mathbf{r}_j$, also forms the triangular lattice. Analytical solutions are obtained for a periodic cell. Particles in the cell are numbered by a pair of indices k, n :

$$\begin{aligned} \mathbf{r}_i - \mathbf{r}_j &= a(k\mathbf{e}_1 + n\mathbf{e}_2), \quad k, n = -N, \dots, N, \\ \mathbf{e}_1 &= \mathbf{i}, \quad \mathbf{e}_2 = -\frac{1}{2}\mathbf{i} + \frac{\sqrt{3}}{2}\mathbf{j}, \quad \mathbf{e}_3 = \mathbf{e}_1 + \mathbf{e}_2, \end{aligned} \quad (33)$$

where $2N + 1$ is the number of particles along one side of the periodic cell; \mathbf{i}, \mathbf{j} are the unit vectors of the Cartesian basis; vectors $\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3$ are shown in Fig. 1. The periodic cell has a diamond shape. Generalized energies $\mathcal{H}_{k, n}, \mathcal{U}_{k, n}$ are defined at the points with indices k, n . In paper [35], it is shown that this numbering is convenient for the analysis of the triangular lattice.

The generalized energies are calculated using difference equations (19) and differential-difference equations (16) and (23). The equations are solved using the discrete Fourier transform. For example, the direct and inverse discrete Fourier transforms of the

generalized total energy $\mathcal{H}_{k, n} = \mathcal{H}(a(k\mathbf{e}_1 + n\mathbf{e}_2))$, have the form

$$\begin{aligned} \hat{\mathcal{H}}_{s, p} &= \sum_{k, n=-N}^N \mathcal{H}_{k, n} e^{-2i(\theta_s k + \theta_p n)}, \quad \theta_s = \frac{\pi s}{2N + 1}, \\ \mathcal{H}_{k, n} &= \frac{1}{(2N + 1)^2} \sum_{s, p=-N}^N \hat{\mathcal{H}}_{s, p} e^{2i(\theta_s k + \theta_p n)}, \end{aligned} \quad (34)$$

where i is the imaginary unit. Hereinafter, the Fourier image is denoted by a hat sign. Indices k, n and s, p are omitted from now for brevity.

Solutions obtained via the discrete Fourier transform (34) describe the processes in finite crystals under periodic boundary conditions. Solutions for infinite crystal are obtained in the limit $N \rightarrow \infty$.

8.2. The Steady State and the Tensor Temperature

Consider the steady-state values of generalized energies \mathcal{H}, \mathcal{U} and tensor temperature (13) in the triangular lattice. The traces of the generalized energies are given by equation (22), and the deviators are expressed in terms of $\text{dev} \mathcal{H}$:

$$\text{dev} \mathcal{H} = \text{dev} \mathcal{U} = \frac{1}{2} \text{dev} \mathcal{H}. \quad (35)$$

Therefore, the problem reduces to calculation of $\text{dev} \mathcal{H}$ from the system of difference equations (19). The following relation is used:

$$\mathcal{D} \cdot \mathcal{H} = \mathcal{H} \cdot \mathcal{D}. \quad (36)$$

The expression (36) is a particular solution of the last equation in (19). Numerical solution of lattice dynamics equations (2) show that formula (36) leads to correct results.

We represent the deviators of tensors $\mathcal{H}, \mathcal{H}_0$ in the Cartesian basis \mathbf{i}, \mathbf{j}

$$\begin{aligned} \text{dev} \mathcal{H} &= H_1(\mathbf{ii} - \mathbf{jj}) + H_2(\mathbf{ij} + \mathbf{ji}), \\ \text{dev} \mathcal{H}_0 &= H_1^0(\mathbf{ii} - \mathbf{jj}) + H_2^0(\mathbf{ij} + \mathbf{ji}). \end{aligned} \quad (37)$$

The discrete Fourier transform (34) is applied to system (19) taking into account formulae (36) and (37). Then projection of the resulting Fourier transforms onto vectors \mathbf{i}, \mathbf{j} , yields

$$\begin{aligned} A_{s, p}(\hat{H}_1 - \hat{H}_1^0) + B_{s, p}(\hat{H}_2 - \hat{H}_2^0) &= 0, \\ B_{s, p} \hat{H}_1 &= A_{s, p} \hat{H}_2, \\ A_{s, p} &= 2\omega_*^2(\sin^2 \theta_p + \sin^2(\theta_s + \theta_p) - 2\sin^2 \theta_s), \\ B_{s, p} &= 2\sqrt{3}\omega_*^2(\sin^2 \theta_p - \sin^2(\theta_s + \theta_p)). \end{aligned} \quad (38)$$

Solving system (38) with respect to \hat{H}_1 , \hat{H}_2 and applying the inverse discrete Fourier transform, we obtain

$$\begin{aligned} \text{dev}\mathcal{H} &= H_1(\mathbf{ii} - \mathbf{jj}) + H_2(\mathbf{ij} + \mathbf{ji}), \\ H_1 &= \frac{1}{(2N+1)^2} \\ &\times \sum_{s,p=-N}^N \frac{A_{s,p}^2 \hat{H}_1^0 + A_{s,p} B_{s,p} \hat{H}_2^0}{A_{s,p}^2 + B_{s,p}^2} \cos(2\theta_s k + 2\theta_p n), \\ H_2 &= \frac{1}{(2N+1)^2} \\ &\times \sum_{s,p=-N}^N \frac{A_{s,p} B_{s,p} \hat{H}_1^0 + B_{s,p}^2 \hat{H}_2^0}{A_{s,p}^2 + B_{s,p}^2} \cos(2\theta_s k + 2\theta_p n), \end{aligned} \quad (39)$$

where θ_s and θ_p are defined by formula (34). In the thermodynamic limit ($N \rightarrow \infty$), sums in formula (39) are transformed into integrals. Solution (39) is obtained under arbitrary initial conditions. Evidently, in a general case $\text{dev}\mathcal{H} \neq 0$, so there is no energy equipartition among spatial directions.

Consider the case when particles have independent random initial velocities and zero initial displacements. Then, $\mathcal{H}_0 = \mathcal{H}_0 \delta_k \delta_n$, where $\mathcal{H}_0 = \frac{m}{2} \langle \mathbf{v}_i^0 \mathbf{v}_i^0 \rangle$. It can be shown that the following identities are satisfied:

$$\begin{aligned} \sum_{s,p=-N}^N \frac{A_{s,p}^2}{A_{s,p}^2 + B_{s,p}^2} &= \sum_{s,p=-N}^N \frac{B_{s,p}^2}{A_{s,p}^2 + B_{s,p}^2}, \\ \sum_{s,p=-N}^N \frac{A_{s,p} B_{s,p}}{A_{s,p}^2 + B_{s,p}^2} &= 0. \end{aligned} \quad (40)$$

Substituting \mathcal{H}_0 into solution (39) and using identities (40), yields for $k = n = 0$

$$\text{dev}\mathcal{H} = \frac{1}{2} \text{dev}\mathcal{H}_0, \quad \text{dev}\mathcal{H} = \frac{1}{4} \text{dev}\mathcal{H}_0. \quad (41)$$

Formula (41) shows that there is no equipartition of kinetic energy among spatial directions in harmonic triangular lattice. If projections of initial velocities on axes x and y are uncorrelated, then formula (41) yields a simple expression for the components of the tensor temperature (13):

$$T_{xx} - T_{yy} = \frac{1}{4} (T_{xx}^0 - T_{yy}^0), \quad (42)$$

where $T_{xx} = \mathbf{i} \cdot \mathcal{T} \cdot \mathbf{i}$, $T_{yy} = \mathbf{j} \cdot \mathcal{T} \cdot \mathbf{j}$; T_{xx}^0 , T_{yy}^0 are initial values of T_{xx} and T_{yy} . Thus, in general, the temperature tensor (13) is not isotropic even in the steady state.

Consider the covariance of velocities in the steady state

$$\langle \mathbf{v}(\mathbf{r}) \mathbf{v}(\mathbf{r} + k \mathbf{a}_\alpha) \rangle = \frac{2}{m} \mathcal{H}(k \mathbf{a}_\alpha). \quad (43)$$

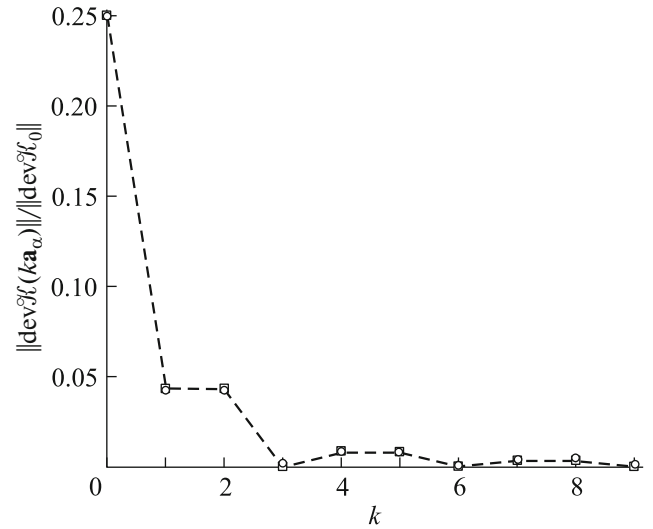


Fig. 2. Generalized kinetic energy in the steady state for harmonic triangular lattice. The value $\|\text{dev}\mathcal{H}(k\mathbf{a}_\alpha)\|$ is proportional to the covariance of velocities for a pair of particles. The distance between particles is equal to ka , where a is an equilibrium distance (see formula (43)). Solid line connects points obtained using formula (39) for $N = 150$; squares and circles correspond to the numerical solution of lattice dynamics equation (2) ($\alpha = 1, 2$).

In the one-dimensional case [17], the covariances are equal to zero for all $k > 0$. In two dimensions, only the spherical parts of tensors (43) are equal to zero (see formula (22)). In the general case, the deviatoric parts of tensors (43) are not equal to zero. They are calculated using equations (14), (35), and (39). Analysis of formula (39) shows that the covariance of velocities is inversely proportional to the square of the distance between the particles. In addition, norm¹⁴ $\|\text{dev}\mathcal{H}(k\mathbf{a}_\alpha)\|$ is independent of the direction given by α .

In order to check the accuracy of analytical solution (39), we compare it with the numerical solution of lattice dynamics equations (2). Hereinafter, the Verlet integration scheme with time-step $5 \times 10^{-3} \tau_*$, $\tau_* = 2\pi/\omega_*$ is used. Periodic boundary conditions are applied. The periodic cell contains 10^6 particles. Initially particles have independent random velocities directed along one of the basis vectors and zero displacements. Comparison of the numerical solution of the lattice dynamic equations (2) with the analytical solution (39) is shown in Fig. 2. It is seen that the solutions are virtually indistinguishable.

Thus, the analytical solution demonstrates that the temperature tensor in a harmonic crystal, generally speaking, is not isotropic ($T_{xx} \neq T_{yy}$). In addition, the velocity covariance for neighboring particles $\langle \mathbf{v}_i \mathbf{v}_j \rangle$ is not equal to zero, i.e. particles' velocities are not statistically independent.

¹⁴Here we use the norm $\|\mathcal{H}\| = \mathcal{H} \cdot \mathcal{H}$.

8.3. Redistribution of Energy Among Spatial Directions

In Section 6, it is shown that the equation (23) for $\text{dev}\mathcal{H}$ describes the redistribution of energy among spatial directions. In the present section, we solve this equation for a triangular lattice.

Suppose that particles have independent random initial velocities and zero initial displacements. We restrict ourselves to the case when components of velocities along the directions \mathbf{i} and \mathbf{j} are independent. Then the initial conditions have the form

$$\begin{aligned} \text{dev}\mathcal{H} &= \text{dev}\mathcal{H}_0 = H_1^0(\mathbf{ii} - \mathbf{jj})\delta_k\delta_n, \\ \dot{\mathcal{H}} &= 0, \quad \ddot{\mathcal{H}} = 0, \quad \ddot{\mathcal{H}} = 0. \end{aligned} \quad (44)$$

Consider the discrete Fourier transform of equation (23),

$$\begin{aligned} \text{dev}\ddot{\mathcal{H}} - 2(\hat{\mathcal{D}} \cdot \text{dev}\ddot{\mathcal{H}} + \text{dev}\ddot{\mathcal{H}} \cdot \hat{\mathcal{D}}) + \hat{\mathcal{D}}^2 \cdot \text{dev}\ddot{\mathcal{H}} \\ - 2\hat{\mathcal{D}} \cdot \text{dev}\ddot{\mathcal{H}} \cdot \hat{\mathcal{D}} + \text{dev}\ddot{\mathcal{H}} \cdot \hat{\mathcal{D}}^2 = 0, \\ \hat{\mathcal{D}} = -4\omega_*^2(\sin^2\theta_s\mathbf{e}_1\mathbf{e}_1 + \sin^2\theta_p\mathbf{e}_2\mathbf{e}_2 \\ + \sin^2(\theta_s + \theta_p)\mathbf{e}_3\mathbf{e}_3). \end{aligned} \quad (45)$$

Tensor $\text{dev}\ddot{\mathcal{H}}$ is represented in the Cartesian basis (37). Corresponding components \hat{H}_1, \hat{H}_2 of tensor $\text{dev}\ddot{\mathcal{H}}$ are related by the first equation of system (38).¹⁵ Multiplying equation (45) by $\mathbf{ii} - \mathbf{jj}$, and taking formula (38) into account, yields an equation for \hat{H}_1 with the corresponding initial conditions:

$$\begin{aligned} \ddot{\hat{H}}_1 - 2\text{tr}\hat{\mathcal{D}}\ddot{\hat{H}}_1 + (A_{s,p}^2 + B_{s,p}^2)\hat{H}_1 - A_{s,p}^2H_1^0 = 0, \\ \hat{H}_1 = H_1^0, \quad \dot{\hat{H}}_1 = 0, \quad \ddot{\hat{H}}_1 = 0, \quad \ddot{\hat{H}}_1 = 0, \end{aligned} \quad (46)$$

where $A_{s,p}$ and $B_{s,p}$ are defined by (39). Solving equation (46) and applying the inverse Fourier transform, yields

$$\begin{aligned} H_1 = \frac{H_1^0}{(2N+1)^2} \sum_{s,p=-N}^N \frac{\cos(2\theta_s k + 2\theta_p n)}{A_{s,p}^2 + B_{s,p}^2} \\ \times \left(A_{s,p}^2 + \frac{B_{s,p}^2}{\Omega_+^2 - \Omega_-^2} (\Omega_+^2 \cos(\Omega_- t) - \Omega_-^2 \cos(\Omega_+ t)) \right), \\ \Omega_{\pm} = 2\omega_*(\sin^2\theta_s + \sin^2\theta_p \\ + \sin^2(\theta_s + \theta_p) \pm \sqrt{3}(\sin^2\theta_s \sin^2\theta_p \\ + (\sin^2\theta_s + \sin^2\theta_p)\sin^2(\theta_s + \theta_p))^{1/2})^{1/2}. \end{aligned} \quad (47)$$

A similar expression for H_2 is obtained using the first equation of system (38). In particular, it is shown

¹⁵This formula follows from conservation law (18).

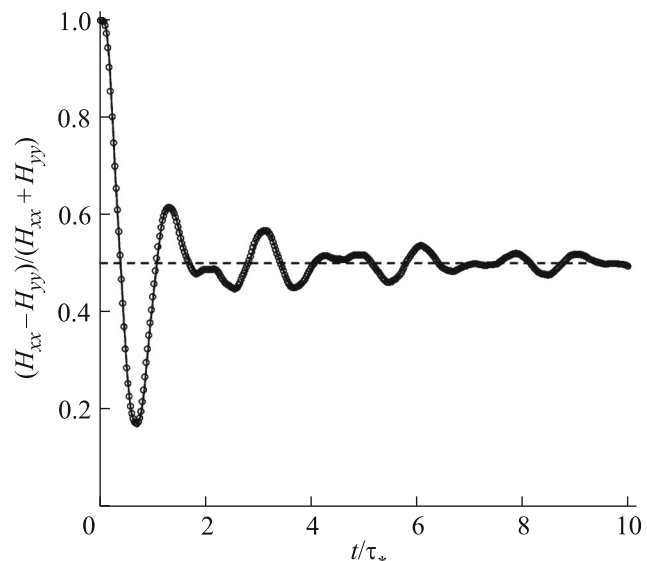


Fig. 3. Redistribution of energy among spatial directions in harmonic triangular lattice. H_{xx}, H_{yy} are components of the generalized total energy $\mathcal{H}(\mathbf{r}_i - \mathbf{r}_j)$ for $i=j$. Solid line—analytical solution (48); circles—numerical solution of lattice dynamics equations (2); dashed line—analytical solution (41) of the steady state problem.

that $H_2 = 0$ for $k = n = 0$. As a result, for $k = n = 0$ we have

$$\begin{aligned} \text{dev}\mathcal{H} = \text{dev}\mathcal{H}_0 \left[1 - \frac{2}{(2N+1)^2} \right. \\ \left. \times \sum_{s,p=-N}^N \frac{B_{s,p}^2 \left(\Omega_+^2 \sin^2 \left(\frac{1}{2} \Omega_- t \right) - \Omega_-^2 \sin^2 \left(\frac{1}{2} \Omega_+ t \right) \right)}{(A_{s,p}^2 + B_{s,p}^2)(\Omega_+^2 - \Omega_-^2)} \right]. \end{aligned} \quad (48)$$

Comparison of analytical solution (48) with the numerical solution of lattice dynamic equations (2) is shown in Fig. 3. Given the scale in the plot, the results agree. The difference between the energies corresponding to x and y direction tends to half of the initial value. This result coincides with the solution of stationary problem (41) $\text{dev}\mathcal{H} = \frac{1}{2}\text{dev}\mathcal{H}_0$.

Thus, the redistribution of energy among spatial directions in a triangular lattice with random initial velocities and zero displacements is described by formula (48). The system tends to the steady state in which relations (41) are satisfied. The characteristic time of the transition process is of the order of ten periods of atomic vibrations τ_* (see Fig. 3).

8.4. Equilibration of the Kinetic and Potential Energies

Consider the equilibration of the kinetic and potential energies. It is described by equation (16) with respect to the generalized Lagrangian \mathcal{L} . Suppose that

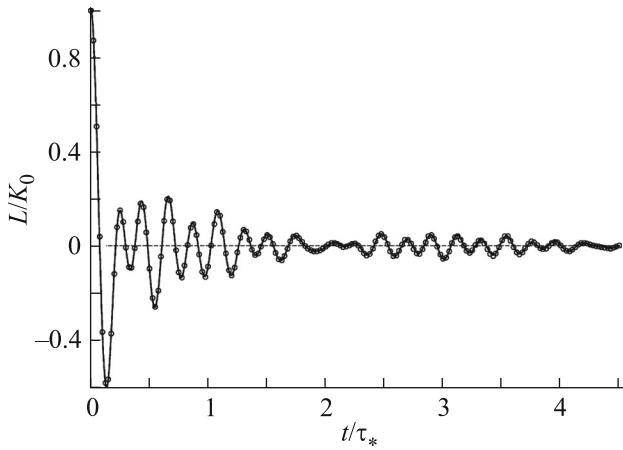


Fig. 4. Equilibration of kinetic and potential energies in harmonic triangular lattice with random initial velocities. Solid line—analytical solution (53); circles—numerical solution of lattice dynamics equations (2).

the particles have independent random initial velocities uniformly distributed among the spatial directions and zero initial displacements. Then initial conditions for equation (16) have the following form

$$\mathcal{L} = \frac{K_0}{2} \delta_k \delta_n \mathcal{F}, \quad \dot{\mathcal{L}} = 0, \quad \ddot{\mathcal{L}} = 4\mathcal{D} \cdot \mathcal{L}, \quad \dddot{\mathcal{L}} = 0, \quad (49)$$

where K_0 is the initial value of the kinetic energy and \mathcal{F} is a unit tensor. In order to solve (16), we assume that $\mathcal{D} \cdot \mathcal{L} = \mathcal{L} \cdot \mathcal{D}$. Then, taking into account initial conditions (49), equation (16) reduces to

$$\ddot{\mathcal{L}} = 4\mathcal{D} \cdot \mathcal{L}. \quad (50)$$

It can be seen that the assumption significantly simplifies equation (16). The comparison with the numerical solution of lattice dynamics equations (2) shows that equation (50) correctly describes the dynamics of the Lagrangian $L = \text{tr} \mathcal{L}|_{i=j}$. Equation (50) is equivalent to a system of three independent equations for vectors $\mathbf{L}_i = \mathcal{L} \cdot \mathbf{e}_i$

$$\ddot{\mathbf{L}}_i = 4\mathcal{D} \cdot \mathbf{L}_i, \quad i = 1, 2, 3. \quad (51)$$

Initial conditions for \mathbf{L}_i have the form

$$\mathbf{L}_i = \frac{K_0}{2} \delta_k \delta_n \mathbf{e}_i, \quad \dot{\mathbf{L}}_i = 0. \quad (52)$$

Equation (51) with initial conditions (52) has a simple mechanical analogy. It is equivalent to the problem of vibrations of a triangular lattice in which one particle has a non-zero initial displacement, while the velocities and displacements of all other particles are equal to zero. The solution of this mechanical problem is

given in Appendix. The analogy yields the following expression for Lagrangian $L = \text{tr} \mathcal{L}|_{i=j}$:

$$L(t) = \frac{K_0}{2(2N+1)^2} \sum_{s,p=-N}^N (\cos(2\Omega_1 t) + \cos(2\Omega_2 t)),$$

$$\Omega_j^4 - 4\omega_*^2 \Omega_j^2 (\sin^2 \theta_s + \sin^2 \theta_p + \sin^2(\theta_s + \theta_p)) + 12\omega_*^4 (\sin^2(\theta_s + \theta_p) \sin^2 \theta_s + \sin^2(\theta_s + \theta_p) \sin^2 \theta_p + \sin^2 \theta_s \sin^2 \theta_p) = 0, \quad j = 1, 2. \quad (53)$$

The second formula in (53) corresponds to the dispersion relation for a triangular lattice [36].

To check the accuracy of formula (53), we carried out a numerical integration of lattice dynamics equations (2). The Verlet integration scheme with time-step $\tau = 10^{-3} \tau_*$ is used. Figure 4 shows the equilibration of kinetic and potential energies. It is seen that analytical solution (53) and numerical solution of the lattice dynamics equations coincide with each other.

Analysis of formula (53) shows that the Lagrangian oscillates with an amplitude that is inversely proportional to time. This is the essential difference from the square lattice, where the Lagrangian decays inversely proportional to the square root of time (see Section 7). The difference between the kinetic and potential energies decays by two orders of magnitude when time is of the order of $10\tau_*$.

8.5. Calculation of Displacement Covariance in Thermal Expansion Problems

In papers [37, 38], it is shown that the displacement covariance plays an important role in describing the thermal expansion of crystals. In particular, the thermal expansion coefficient for an anharmonic triangular lattice depends on the ratio between the components of the following tensor in the steady state:

$$\mathcal{A} = \langle (\mathbf{u}(\mathbf{r} + \mathbf{a}_\alpha) - \mathbf{u}(\mathbf{r}))(\mathbf{u}(\mathbf{r} + \mathbf{a}_\alpha) - \mathbf{u}(\mathbf{r})) \rangle = 2\xi(0) - \xi(\mathbf{a}_\alpha) - \xi(-\mathbf{a}_\alpha). \quad (54)$$

Without loss of generality, we consider the case $\alpha = 1$. Then, components $A_{xx} = \mathbf{i} \cdot \mathcal{A} \cdot \mathbf{i}$ and $A_{yy} = \mathbf{j} \cdot \mathcal{A} \cdot \mathbf{j}$ of tensor \mathcal{A} in the Cartesian basis (33) characterize the longitudinal and transverse deformations of the bonds caused by the thermal motion. In paper [38], it is shown that the thermal expansion coefficient of the triangular lattice essentially depends on the ratio A_{yy}/A_{xx} .

We calculate tensor \mathcal{A} in the framework of the harmonic crystal model considered in the present paper. The diamond-shaped periodic cell is considered (see Eq. (33)). Equations (7) for covariances of displacements are solved numerically with the following initial conditions:

$$\xi = 0, \quad \dot{\xi} = 0, \quad \kappa = \kappa_0 \delta_k \delta_n \mathcal{F}, \quad \dot{\kappa} = 0. \quad (55)$$

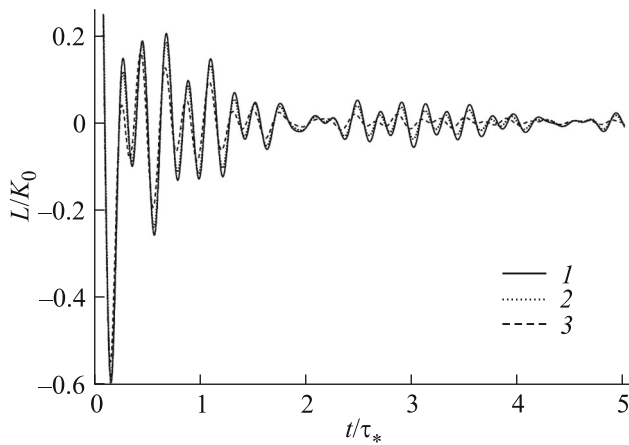


Fig. 5. Equilibration of kinetic and potential energies in triangular lattice with Lennard-Jones interactions. Initial velocities are randomly distributed in a circle with radius v_0 . v_0/v_d : (1) 0.05, (2) 0.25, and (3) 0.5.

Note that the value κ_0 does not effect the ratio A_{yy}/A_{xx} . The Verlet integration scheme with time-step $10^{-3}\tau_*$ is used. The solution yields the following relation between the components of tensor \mathcal{A}

$$\frac{A_{yy}}{A_{xx}} \approx 1.43. \quad (56)$$

Formula (56) is in a good agreement with the results of molecular dynamics simulations carried out for the Lennard-Jones crystal in paper [38], where the following result was obtained: $A_{yy}/A_{xx} \approx 1.435$.

Thus, it is possible to estimate the ratio between the longitudinal and transverse deformations of the bonds in a harmonic crystal. This estimate is required in order to calculate the thermal expansion coefficient in crystals using the approach outlined in papers [37, 38].

9. INFLUENCE OF NONLINEARITY

In this section, we investigate the influence of weak nonlinearity on two transient thermal processes described previously: (i) equilibration of kinetic and potential energies and (ii) redistribution of the kinetic energy among spatial directions.

Two-dimensional triangular lattice is considered. The nearest neighbors interact via the Lennard-Jones potential:

$$\Pi(r) = \varepsilon \left[\left(\frac{a}{r} \right)^{12} - 2 \left(\frac{a}{r} \right)^6 \right], \quad (57)$$

where ε is the bond energy; a is the equilibrium distance. Periodic boundary conditions are used. Initially, the particles have independent random velocities uniformly distributed in a circle of radius v_0 . The dissociation velocity $v_d = \sqrt{2\varepsilon/m}$ is used as a “scale

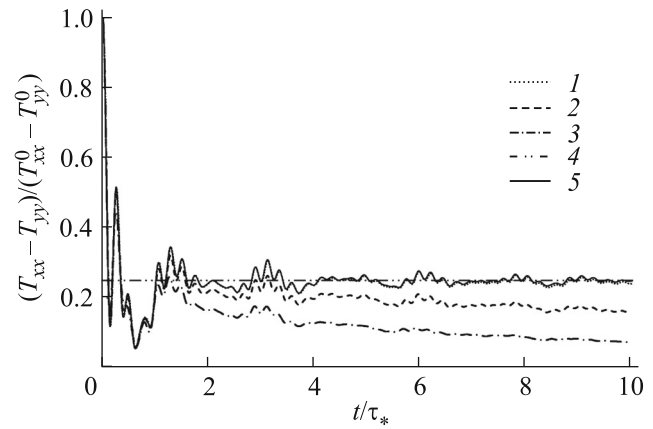


Fig. 6. Redistribution of energy among spatial directions in triangular lattice with Lennard-Jones interactions. Initial velocities are randomly distributed in a circle with radius v_0 . v_0/v_d : (1) 0.05, (2) 0.25, (3) 0.5, (4) analytical solution of steady problem for harmonic triangular lattice, and (5) numerical solution of lattice dynamics equations (2).

factor.” The initial displacements of the particles are equal to zero.

Varying the amplitude of the initial velocities of the particles (the temperature), one can change the influence of the non-linearity on the behavior of the system. We show that at low velocities of the particles (low temperatures) the transient thermal processes in the Lennard-Jones crystal are well described by a harmonic model.

Consider the effect of nonlinearity on the equilibration of the kinetic and potential energies. The dependence of the Lagrangian on time is obtained using molecular dynamics simulation and it is shown in Fig. 5. It is seen that transition to the steady state is accompanied by equilibration of the kinetic and potential energies. In the case $v_0 = 0.05v_d$, the numerical solution for $L(t)$ practically coincides with the analytical solution for the harmonic crystal (53). An increase of initial velocities leads to faster equilibration of kinetic and potential energies than in the harmonic crystal.

Consider the effect of non-linearity on the redistribution of energy among the spatial directions. Initial particle velocities are directed along the x -axis, parallel to one of the basis vectors of the lattice. Difference between the components of the temperature tensor T_{xx} , T_{yy} corresponding to x and y directions is calculated using molecular dynamics simulations. The time dependence of $T_{xx} - T_{yy}$ is plotted in Fig. 6. The curves are obtained by averaging over 25 realizations with random initial velocities. The figure shows that at times of the order of τ_* , the value $T_{xx} - T_{yy}$ decreases by approximately a factor of 4 predicted by the harmonic model. At larger times, it tends to zero relatively slowly.

Thus, the transition to a steady state in weakly anharmonic crystals has two time scales. At short times (in the order of a few periods τ_*), the transient processes are well described by a harmonic crystal model. At larger times ($t \gg \tau_*$), a new evolutionary process caused by the non-linearity is observed. In particular, nonlinearity leads to equipartition of kinetic energies among spatial directions. Time required for the equipartition depends on the magnitude of nonlinearity (the temperature).

10. CONCLUSIONS

In the present paper, an analytical description of two transient thermal processes, notably (i) equilibration of kinetic and potential energies and (ii) redistribution of the kinetic energy among spatial directions was proposed. A closed system of equations with deterministic initial conditions describing the two processes in two-dimensional and three-dimensional cases was derived. It was shown that in the steady state the kinetic and potential energies are equal. Kinetic energy is redistributed among spatial directions, however, the equipartition theorem is not satisfied in general. In other words, the kinetic temperature exhibits tensor properties. A system of equations relating the temperature tensor in the steady state with the initial conditions was derived.

Square and triangular lattices were studied. In the square lattice, there is no energy redistribution among spacial directions. Equilibration of the kinetic and potential energies corresponding to one direction is described by the Bessel function. In the triangular lattice, the energy is redistributed among spatial directions. However, the equipartition theorem is not satisfied. In addition, the covariance of particle velocities $\langle \mathbf{v}_i \mathbf{v}_j \rangle$, in general, is not equal to zero even in the steady state. It is inversely proportional to the square of the distance between the particles. The difference between the kinetic and potential energies undergoes oscillations with an amplitude inversely proportional to time. A characteristic time of the decay of the oscillations is of the order of ten periods of atomic vibrations. In a square lattice, similar oscillations decay inversely proportional to the square root of time. The influence of nonlinearity on the transition towards the steady state is investigated numerically. It is shown that a small nonlinearity causes a slow process that is superimposed on the fast process studied in the harmonic case. Thus, the results of the paper are relevant to description of fast transients processes in weakly anharmonic crystals.

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APPENDIX

OSCILLATIONS OF THE TRIANGULAR LATTICE

Consider the triangular lattice consisting of particles with masses m , connected by springs of stiffness $4C$. The boundary conditions are periodic. The periodic cell has a diamond shape. A side of the cell consists of $2N + 1$ particles. The radius vectors of the particle are given by formula (33). The equations of motion have the form

$$\ddot{\mathbf{u}}_{k,n} = 4\mathcal{D} \cdot \mathbf{u}_{k,n}. \quad (\text{A.1})$$

Initially, the central particle ($k = 0, n = 0$) is displaced along the bond \mathbf{e}_1 by u_0 . The initial velocities and displacements of the remaining particles are equal to zero. We introduce the new variables

$$\begin{aligned} \mathbf{u}_{k,n} &= w_1 \mathbf{e}_1 + w_2 \mathbf{e}_2, & w_1 &= \frac{2}{3}(2u_1 + u_2), \\ w_2 &= \frac{2}{3}(2u_2 + u_1), & u_i &= \mathbf{u}_{k,n} \cdot \mathbf{e}_i, \end{aligned} \quad (\text{A.2})$$

where vectors \mathbf{e}_i are determined by formula (33).

Hereinafter, indices k, n of variables w_1, w_2, u_1, u_2 are omitted for brevity. Substitution of formula (A.2) into the equations of motion, yields

$$\begin{aligned} \ddot{w}_1 &= 2\omega_*^2(\Delta_1^2(2w_1 - w_2) + \Delta_3^2(w_1 + w_2)), \\ \ddot{w}_2 &= 2\omega_*^2(\Delta_2^2(2w_2 - w_1) + \Delta_3^2(w_1 + w_2)). \end{aligned} \quad (\text{A.3})$$

The initial conditions have the form

$$\begin{aligned} \mathbf{u}_{k,n} &= u_0 \delta_k \delta_n \mathbf{e}_1, & w_1 &= u_0 \delta_k \delta_n, \\ w_2 &= 0, & \dot{w}_1 &= \dot{w}_2 = 0. \end{aligned} \quad (\text{A.4})$$

We apply the discrete Fourier transform (34) to equation (A.3), with respect to indices k, n and use the identities

$$\begin{aligned} \Phi(\Delta_1^2 g_{k,n}) &= -4 \sin^2 \theta_s \hat{g}_{s,p}, \\ \Phi(\Delta_2^2 g_{k,n}) &= -4 \sin^2 \theta_p \hat{g}_{s,p}, \\ \Phi(\Delta_3^2 g_{k,n}) &= -4 \sin^2(\theta_s + \theta_p) \hat{g}_{s,p}, \\ \hat{g}_{s,p} &= \Phi(g_{k,n}), & \theta_s &= \frac{\pi s}{2N+1}. \end{aligned} \quad (\text{A.5})$$

As a result, for the Fourier images $\hat{w}_i = \Phi(w_i)$ we have

$$\begin{aligned} \ddot{\hat{w}}_1 &= -8\omega_*^2[(2 \sin^2 \theta_s + \sin^2(\theta_s + \theta_p))\hat{w}_1 \\ &\quad + (\sin^2(\theta_s + \theta_p) - \sin^2 \theta_s)\hat{w}_2], \\ \ddot{\hat{w}}_2 &= -8\omega_*^2[(\sin^2(\theta_s + \theta_p) - \sin^2 \theta_p)\hat{w}_1 \\ &\quad + (2 \sin^2 \theta_p + \sin^2(\theta_s + \theta_p))\hat{w}_2]. \end{aligned} \quad (\text{A.6})$$

Eigenfrequencies Ω_1 and Ω_2 of system (A.6) are given by

$$\begin{aligned} & \Omega_j^4 - 16\omega_*^2 \Omega_j^2 (\sin^2 \theta_s + \sin^2 \theta_p \\ & + \sin^2(\theta_s + \theta_p)) + 192\omega_*^4 (\sin^2(\theta_s + \theta_p) \sin^2 \theta_s \\ & + \sin^2(\theta_s + \theta_p) \sin^2 \theta_p \\ & + \sin^2 \theta_s \sin^2 \theta_p) = 0, \quad j = 1, 2. \end{aligned} \quad (\text{A.7})$$

The initial conditions for \hat{w}_1, \hat{w}_2 are as follows:

$$\hat{w}_1 = u_0, \quad \hat{w}_2 = 0, \quad \dot{\hat{w}}_1 = \dot{\hat{w}}_2 = 0. \quad (\text{A.8})$$

Solving system (A.6) with initial conditions (A.8) and applying the inverse discrete Fourier transform, yields

$$\begin{aligned} \mathbf{u}_{k,n} &= w_1 \mathbf{e}_1 + w_2 \mathbf{e}_2, \\ w_1 &= \frac{u_0}{2(2N+1)^2} \\ & \times \sum_{s,p=-N}^N \cos(2\theta_s k + 2\theta_p n) (\cos(\Omega_1 t) + \cos(\Omega_2 t)) \quad (\text{A.9}) \\ & + 16\omega_*^2 \frac{\sin^2 \theta_s - \sin^2 \theta_p}{\Omega_1^2 - \Omega_2^2} (\cos(\Omega_1 t) - \cos(\Omega_2 t)), \\ w_2 &= \frac{8u_0}{(2N+1)^2} \sum_{s,p=-N}^N \frac{\omega_*^2 (\sin^2(\theta_s + \theta_p) - \sin^2 \theta_p)}{\Omega_1^2 - \Omega_2^2} \\ & \times (\cos(\Omega_1 t) - \cos(\Omega_2 t)) \cos(2\theta_s k + 2\theta_p n). \end{aligned}$$

Formulas (A.9) give an exact solution for the problem of oscillations in the triangular lattice, where one particle has an initial displacement.

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