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

Energy Oscillations in a One-Dimensional Crystal

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Oscillations of the kinetic and potential energies in a one-dimensional crystal (the chain of particles) are considered. An analytical solution for the linear interaction of particles, random initial velocities, and zero initial displacements is derived. It is shown that the time dependence of energies is expressed by the Bessel function, and the period and the damping rate of oscillations are determined. Analytical conclusions are confirmed by computer modeling. According to the results found, in order to describe high-speed transient processes, apart from the consideration of velocities dispersion (which determines the temperature in the equilibrium statistical mechanics), the correlations of velocities of different particles should be considered. In particular, the damping of energy oscillations is associated with the fact that correlations associating the motion of remote particles are excited.

In recent decades, the methods of mechanics of discrete media have widely been used to describe non-equilibrium processes in matter [1−3]. Interest in discrete approaches has especially risen in connection with the development of nanotechnologies [4, 5]. However, the analysis of nonequilibrium thermal processes in discrete media even for such a simple model as ideal crystals under classic (nonquantum) description remains a serious problem. For example, for one-dimensional crystal the thermal elasticity equations can be derived in the adiabatic approximation [3, 6], however the description of heat transfer can diverge with the conclusions of classic heat conductivity theory [7, 8].

One of the theoretical questions in the mechanics of discrete media is associated with high-frequency oscillations of the kinetic and potential energies, which are known well by the results of numerical modeling [9]. In particular, if at the initial instant the particles are ordered into the ideal crystal lattice and their velocities are specified randomly, then the dynamic transition of the kinetic energy into the potential energy of the bonds deformation is initiated in the crystal. This transition leads to the distribution of the internal energy between the kinetic and deformation degrees of freedom, which are determined by the virial theorem [10]. However, the transition is accompanied by high-frequency oscillatory process with decreasing amplitude, which still has no theoretical interpretation.

In this study, in order to investigate the mentioned processes, we selected the model of a one-dimensional crystal. This is a simple model, which makes it possible, on the one hand, to obtain the transition from the discrete system to a continual one, and on the other hand, to demonstrate radical distinctions, which are implemented for such systems [11−13]. Below we propose a method for the analytical description of such energy oscillations and give an exact solution of the corresponding mathematical problem as well as perform a comparison with the results of numerical modeling.

Let us consider a one-dimensional crystal in the form of a chain of identical particles with mass m, which are connected by identical linear springs with stiffness C. The dynamic equations of the chain have the form

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

where u_k is the displacement of the kth particle and k is the integer index. Let us consider that periodicity conditions are fulfilled: $u_{k+N} = u_k$, where $N \gg 1$ is the number of independent particles.

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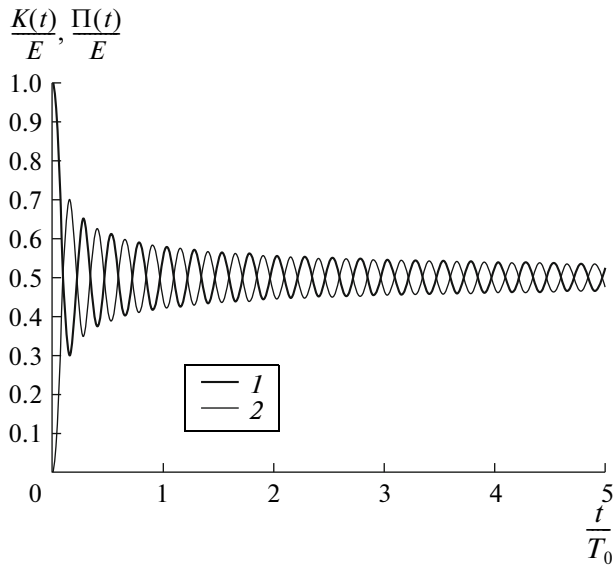*e-mail: akrivtsov@bk.ru*

$$\frac{K(t)}{E}, \frac{\Pi(t)}{E}$$

Fig. 1. Oscillations of the (*1*) kinetic and (*2*) potential energies in a one-dimensional crystal.

Let us introduce the operator of averaging by the index for arbitrary quantity f_k, which characterizes the motion of the kth particle,

$$\langle f_k \rangle = \frac{1}{N}\sum_{k=1}^{N} f_k. \qquad (2)$$

In this case, the specific (per particle) kinetic, potential, and total energy can be determined by the formulas

$$K = \frac{1}{2}m\langle v_k^2 \rangle, \quad \Pi = \frac{1}{2}C\langle \varepsilon_k^2 \rangle, \quad E = K + \Pi, \quad (3)$$

where particle velocities $v_k = \dot{u}_k$ and deformations of bonds $\varepsilon_k = u_k - u_{k-1}$ are introduced. It is evident that the total energy is constant, while the kinetic and potential energies depend on time t.

Let us admit that the displacements of particles equal zero at $t = 0$, while the velocities are distributed randomly, which corresponds to $\Pi = 0$, $K = E$. The dynamics of varying the energies obtained by the numerical integration of Eqs. (1) under the mentioned initial conditions is shown in Fig. 1. The variation in energies is calculated for $N = 10^6$ and $0 \leq t \leq 5T_0$, where $T_0 \overset{\text{def}}{=} \frac{2\pi}{\omega_0}$. Even for such a short time interval, the convergence of energies to the limiting value $E/2$ is quite noticeable, which agrees with the virial theorem [10]. In this case, the variation in energies has an oscillatory character with the period close to $T_0/4$.

Let us derive the analytical expressions that make it possible to describe the energy oscillations. In order to

do this, following [14], let us introduce generalized energies

$$K_n \overset{\text{def}}{=} \frac{1}{2}m\langle v_k v_{k+n} \rangle, \quad \Pi_n \overset{\text{def}}{=} \frac{1}{2}C\langle \varepsilon_k \varepsilon_{k+n} \rangle, \qquad (4)$$

where averaging is performed by repeating index k. Formulas (4) at $n = 0$ give usual energies (3). If the latter are determined by the dispersions of velocities and deformations, then the generalized ones are determined by correlations of the same quantities for particles, the index of which differs by n.

Differentiation of the generalized energies with the use of dynamic equations (1) allows us to derive the following identities:

$$\dot{K}_n + \dot{\Pi}_n = 0 \Rightarrow E_n \overset{\text{def}}{=} K_n + \Pi_n = \text{const}, \qquad (5)$$

$$\ddot{\Pi}_n = -2\omega_0^2(L_{n-1} - 2L_n + L_{n+1}), \quad L_n \overset{\text{def}}{=} K_n - \Pi_n. \ (6)$$

Identity (5) means that the conservation law similar to the conservation law of the total mechanical energy is fulfilled for the generalized energies; quantity E_n serves as a generalized total energy. When deriving identities (5) and (6), we used a postulate that the values of average quantities calculated for the chain are invariable with its reflection. This postulate is valid for $N \to \infty$ and makes it possible to use equality $\langle f_k g_{k+n} \rangle = \langle f_k g_{k-n} \rangle$ for any f_k, g_k, and any integer n.

Excluding quantities K_n and Π_n from identities (5) and (6), we derive the differential-difference equation for the generalized Lagrangian function L_n:

$$\ddot{L}_n = 4\omega_0^2(L_{n-1} - 2L_n + L_{n+1}), \qquad (7)$$

which coincides in form with the dynamic equation of chain (1) and differs only by the value of the coefficient on the right side. By virtue of the periodicity of the chain and the properties of the averaging operator, quantities L_n are periodic and even by index n: $L_{n+N} = L_n$, $L_{-n} = L_n$. The initial values of quantities L_n and $\dot{L}_n$, which are determined by dispersion and correlations of velocities and displacements of particles at $t = 0$, serve as the initial conditions for Eq. (7).

Let us assume that the initial velocities of various particles are independent and the initial displacements are absent. Then, using definitions (4), we derive at $t = 0$

$$L_n = E\delta_n, \quad \dot{L}_n = 0, \quad 0 \leq n < N, \qquad (8)$$

where δ_n is the Kronecker symbol equal to the unit at $n = 0$ and equal to zero in all other cases.

Considering (7) as the set of linear differential equations with initial conditions (8), we can derive the

analytical solution, which takes the form in the limit $N \to \infty$:

$$L_n(t) = EJ_{2n}(4\omega_0 t), \tag{9}$$

where $J_k(\tau)$ is the first-order Bessel function [15]. According to the derived solution, the Lagrangian function $L = L_0(t)$ satisfies the differential Bessel equation

$$\ddot{L} + \frac{1}{t}\dot{L} + 16\omega_0^2 L = 0, \tag{10}$$

which can be interpreted as the equation of oscillations of the material point under the effect of a linear spring and viscous friction force with the coefficient inversely proportional to time. At large t, formula (9) can be presented [15] in the form

$$L_n(t) = (-1)^n \frac{E}{\sqrt{2\pi\omega_0 t}} \cos\left(4\omega_0 t - \frac{\pi}{4}\right) + O(t^{-3/2}). \tag{11}$$

Thus, oscillations occur with frequency $4\omega_0$, while the amplitude of oscillations is inversely proportional to the root of time. With the use of solution (9), the specific kinetic and potential energies can be represented in the form

$$K(t) = \frac{E}{2}(1 + J_0(4\omega_0 t)),$$
$$\Pi(t) = \frac{E}{2}(1 - J_0(4\omega_0 t)). \tag{12}$$

Figure 2 presents the results of calculating the Lagrangian function $L(t)$: for the numerical solution of the initial problem for chain (1); for the numerical solution of initial problem (7), (8) for the generalized Lagrangian; and analytical solution (9). The numerical solution of Eqs. (1) and (7) was undertaken by the method of central differences with an integration step of $0.01 T_0$. The initial velocities for the chain (1) were specified using a randomizer with a uniform distribution. It is seen from Fig. 2 that all three plots are almost indistinguishable in the accepted scale. We note that in contrast to $N = 10^6$ steps necessary to attain the required accuracy in the course of the numerical solution of chain (1), it was sufficient to have $N = 10^2$ for Eqs. (7).

Thus, we derived an exact analytical solution, according to which the Lagrangian function for the chain with the stochastic initial conditions varies following the same law, according to which the central particle for the chain with the deterministic initial conditions moves. The variation in the kinetic and potential energies of the system under consideration is described by the Bessel function, the oscillation period of which is $T_0/4$, while the amplitude of oscillations is
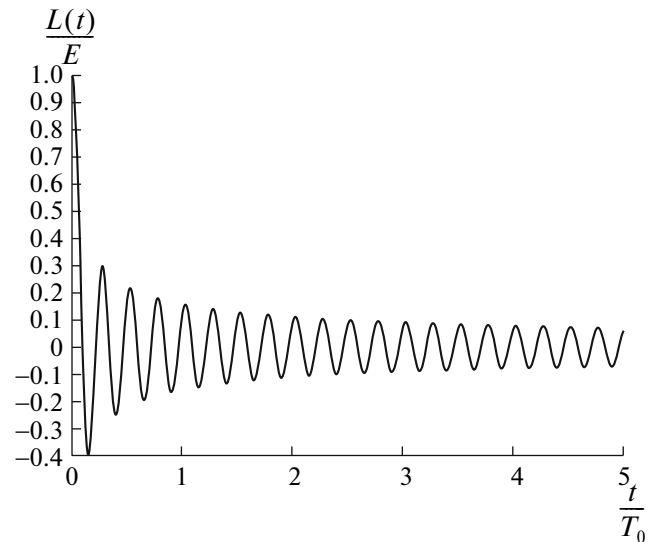

Fig. 2. Oscillations of the Lagrangian function.

inversely proportional to the root of time. It follows from the found solution that the damping of oscillations of energies is determined by excitation of correlations, which associates the motion of the particles remote from each other. The oscillation period of energies is very small; therefore, it is more correct to associate the temperature in the course of these oscillations with the total energy rather than with the kinetic energy, which constantly transforms into the potential energy and vice versa. The temperature can be associated with the kinetic energy as is accepted in equilibrium statistical mechanics only after damping the transient process, for which times of about ten periods T_0 are required.

The derived solution, on the one hand, makes it possible to describe the oscillations of energies, which appear when solving the problems by the molecular dynamics methods. On the other hand, similar oscillations can appear in actual solids during fast transient processes, for example, under the effect of femtosecond laser pulses. According to [13], oscillations of a similar nature can cause destruction in discrete systems. In addition, processes considered in the article can serve for the description of heat conductivity and internal friction in crystalline solids.

REFERENCES

1. A. N. Andreev, et al., *Mechanics—from Discrete to Continuous*, Ed. by V. M. Fomin (Sib. Otd. Ross. Akad. Nauk, Novosibirsk, 2008) [in Russian].
2. W. G. Hoover, World Sci. Adv. Ser. Nonlin. Dyn. **25** (2006).
3. A. M. Krivtsov, *Deformation and Fracture of Solids with Microstructure* (Fizmatlit, Moscow, 2007) [in Russian].

4. R. V. Gol'dshtein and N. F. Morozov, Fiz. Mezomekh. **10** (5), 17 (2007).

5. A. M. Krivtsov and N. F. Morozov, Phys. Solid State **44** (12), 2260 (2002).

6. A. M. Krivtsov, Chaos, Solit. Fract. **17** (1), 79 (2003).

7. H. Nakazawa, Prog. Theor. Phys. Suppl. **45**, 231 (1970).

8. A. A. Le-Zakharov and A. M. Krivtsov, Doklady Phys. **53** (5), 261 (2008).

9. M. P. Allen and A. K. Tildesley, *Computer Simulations of Liquids* (Clarendon, Oxford, 1987).

10. L. D. Landau and E. M. Lifshits, *Mechanics. Vol. 1. Theoretical Physics* (Fizmatlit, Moscow, 2004) [in Russian].

11. L. I. Slepyan, *Unsteady Elastic Waves* (Sudostroenie, Leningrad, 1972) [in Russian].

12. N. F. Morozov and M. V. Paukshto, *Discrete and Hybrid Models* (St. Petersburg Gos. Univ., St. Petersburg, 1995) [in Russian].

13. Yu. V. Petrov, A. A. Gruzdkov, and N. A. Kazarinov, Doklady Phys. **53** (11), 595 (2008).

14. A. M. Krivtsov, *Proc. XXXIV Summer School "Advanced Problems in Mechanics"* (St. Petersburg, 2007) pp. 261–273.

15. *Handbook for Special Functions*, Ed. by M. Abramovits and I. Stigan (Nauka, Moscow, 1979) [in Russian].

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