

## INFLUENCE OF NONLINEAR INTERACTIONS AND BOUNDARY EFFECTS ON THE PROPAGATION OF ENERGY IN A ONE-DIMENSIONAL PARTICLE CHAIN

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*A one-dimensional system (chain) of particles interacting with each other and with the substrate has been investigated by the method of computer modeling. Particles at the boundaries of the chain, which are considered separately, represent self-oscillating systems. The influence of the parameters of a system on the transfer of energy by the chain has been studied; the behavior of the system in the transient and steady-state regimes of motion has been investigated. It has been shown that the stationary states of the system are characterized by a nonuniform distribution of the average particle velocities (temperatures) squared over the chain's length. A correlation between the increase in the thermal resistance of a system and the enhancement of its structuring has been established.*

**Introduction.** The propagation of energy along one-dimensional structures has been widely investigated [1] both in connection with the problems of substantiation of the Fourier law of heat conduction [2, 3] and in view of the necessity of understanding the processes of transmission of energy in actual quasi-one-dimensional systems (biological and organic molecules, anisotropic crystals, nano-size tubes, etc.) [4–6]. The emphasis is on the process of propagation of energy along a one-dimensional system for which, for example, the energy flux is represented as the heat flux and is written in the form of the Fourier law

$$J = -\kappa \nabla T. \quad (1)$$

The final objective of statistical-mechanical theory is derivation of an equation similar to (1) from the "first principles," i.e., from the equations of motion, written for the mechanical system in question with a large number of degrees of freedom without additional approximations. Such a problem has not been solved completely up to the present time. For a crystal where energy is transferred through lattice (phonon) vibrations, the first and the most elementary attempt at constructing heat-conduction theory based on the kinetic Boltzmann equation for phonons gave a microscopic base for the Fourier law [7]. Ever since then the Boltzmann approach has become one basic approach in the theory of heat conduction of the lattice. One-dimensional systems attract researchers by their relative simplicity in solving fundamental problems of heat conduction and by the presence of prototypes among actual physical objects.

In investigating heat conduction by computer modeling, one often considers the stationary state of a system, which is held using thermostats located at the system's boundaries. It is precisely the propagation of energy along the system that is usually studied, whereas the effects developing at the boundaries where the system is in contact with the thermostats and the influence of the parameters of the thermostats have not been adequately studied. The problem of boundary effects is topical in connection with the investigation of heat-transfer processes and the existing trends toward the development and adoption of composite and nano-structured materials, since the phenomena at the boundaries between mesoscopic generating elements are of considerable importance in them. Furthermore, it is not necessarily correct to consider systems located at the ends of small-size objects as thermostats in view of their limited heat capacity and the insufficient, in many cases, number of degrees of freedom. In the present work, we consider, as the energy source and consumer, self-oscillating subsystems capable of ensuring energy fluxes of any high value but characterized

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by a small number of degrees of freedom and a low stochasticity level. Modeling is performed based on the equations of motion of classical mechanics.

Many processes, particularly electronic ones, occurring in nano-size systems require a quantum-mechanical description. At the same time, it is common knowledge that classical mechanics adequately reflects the behavior of ensembles of particles at the atomic level (see [8, 9]) if the characteristic frequencies of the processes are not very high (are limited to values of the order of ten THz). In this work, we investigate lattice characteristics that refer to the motion of atoms composing a system, and classical description seems quite justified.

**Equations of Motion of a System of Interacting Particles.** Let us consider a one-dimensional system of  $n + 2$  particles of the same mass  $m$ , interacting with each other and with the substrate via linear elastic bonds of rigidity  $c$  and  $c_1$  respectively and through nonlinear cubic forces characterized by the coefficient  $\chi$ . The first and last bodies of the chain are capable of exchanging energy with sources of unlimited power via velocity-dependent nonlinear interactions; in view of this fact, we can consider these sources as specific thermostats. When  $n \approx 100$ , the size of the system is several tens of nanometers.

As the generalized coordinates we take the displacement of weights from their equilibrium positions; they are denoted as  $x_j$  ( $j = 0, 1, 2, \dots, n + 1$ ). The system of  $n + 2$  differential equations of motion has the form

$$\begin{aligned} m_0 \ddot{x}_0 &= -cx_0 + \mu_0 \dot{x}_0 - \gamma_0 \dot{x}_0^3 + c(x_1 - x_0) + \chi(x_1 - x_0)^3, \\ m_j \ddot{x}_j &= -c(x_j - x_{j-1}) + c(x_{j+1} - x_j) - c_1 x_j + \chi[(x_{j+1} - x_j)^3 - (x_j - x_{j-1})^3], \quad j = 1, \dots, n, \\ m_{n+1} \ddot{x}_{n+1} &= -cx_{n+1} + \mu_{n+1} \dot{x}_{n+1} - \gamma_{n+1} \dot{x}_{n+1}^3 - c(x_{n+1} - x_n) - \chi(x_{n+1} - x_n)^3. \end{aligned} \quad (2)$$

The interaction with the thermostats is modeled by introducing of two additional terms into the equations of motion of the zero and  $(n + 1)$ th particles; one of the terms simulates negative viscosity (coefficients  $\mu_0$  and  $\mu_{n+1}$ ), whereas the other simulates resistance forces cubic in velocity (coefficients  $\gamma_0$  and  $\gamma_{n+1}$ ). Thus, particles (considered separately) at the boundaries are self-oscillating systems that can consume or give up energy to the ambient medium. Such thermostats are close to a Nose–Hoover thermostat [10, 11] in properties. In this case, we have eight parameters ( $\mu_0$ ,  $\mu_{n+1}$ ,  $\gamma_0$ ,  $\gamma_{n+1}$ ,  $c$ ,  $c_1$ ,  $\chi$ , and  $m$ ) characterizing the system.

It is convenient to pass to a dimensionless form, for which purpose we introduce  $\tau = \sqrt{m/c}$  and  $\lambda = m/\sqrt{\mu_0 \gamma_0}$  as units of time and length respectively and use the dimensionless relations of the parameters

$$\alpha_1 = c_1/c, \quad \alpha_2 = \mu_0/\mu_{n+1}, \quad \alpha_3 = \gamma_0/\gamma_{n+1}, \quad \alpha_4 = cm/\mu_0^2, \quad \alpha_5 = \chi\lambda^2/c \quad (3)$$

rather than the parameters themselves. Then the system of differential equations of motion is represented in the form

$$\begin{aligned} \ddot{\bar{x}}_0 &= -\bar{x}_0 + \dot{\bar{x}}_0/\sqrt{\alpha_4} - \sqrt{\alpha_4} \dot{\bar{x}}_0^3 + \bar{x}_1 - \bar{x}_0 + \alpha_5 (\bar{x}_1 - \bar{x}_0)^3, \\ \ddot{\bar{x}}_j &= -\bar{x}_j + \bar{x}_{j-1} + \bar{x}_{j+1} - \bar{x}_j - \alpha_1 \bar{x}_j + \alpha_5 [(\bar{x}_{j+1} - \bar{x}_j)^3 - (\bar{x}_j - \bar{x}_{j-1})^3], \quad j = 1, \dots, n, \\ \ddot{\bar{x}}_{n+1} &= -\bar{x}_{n+1} + \dot{\bar{x}}_{n+1}/(\alpha_2 \sqrt{\alpha_4}) - \dot{\bar{x}}_{n+1}^3 \sqrt{\alpha_4}/\alpha_3 - \bar{x}_{n+1} + \bar{x}_n - \alpha_5 (\bar{x}_{n+1} - \bar{x}_n)^3, \end{aligned} \quad (4)$$

where  $\bar{x}$ ,  $\dot{\bar{x}}$ , and  $\ddot{\bar{x}}$  are the dimensionless coordinate, velocity, and acceleration respectively ( $\bar{x} = x/\lambda$ ).

Thus, the problem is reduced to investigation of the behavior of the system as a function of dimensionless parameters, and passage to dimensional quantities can be carried out based on the similarity and dimensional theory [12, 13].

Let us introduce the dimensionless form of the system's internal energy  $\bar{E}$ :

$$E = (m\lambda^2/\tau^2) \bar{E}, \quad (5)$$

$$\bar{E} = \sum_{k=0}^{n+1} \frac{1}{2} \dot{\bar{x}}_k^2 + \sum_{k=1}^{n+1} \frac{1}{2} (\bar{x}_k - \bar{x}_{k-1})^2 + \sum_{k=1}^{n+1} \frac{1}{4} \alpha^5 (\bar{x}_k - \bar{x}_{k-1})^4 \frac{1}{2} \dot{\bar{x}}_0^2 + \frac{1}{2} \dot{\bar{x}}_{n+1}^2 + \sum_{k=1}^n \frac{1}{2} \alpha_1 \dot{\bar{x}}_k^2. \quad (6)$$

Expressions for the powers of dissipative forces acting on the zero and  $(n+1)$ th bodies have the form

$$N_0 = (\mu_0 \dot{\bar{x}}_0 - \gamma_0 \dot{\bar{x}}_0^3) \dot{\bar{x}}_0, \quad (7)$$

$$N_{n+1} = (\mu_{n+1} \dot{\bar{x}}_{n+1} - \gamma_{n+1} \dot{\bar{x}}_{n+1}^3) \dot{\bar{x}}_{n+1}. \quad (8)$$

With account for relations (3) between the parameters, we write (7) and (8) in dimensionless form ( $N = (\lambda^2/\tau^3)\bar{N}$ ):

$$\bar{N}_0 = (\dot{\bar{x}}_0^2 - \alpha_4 \dot{\bar{x}}_0^4) / \sqrt{\alpha_4}, \quad (9)$$

$$\bar{N}_{n+1} = (\alpha_3 \dot{\bar{x}}_{n+1}^2 - \alpha_1 \alpha_4 \dot{\bar{x}}_{n+1}^4) / (\alpha_1 \alpha_3 \sqrt{\alpha_4}). \quad (10)$$

Averaging over the period of self-oscillations, for the average powers we obtain

$$\langle \bar{N}_0 \rangle = \bar{a}_0^2 \bar{k}_0^2 (1 - 3\alpha_4 \bar{a}_0^2 \bar{k}_0^2 / 4) / 2 \sqrt{\alpha_4}, \quad (11)$$

$$\langle \bar{N}_{n+1} \rangle = \bar{a}_{n+1}^2 \bar{k}_{n+1}^2 (\alpha_3 - \alpha_1 \alpha_4 \bar{a}_{n+1}^2 \bar{k}_{n+1}^2) / (\alpha_1 \alpha_3 \sqrt{\alpha_4}), \quad (12)$$

where  $\bar{a}_j$  and  $\bar{k}_j$  are the dimensionless amplitude and frequency of oscillations of the corresponding body ( $j = 0$  and  $n+1$ ). We note that, in dimensionless form, the amplitude of oscillations of an isolated zero body [14, 15] is determined by the dependence  $\bar{a}_{0\text{is}}^2 = 4/(3\alpha_4)$ , and the frequency of its oscillations is equal to unity. The right-hand sides of Eqs. (9) and (10) vanish. Since the parameters  $\mu$  and  $\gamma$  at the left and right ends of the chain differ, the amplitudes of steady-state oscillations also differ from their values for isolated bodies, leading to the energy flux along the chain. In the steady-state regime, we have  $\langle \bar{N}_0 \rangle = -\langle \bar{N} \rangle_{n+1}$ .

**Results of Computer Modeling and Their Analysis.** The resulting system of differential equations of motion (4) is nonlinear, and the possibilities of investigating it analytically are limited. Therefore, we should study first the features of its numerical solutions depending on the selection of the values of dimensionless parameters, which will enable us to work out methods of approximate analytical behavior of the system. The energy fluxes and the amplitudes, periods, and phases of oscillations of individual bodies of the system and of the last bodies, in particular, can act as the characteristics under study. It is important to consider transient processes leading to steady states and possible spatial distributions of the characteristics of motion in steady-state regimes.

Integration of the equations of motion for  $n = 98$  has been performed in the MatLab environment according to the Adams–Bashforth–Moulton multistep algorithm of variable order [16]. It was only the zero particle (left end of the chain) that was excited at the initial instant, whereas the remaining particles were at rest. Figure 1 gives results of the integration of the equations of motion for the system with parameters  $\alpha_1 = 0.5$ ,  $\alpha_2 = 2$ ,  $\alpha_3 = 0.1$ ,  $\alpha_4 = 1$ , and  $\alpha_5 = 0$ . As might be expected, excitation propagates over the chain with a certain velocity.

In the behavior of the system, we track two starting periods during which a perturbation first reaches the right end, after which the reflected wave returns to the left end. The first body behaves stably until the reflected perturbation returns. Then the amplitude of its oscillations somewhat increases and nearly attains a stationary value. The body at the right end of the chain reaches the stationary regime practically as soon as the perturbation arrives.

Figure 2 shows a fragment (corresponding to the steady-state regime of motion) of Fig. 1 on a larger scale. We easily track the periodicity of motion of the last left and right bodies of the system with the same period of 5.2

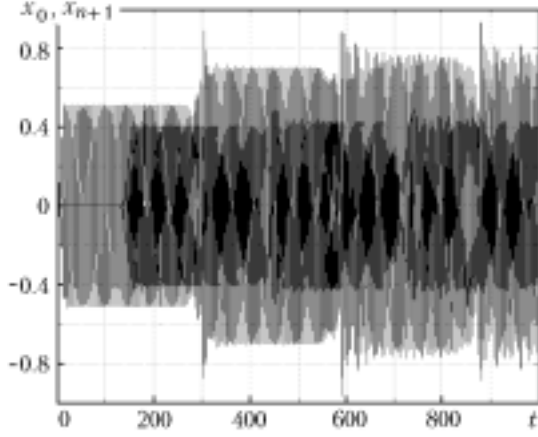


Fig. 1. Coordinate vs. time for the zero (gray background) and  $(n + 1)$ th (black background) bodies.

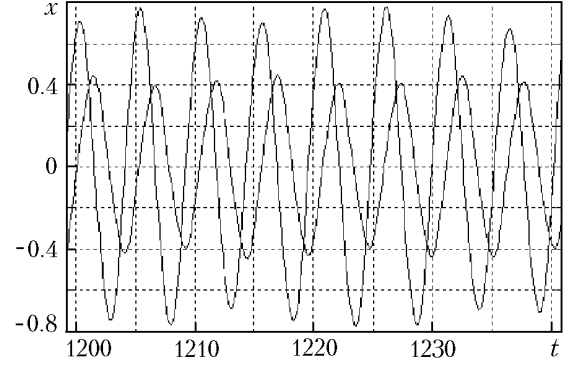


Fig. 2. Dimensionless coordinate of the last left (with a larger amplitude) and right bodies of the system vs. time in the steady-state regime of motion.

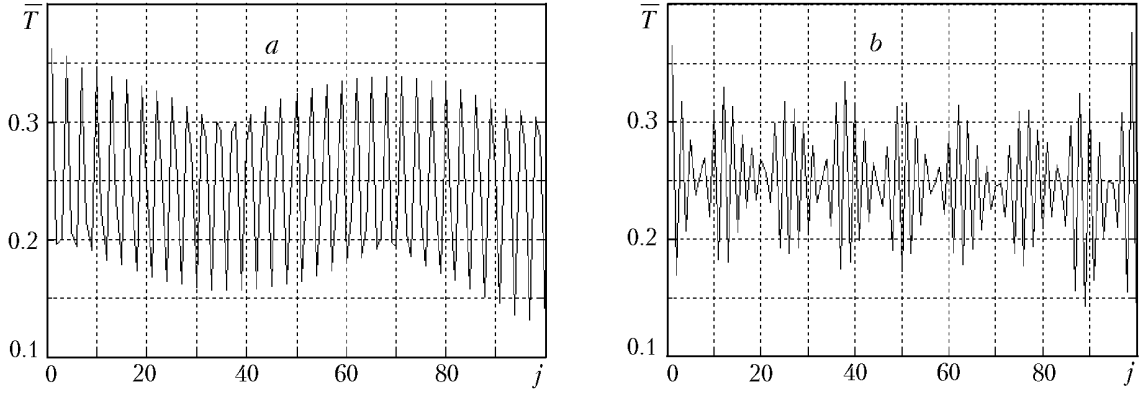


Fig. 3. Influence of the parameter  $\alpha_1$  on the distribution of the average kinetic energy of particles along the chain for  $\alpha_2 = 2$ ,  $\alpha_3 = 0.1$ ,  $\alpha_4 = 1$ , and  $\alpha_5 = 0$ : a)  $\alpha_1 = 0.125$ ; b)  $0.5$ .

dimensionless units and a constant phase shift of nearly  $\pi/2$ . We note that the oscillation period is  $2\pi \cong 6.28$  for an isolated self-oscillating system with the parameters of the last left body.

Another important feature of the motion of the last bodies is the variability of their amplitudes. We observe beats with a period of several fundamental periods of oscillations. This means that the motion of the bodies in question is characterized by two close frequencies; the amplitude of oscillations at the fundamental frequency is substantially larger than the secondary one, since the variations of the total amplitude are small.

Of interest is information on the motion of the bodies of the system depending on their location in the chain. In the context of this work, an important characteristic of motion of the bodies is their average velocity squared or the dimensionless temperature.

Figure 3 shows the influence of the parameter  $\alpha_1 = c_1/c$  on the form of the dependence of the dimensionless temperature  $\bar{T}$  (determined as the average kinetic energy of a particle  $\bar{T}_j = \langle \bar{x}_j^2 \rangle / 2$ ) on the particle number in the system (numbering is from the left particle). The energy distribution in the chain is characterized by nonuniformities with a minimum wavelength where any two neighboring particles are nearly antiphased, and these short-wave oscillations are modulated by waves of much longer length. When  $\alpha_1 = 0.5$  the period of the modulating wave is equal to approximately 60, whereas when  $\alpha_1 = 0.125$  it decreases to approximately 10. Here the phenomenon of beats is observed in the coordinate space, and, by analogy with beats in time, it can be noted that the propagating waves are characterized by two close wave numbers. Each wave number corresponds to its circular frequency, so that beats in the co-

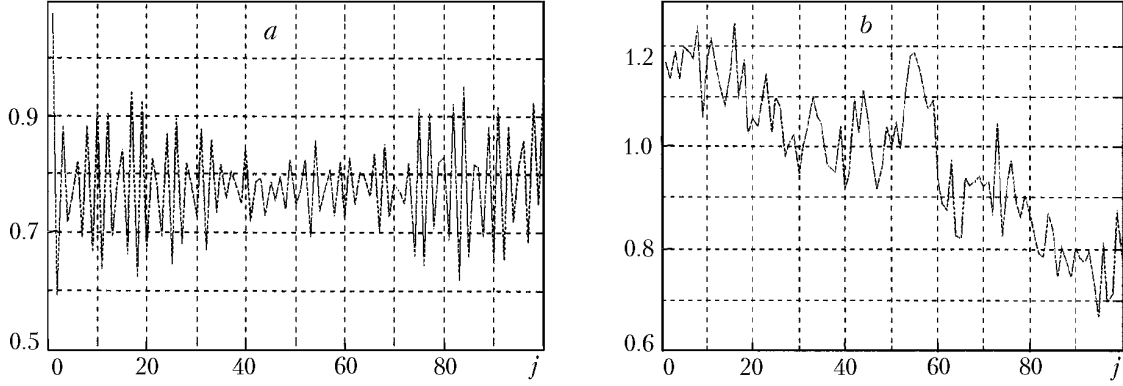


Fig. 4. Influence of the parameter  $\alpha_5$  on the distribution of the average kinetic energy of particles along the chain for  $\alpha_1 = 0.1$ ,  $\alpha_3 = 1$ , and  $\alpha_4 = 1$ : a)  $\alpha_5 = 0.02$ ; b)  $0.04$ .

ordinate space and in time are interrelated and steady-state motion is characterized by the superposition of standing waves. The interaction between nonlinear subsystems and feedback is established via the linear chain at its ends, and the resulting system shows a certain self-organization.

The parameter  $\alpha_2$  influences the amplitude of short-wave oscillations of the average kinetic energy of particles. An increase by an order of magnitude in this parameter caused the amplitude to increase by approximately one-third, whereas the average energy of the entire system, controlled by the parameter  $\alpha_4$ , remains the same for all systems and equal to about 0.25 per particle.

The parameter  $\alpha_3$  influences the amplitude of oscillations of the average kinetic energy over the chain length, but in this case its decrease causes the amplitude to increase now. The reason is that the coefficients  $\mu$  and  $\gamma$  exert an opposite influence on the energy exchange of the system with the ambient medium. We note that decrease in  $\alpha_3$  causes the average energy of the entire system somewhat to increase.

An important role is played by the parameter  $\alpha_5$ , reflecting the influence of nonlinear interparticle interactions on the process of transfer of energy. When the value of this parameters is low ( $\alpha_5 = 0.02$ ), the character of distribution of the average kinetic energy of particles along the system (Fig. 4a) is close to the case of the absence of nonlinear interaction (Fig. 3b), but already for  $\alpha_5 = 0.04$  a considerable temperature gradient appears (Fig. 4b) and the signs of periodic variations of root-mean-square velocities disappear.

Although the average kinetic energy undergoes substantial variations from body to body, we can observe the temperature gradient if averaging over several neighboring particles is introduced. At the same time, if we determine the temperature difference from the difference of the average kinetic energies of the last left and right particles, we obtain a much higher value of the temperature gradient. This means that the boundary effects due to the conjugations of the harmonic chain to anharmonic thermostats increase the total thermal resistance of the system by an order of magnitude.

Let us perform numerical evaluations, avoiding the appearance of the parameters of the thermostats in them. The time scale is determined by the interparticle interaction and the mass of particles. We take the characteristic molecular time  $\tau = 10^{-13}$  sec, the characteristic interparticle distance  $l_0 = 3 \cdot 10^{-10}$  m, and the mass of a particle  $m = 10^{-25}$  kg. We write  $\kappa = |J|/\nabla T$  for the thermal conductivity. Here the heat flux is referred to unit area, and its representation by the dimensionless energy flux introduced above has the form

$$J = \bar{J} \lambda^2 / l_0^2 \tau^3. \quad (13)$$

In turn, for the temperature gradient, we have  $\nabla T = \Delta T / (100 l_0) = 0.01 \Delta \bar{T} \lambda^2 / (\tau^2 l_0 k_B)$ , where  $\Delta T$  is the difference of the temperatures at the ends of the chain and  $100 l_0$  is the chain length. Thus, we have

$$\kappa = 100 k_B \bar{J} / (l_0 \tau \Delta \bar{T}). \quad (14)$$

Here, using  $\bar{J} = 0.17$  and the estimate  $\Delta\bar{T} = 0.04$  obtained above, we find  $\kappa \approx 200$  W/(m·K) for the thermal conductivity, which is comparable to the thermal conductivity of diamond (400–1000 W/(m·K) [17]), since diamond corresponds to the greatest extent to the model in question in view of the low level of its imperfection and anharmonicity.

The evaluation of the thermal conductivity obtained remains true in a wide range of variation of the parameters of the thermostats and, consequently, is, indeed, a characteristic of the one-dimensional particle chain in question. However, in certain numerical experiments, the dimensionless difference of the temperatures at the chain's ends is substantially higher than that in other experiments; therefore, the thermal conductivity will be much lower. The reason is the stronger nonuniformity of the temperature distribution over the chain length, which follows from a comparison of Fig. 3a and 3b.

Introduction of nonlinear terms into the equations of motion leads to a substantial increase in the difference of the temperatures at the boundaries of the system and accordingly to a significant decrease in the thermal conductivity. Thus, with increase in the coefficient  $\alpha_5$  of the cubic terms of the forces from 0 to 0.1, the effective thermal conductivity decreased by more than an order of magnitude.

In accordance with the theory of heat conduction of crystals that is based on the introduction of the ideas of phonons as quasiparticles, the thermal resistance is caused by the scattering of phonons on different imperfections of the crystal structure: defects, dislocations, etc. In the case in question, the interaction of the system with the thermostats causes structure formation, and the more pronounced these structures, the smaller the thermal conductivity. We can assume that, as the size of the system (number of particles in the chain) increases, its structurization will become less pronounced and, as consequence, the thermal conductivity will increase. This effect was observed in many numerical experiments [1].

Furthermore, it should be noted that an abnormally high thermal resistance capable of decreasing the effective thermal conductivity of the system by an order of magnitude appears at the points of contact of the thermostats and the chain. A more detailed investigation of this effect will enable one to study the nature of the heat-transfer coefficient, whose knowledge is necessary for consideration of the thermal processes occurring in contact of different bodies or their parts.

## CONCLUSIONS

The investigation performed has enabled us to establish a number of features of the processes of transfer of energy in a one-dimensional chain of linearly interacting particles.

The self-oscillating systems located at the ends of the chain and selected as thermostats are capable, in the steady-state regime, of ensuring an ordered transfer of energy with the corresponding selection of the parameters of the thermostats. The self-oscillating systems mentioned move in the regime close to the limiting cycle but with smeared contours because of the (nearly periodic) variations of the amplitude of their oscillations. The parameters of the limiting cycles significantly differ from their values for isolated self-oscillating systems; moreover, the mutual influence of the thermostats through the particle chain connecting them is established. Particles at the chain's ends oscillate with a time-independent difference of phases.

After a certain time interval, a steady-state regime with a practically constant (in averaging over the self-oscillating period) energy flux is established in the system. The duration of the transient process exceeds the time of run of a perturbation in the chain several times. The stationary states of the system are characterized by a nonuniform distribution of the average particle velocities (temperature) squared along the chain length. The main nonuniformity is determined by the wavelength comparable to a doubled equilibrium interparticle distance. This nonuniformity is modulated by a wave with a period from ten to sixty interparticle distances, i.e., comparable to the system's size.

The presence of periodic variations of the amplitudes of oscillations of the thermostats and two scales of spatial nonuniformities of the stationary states of the system suggest that the transfer of energy is mainly by waves with two close wave numbers and frequencies leading to beats in both time and coordinate space. This fact can be used in constructing, in the future, an approximate analytical theory of behavior of the nonlinear system in question.

Numerical evaluations of the thermal conductivity of the chain have shown that it is comparable to the value of this coefficient for diamond, whose crystals are characterized by low levels of imperfection and anharmonicity. A

correlation between the increase in the thermal resistance of the system and the enhancement of its structurization has been established. A conclusion on the influence of the conjugations of different subsystems on the effective thermal conductivity and on the possibility of using the data obtained for investigation of the nature of the heat-transfer coefficients has been drawn. It has been shown that introduction of nonlinear interparticle interactions leads to a substantial decrease in the thermal conductivity.

## NOTATION

$a_j$  ( $j = (0, n + 1)$ ), amplitudes of oscillations of particles, m;  $a_{0is}$ , steady-state amplitude of self-oscillations of an isolated zero particle, m;  $c$  and  $c_1$ , coefficients of linear interaction between particles and with the substrate, N/m;  $E$ , energy, J;  $J$ , heat flux,  $W/m^2$ ;  $k$ , circular frequency,  $sec^{-1}$ ;  $k_B$ , Boltzmann constant, J/K;  $l_0$ , equilibrium interparticle distance;  $m$ , particle mass, kg;  $N$ , power, W;  $n$ , number of particles in the system;  $T$ , temperature, K;  $x_j$ , coordinate of the  $j$ th particle, m;  $a_i$  ( $i = 1, 5$ ), dimensionless parameters;  $\gamma$ , coefficient of the resistance (cubic in velocity) to the motion of particles,  $kg \cdot sec/m^2$ ;  $\kappa$ , thermal conductivity,  $W/(m \cdot K)$ ;  $\lambda$  and  $\tau$ , length and time units respectively, m and sec;  $\mu$ , coefficient of negative resistance, kg/sec;  $\chi$ , parameter of nonlinear (cubic) interparticle interaction,  $kg/(sec^2 \cdot m^2)$ . Subscripts: is, isolated; bar, dimensionless quantity.

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