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Energy Oscillations in a One-Dimensional Harmonic Crystal on an Elastic Substrate

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Abstract—A one-dimensional harmonic crystal on an elastic substrate is considered as a stochastic system into which randomness is introduced through initial conditions. The use of the particle velocity and displacement covariances reduces the stochastic problem to a closed deterministic problem for statistical characteristics of particle pairs. An equation of rapid motion that describes oscillations of potential and kinetic energy components of the system has been derived and solved. The obtained solutions are used to determine the character and to estimate the time of decay of the transient process that brings the system to thermodynamic equilibrium.

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1. INTRODUCTION

Nanoscale mechanics of materials has special features [1, 2] that are largely related to the discreteness of the atomic structure of matter [3, 4]. Discreteness, among other things, significantly affects wave processes in the medium, thus introducing dispersion into the law of propagation of mechanical waves [5]. A classic example of such systems is a chain of masses on an elastic substrate described by a harmonic (linear) interaction [6]. This chain can serve as a model of carbon nanofibers formed on the surface of the silicon substrate. Mechanical waves propagating in such a system obey a dispersion-filtration law characterized by the lower and upper cutoff frequencies (cutoffs). Similar effects arise in nanostructures, specifically, in an array of parallel nanosized crystals grown perpendicular to the substrate. Eremeyev et al. [7, 8] found that the wave dispersion law in such an array is a discontinuous function of frequency. Special features of thermomechanical processes in discrete systems are negative thermal expansion [9, 10] and the possibility of structural transitions [11, 12]. The diversity of thermal phenomena makes a description of heat transfer in discrete media very difficult.

In an ideal single crystal, analytical and computer investigations show a sufficient disagreement with the classical thermal conductivity based on the Fourier law [6, 13, 14]. The disagreement can be reduced or even completely eliminated with the use of special interaction laws [15–18] or quite complex structures [19, 20]. However, recently derived experimental results [21–23] demonstrate that the Fourier conduction law is really broken in low-dimensional nanostructures. This has awakened interest in simple lattice models, in particular, in one-dimensional harmonic crystals where the mentioned anomalies are most pronounced [24–26].

Compared with continuum models of heat transfer by waves at the nano- and microlevels [27–29], thermal processes in discrete media exhibit important distinctions. Thus, sudden heating initiates high-frequency oscillations in a discrete system, which are related to the establishment of an equality of potential and kinetic energy according to the virial theorem [4, 30]. This process has been long observed in computer simulations [31]. Its analytical description was apparently pioneered by Krivtsov [32] who used Bessel functions to describe damped oscillations of energy in a one-dimensional harmonic crystal without a substrate. The solution by Krivtsov [32] is also interesting regarding its use for the description of heat transfer in the crystal after the decay of the mentioned transient process [33–35]. In addition, the Fourier law was replaced by the heat conduction law for a one-dimensional crystal [33, 34].

The present paper is devoted to an investigation of high-frequency energy oscillations using the harmonic model of a one-dimensional crystal on an elastic substrate, which presents a generalization of the model discussed earlier [32]. The approach proposed in this paper is based on previous papers [32, 35, 36]. It provides dynamic equations for statistical characteristics of the crystal and an analytical description of thermal processes in the crystal. The crystal is considered to be a stochastic system, into which randomness is introduced through initial conditions. Deterministic dynamic equations are deduced for the particle velocity and displacement covariance. The solution of these equations yields an accurate analytical representation and approximate asymptotic formulae describing the transient process that brings the system to the state of thermodynamic equilibrium. The analytical results are confirmed by computer simulation.

2. DYNAMIC EQUATIONS OF A CHAIN

Consider a chain composed of identical masses m connected by springs of stiffness C_0. The chain is on an elastic substrate of stiffness C_1. Then the dynamic equation of chain particles has the form

$$\ddot{u}_n = (\omega_0^2\Delta_n^2 - \omega_1^2)u_n, \tag{1}$$

$$\omega_0 \overset{\text{def}}{=} \sqrt{C_0/m},\ \omega_1 \overset{\text{def}}{=} \sqrt{C_1/m},$$

where u_n is the displacement of the nth particle, Δ_n^2 is the second-order difference operator:

$$\Delta_n^2 u_n \overset{\text{def}}{=} u_{n-1} - 2u_n + u_{n+1}, \tag{2}$$

n is the index that takes integer values. Equation (3) can be written as

$$\ddot{u}_n = \omega_0^2(u_{n-1} - (2+\epsilon)u_n + u_{n+1}), \tag{3}$$

$$\epsilon \overset{\text{def}}{=} \omega_1^2/\omega_0^2 = C_1/C_0.$$

For analytical constructions, the crystal is rendered infinite. The approximate model of the infinite crystal used for the numerical analysis is a chain consisting of $N \gg 1$ particles subject to the periodicity condition $u_{k+N} = u_k$.

We consider initial conditions corresponding to an instanteneous thermal disturbance

$$u_n|_{t=0} = 0,\ \dot{u}_n|_{t=0} = \sigma\rho_n, \tag{4}$$

where ρ_n is the independent random variables with zero expectation and unit variance and σ is the deviation of initial velocities. Initial conditions (4) can be interpreted as an ultrashort laser pulse applied to the crystal [37]. We assume that initial condition (4) is statistically homogeneous in space, i.e. all statistical characteristics ρ_n are independent of n.

3. DETERMINATION OF NONLOCAL ENERGY

For heat transfer problems in a one-dimensional crystal, a covariance matrix was first used by Rieder et al. [38] who found steady-state heat flow between hot and cold heat reservoirs. Following [32, 33], we introduce the nonlocal (covariant) kinetic energy

$$K_n \overset{\text{def}}{=} \frac{1}{2}m\langle v_s v_{s+n}\rangle, \tag{5}$$

where $v_s \overset{\text{def}}{=} \dot{u}_s$ is the particle velocity and triangular brackets stand for the expectation value. Nonlocal potential energy acquires the form

$$\Pi_n \overset{\text{def}}{=} \frac{1}{2}C_0\langle\varepsilon_s\varepsilon_{s+n}\rangle + \frac{1}{2}C_1\langle u_s u_{s+n}\rangle, \tag{6}$$

where $\varepsilon_s \overset{\text{def}}{=} u_{s+1} - u_s$ is the bond strain. If conventional energy is determined by the velocity and strain dispersion, then nonlocal energy is defined by covariance[1] of the same values for a pair of particles whose position indices differ by n. Since the crystal is in the statistically homogeneous state, the introduced quantities are independent of the position index s but they essentially depend on the correlation index n. At $n = 0$, formulae (5) and (6) allow for the conventional energy

$$\Pi_0 = \frac{1}{2}C_0\langle\varepsilon_s^2\rangle + \frac{1}{2}C_1\langle u_s^2\rangle,$$

$$K_0 = \frac{1}{2}m\langle v_s^2\rangle,\ E_0 = \Pi_0 + K_0. \tag{7}$$

For computer simulation, the expectation in the covariance calculation can be approximately replaced by averaging over all possible values of s in the crystal.

The use of the energy term for the introduced quantities is related to the fact that the total nonlocal energy

$$E_n \overset{\text{def}}{=} K_n + \Pi_n$$

remains unaltered. Let us demonstrate it. Use dynamic equation (3) to calculate the time derivative of nonlocal kinetic energy

$$\dot{K}_n = m\langle v_s\dot{v}_{s+n}\rangle = (C_0\Delta_n^2 - C_1)\langle v_s u_{s+n}\rangle. \tag{8}$$

The latter equation is deduced with the covariance symmetry identity [32]

$$\langle f_{s+n}g_s\rangle = \langle f_s g_{s+n}\rangle. \tag{9}$$

By using the representation $\langle\varepsilon_s\varepsilon_{s+n}\rangle = -\Delta_n^2\langle u_s u_{s+n}\rangle$ [32], we calculate the derivative of potential energy

$$\dot{\Pi}_n = -C_0\Delta_n^2\langle v_s u_{s+n}\rangle + C_1\langle v_s u_{s+n}\rangle$$

$$= (C_1 - C_0\Delta_n^2)\langle v_s u_{s+n}\rangle = -\dot{K}_n. \tag{10}$$

[1] For centered random variables, the covariance presents an expectation value of their product.

From equality (10) it follows that the system conserves the total energy. Thus, nonlocal energy E_n obeys the law of conservation of energy similar to that of mechanical energy.

4. DYNAMICS OF NONLOCAL ENERGY

We obtain analytical equations to describe high-frequency oscillations of potential and kinetic energy in a crystal. Dynamic equation (1) of the chain is used to calculate the second derivative of potential energy

$$\ddot{\Pi}_n = (C_1 - C_0\Delta_n^2)(\langle v_s v_{s+n}\rangle + \langle \ddot{u}_s u_{s+n}\rangle) = 2(\omega_1^2 - \omega_0^2\Delta_n^2)L_n, \quad (11)$$

where $L_n \overset{\text{def}}{=} K_n - \Pi_n$ is the nonlocal Lagrangian of the system. Differentiating the Lagrangian twice with respect to time and considering for $\ddot{\Pi}_n = -\ddot{K}_n$ (10), we derive

$$\ddot{L}_n = 4(\omega_0^2\Delta_n^2 - \omega_1^2)L_n, \quad (12)$$

or in the explicit form

$$\ddot{L}_n = 4\omega_0^2(L_{n-1} - (2+\epsilon)L_n + L_{n+1}). \quad (13)$$

The resulting equation for L_n, as with the case of no substrate [32], differs from the dynamic equation of the chain (3) only by a doubled partial frequency ω_0.

5. ANALYTICAL SOLUTION

Initial values of L_n and $\dot{L}_n$ determined by dispersions and particle velocity and displacement covariances at the initial moment are taken as initial conditions for Eq. (13). According to initial conditions (4), different particles have independent initial velocities and zero initial displacements. Then, using the definitions of nonlocal potential and kinetic energies (5), (6) we obtain

$$L_n|_{t=0} = E\delta_n, \quad \dot{L}_n|_{t=0} = 0, \quad (14)$$

where $E = m\sigma^2/2$ is the total energy of the chain and δ_n is the discrete function[2].

Thus, the dynamics of energy in the stochastic problem (3), (4) is determined from the deterministic initial problem (13), (14). This means that the progress of a random process is completely determined by initial conditions (14) while energy oscillations are independent of the initially selected velocity distribution function.

With initial conditions (14), Eq. (13) is solved using the discrete Fourier transform [39] to give:

$$L_n = \frac{2E}{\pi}\int_0^{\pi/2} \cos(2\sqrt{4\sin^2 p + \epsilon}\,\omega_0 t)\cos(2pn)\mathrm{d}p. \quad (15)$$

A similar expression was obtained by Gendelman et al. [40] when studying a sinusoidal thermal disturbance in the crystal on the substrate. For conventional energy, the correlation coefficient n is zero. By using the notation $L \overset{\text{def}}{=} L_0$, from (15) we derive

$$L = \frac{E}{\pi}\int_0^{\pi} \cos(2\sqrt{4\sin^2 p + \epsilon}\,\omega_0 t)\mathrm{d}p. \quad (16)$$

After the Lagrangian is found, the kinetic and potential energies are calculated according to the formulae

$$K(t) = E\frac{1+L(t)}{2}, \quad \Pi(t) = E\frac{1-L(t)}{2}. \quad (17)$$

Write Lagrangian values (15) for the two extreme cases

$$\epsilon = 0: \; L = EJ_0(4\omega_0 t) \approx \frac{E}{\sqrt{2\pi\omega_0 t}}\cos(4\omega_0 t - \pi/4), \qquad \epsilon = \infty: \; L = E\cos(2\omega_1 t). \quad (18)$$

Here we use the identity $\sqrt{\epsilon}\omega_0 = \omega_1$. In the first case ($\epsilon = 0$), there is no substrate and a solution coincides with the solution obtained previously [32]. In accordance with properties of the Bessel function, the Lagrangian describes damped oscillations with a frequency and amplitude inversely proportional to the square root of time (an approximate formula is valid for not too short times). In the second case ($\epsilon = \infty$), particles do not interact and consequently perform undamped oscillations with the same frequency and phase (since all of them are simultaneously excited at $t = 0$). Energies as quadratic functions of displacements and coordinates oscillate with a doubled frequency $2\omega_1$, where the frequency ω_1 is determined by the substrate stiffness.

Represent solution (15) in the form convenient for the asymptotic analysis. To do this, we calculate the Laplace time transform of the integrand in (15). After reverse Laplace transformation, integration over p yields

$$L = E\frac{\mathrm{d}}{\mathrm{d}t}\int_0^t J_0(2\sqrt{4+\epsilon}\,\omega_0(t-\tau))J_0(2\sqrt{\epsilon}\omega_0\tau)\mathrm{d}\tau. \quad (19)$$

The transformation data are detailed in Appendix A1. The value $\sqrt{4+\epsilon}\,\omega_0$ in expression (19) is equal to the upper cutoff frequency while $\sqrt{\epsilon}\omega_0$ corresponds to the lower cutoff frequency for the chain on the elastic substrate (3). The calculation of the time derivative t leads to the expression

$$\frac{L}{E} = J_0(2\sqrt{4+\epsilon}\,\omega_0 t) - 2\sqrt{\epsilon}\omega_0 \times\int_0^t J_0(2\sqrt{4+\epsilon}\,\omega_0(t-\tau))J_1(2\sqrt{\epsilon}\omega_0\tau)\mathrm{d}\tau. \quad (20)$$

[2] $\delta_n = 1$ for $n = 0$ and $\delta_n = 0$ for $n \neq 0$.

6. SOFT SUBSTRATE

At small values ϵ, from formula (20) we obtain the following asymptotic representation of the Lagrangian as the sum of two Bessel functions (the asymptotic development is given in Appendix A2):

$$\frac{L}{E} \approx J_0(2\sqrt{4+\epsilon}\,\omega_0 t) - \frac{1}{2}\sqrt{\epsilon} J_1(2\sqrt{\epsilon}\omega_0 t). \qquad (21)$$

The numerical analysis shows that the formula has a negligible error up to $\epsilon = 1$ (see Appendix A3). Figure 1 illustrates the solution of (20) and its slow component $\sqrt{\epsilon}J_1(2\sqrt{\epsilon}\omega_0 t)/2$, on which high-frequency oscillations $J_0(2\sqrt{4+\epsilon}\,\omega_0 t)$ are superimposed. Both slow and high-frequency components of oscillations damp according to properties of the Bessel functions, in proportion to $1/\sqrt{t}$.

From (21) it is easy to derive constraints for the Lagrangian. For the Bessel function we estimate

$$|J_0(2x)| < \frac{1}{\sqrt{\pi x}}, \qquad (22)$$

where bounding functions can be considered to be envelopes to a high accuracy. Summarizing the constraints for each of the Bessel functions entering (21), we obtain the estimate for $L(t)$

$$|L(t)| < L_*(t), \quad L_*(t) = \left(\frac{1}{\sqrt[4]{4+\epsilon}} + \frac{\sqrt[4]{\epsilon}}{2}\right)\frac{E}{\sqrt{\pi\omega_0 t}}. \qquad (23)$$

The bounding functions $\pm L_*(t)$ are shown by dashed lines in Fig. 1.

It is easy to show that the following inequality holds

$$L_*(t) \geq L_*(t)|_{\epsilon=0} = \frac{E}{\sqrt{2\pi\omega_0 t}}. \qquad (24)$$

According to (24), in the crystal on the elastic substrate a balance between potential and kinetic energy (damping of Lagrangian oscillations) is established slower than that in the free crystal ($\epsilon = 0$). This agrees well with the fact that in the extreme case when particles interact with the substrate and do not interact with each other ($\epsilon = \infty$) no damping occurs (see the second formula in (18)).

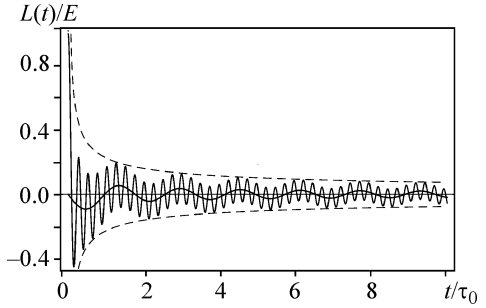

Fig. 1. Lagrangian oscillations for the soft substrate (ϵ = 0.1). The solid line shows the slow component of the signal. The dashed lines show bounding functions (23). The time scale $\tau_0 = 2\pi/\omega_0$.

It was previously found [32] that in the case of no substrate the time dependence of the Lagrangian is described by the differential Bessel equation

$$\ddot{L} + \frac{1}{t}\dot{L} + 16\omega_0^2 L = 0. \qquad (25)$$

This equation is evidently satisfied by the Lagrangian $L(t) = EJ_0(4\omega_0 t)$ derived in (18) at $\epsilon = 0$. We obtain a generalization of (25) for a soft elastic substrate. Consider asymptotic representation (21). Combining differential operators corresponding to Bessel functions of the zero and first orders, we obtain

$$(t^2\partial_t^2 + t\partial_t + 4\epsilon\omega_0^2 t^2 - 1)(16t^2\omega_0^2 + 1)^{-1}$$
$$\times(t^2\partial_t^2 + t\partial_t + 4(4+\epsilon)\omega_0^2 t^2)L(t) = 0. \qquad (26)$$

The time function $(16t^2\omega_0^2 + 1)^{-1}$ is introduced to reduce the factor that arises due to the noncommutation of these operators. Resulting differential equation (26) is of the fourth order with respect to time, which is typical of systems with two coupled oscillators. In addition, this equation is transient and reversible, similarly to (25). A solution of Eq. (26) is function (21) with the initial conditions

$$t = 0: L = E, \ \dot{L} = -\frac{1}{2}E\omega_0\epsilon,$$
$$\ddot{L} = -2E\omega_0^2(4+\epsilon), \ \dddot{L} = \frac{3}{2}E\omega_0^3\epsilon^2. \qquad (27)$$

Note that $\dot{L}|_{t=0} = 0$ according to initial conditions (14). Initial conditions (27) set a small nonzero value for $\dot{L}|_{t=0}$. This discrepancy is due to the approximate character of formula (21). At $\epsilon = 0$, Eq. (26) can be partially integrated, which gives initial equation (25) for $L(t)$ corresponding to the right bracket in (26). Thus, the equation of Lagrangian oscillations (27) is a generalization of Eq. (25) for the chain on the soft substrate. At the moment it is unclear whether it is possible to construct a similar equation for an arbitrary stiffness of the substrate.

7. HARD SUBSTRATE

From the numerical analysis of the diagram of (20) at high ϵ it follows that the solution may be approximately represented as a product of a low-frequency Bessel function and high-frequency harmonic oscillations. Frequencies are defined by characteristic frequencies of dependence (19)

$$\Omega_1 \overset{\text{def}}{=} (\sqrt{4+\epsilon} + \sqrt{\epsilon})\omega_0, \ \Omega_2 \overset{\text{def}}{=} (\sqrt{4+\epsilon} - \sqrt{\epsilon})\omega_0, \qquad (28)$$

where Ω_1 and Ω_2 are the sum and difference of the cut-off frequencies for the chain on the substrate. From the analytical and numerical analysis of formula (20), the fol-

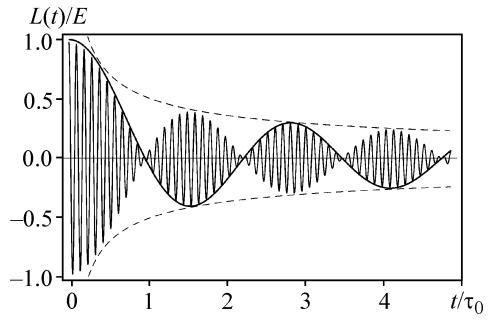

Fig. 2. Lagrangian oscillations for the hard substrate (ϵ = 24). The solid line shows an envelope, the dashed lines show bounding functions (30).

lowing asymptotic representation has been empirically obtained:

$$L \approx EJ_0(\Omega_2 t)\cos(\Omega_1 t). \tag{29}$$

According to formula (29), beats occur in the system: the envelope curve $J_0(\Omega_2 t)$ restricts the wave packet filled with a high-frequency signal $\cos(\Omega_1 t)$ (Fig. 2). In accordance with properties of the Bessel function, the envelope amplitude is attenuated as $1/\sqrt{t}$. The numerical analysis shows that formula (29) is asymptotically exact at high ϵ (see Appendix A3), which however requires further analytical verification.

Using formula (29) and estimate (22), we obtain constrains for the Lagrangian

$$|L(t)| < L_*(t), \tag{30}$$

$$L_*(t) = \frac{E}{\sqrt{\Omega_2 t\,\pi/2}} = \frac{\sqrt{2}E}{\sqrt{\pi(\sqrt{4+\epsilon}-\sqrt{\epsilon})\omega_0 t}}.$$

The bounding functions $\pm L_*(t)$ are shown by dashed lines in Fig. 2. At $\epsilon \to \infty$, $\Omega_1 \to 2\omega_1$ and $\Omega_2 \to 2\omega_0^2/\omega_1 \to 0$ hold to give $L \to E\cos(2\omega_1 t)$ from approximate formula (29), which coincides with (18) obtained previously by exact formula (16). At $\epsilon \to \infty$ estimate (23) yields an overestimated result $L_* \to \infty$. The simplest estimation formula that is valid for arbitrarily large ϵ has the form

$$L_*(t) = \min\left(E, \frac{E}{\sqrt{\Omega_2 t\,\pi/2}}\right). \tag{31}$$

8. APPROXIMATION AND NUMERICAL SOLUTION

Lagrangian oscillations obtained by solving (20) at different ratios of stiffnesses of the substrate and springs between particles resemble oscillations in the system with two degrees of freedom in viscous friction. Figures 1 and 2 exhibit a typical behavior of such a system, i.e. frequency aliasing and beating. However, in contrast to the system in viscous friction, damping is described by a power law rather than by an exponential curve, i.e. amplitudes are inversely proportional to the square root of time.

Figure 3a plots a solution of (20) at equal stiffnesses of springs connecting masses with each other and with the substrate. This case is satisfactorily approximated by each of approximate formulae (21) and (29). The main differences are observed at the extrema where both asymptotic representations somewhat underestimate the exact solution as to amplitude (see Fig. 3a). Thus, the found approximate solutions provide a good approximation: solution (21) for $C_1 \le C_0$ and solution (29) for $C_1 \ge C_0$, thereby covering all possible ratios of stiffnesses.

The analytical results are verified by computer simulation. The system of discrete dynamic equations of the chain (3) with stochastic initial conditions (4) is solved numerically by a central difference method with the integration step $0.001\tau_0$, where $\tau_0 = 2\pi/\omega_0$. Initial velocities are set by a random number generator with a uniform distribution. Expectation is calculated as the average

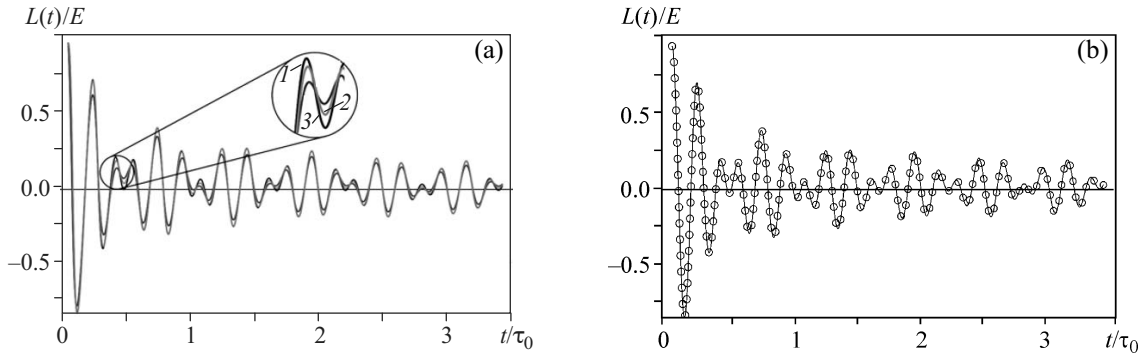

Fig. 3. Energy oscillations at equal stiffnesses: ϵ = 1 ($C_1 = C_0$). *1*—exact solution (20); *2*—asymptotic behavior (21); *3*—asymptotic behavior (29) (a), comparison of the exact solution (solid line) and the solution obtained by computer simulation (circles) (b).

over the crystal. The chain consists of 20 000 particles to provide the required accuracy of the numerical solution. As can be seen graphically, the numerical and analytical solutions agree on the assumed scale. A similar agreement is obtained for the soft and hard substrates.

9. CONCLUSION

We consider discrete dynamic equations of an infinite crystal with stochastic initial conditions. The used approach allows a stochastic problem for particle displacements to be reduced to a closed deterministic problem for statistical characteristics of particle pairs. It is thus found that the Lagrangian of the system satisfies the equation of displacement of a particle in the chain with deterministic initial conditions. In the problem of an instanteneous thermal disturbance, the initial condition for this equation is a displacement of a particle by value E. As the number of particles is infinite, the chain comes to equilibrium in time. Consequently, the Lagrangian vanishes with time; a transient process ends with the balance between kinetic and potential energy, which agrees with the virial theorem. In general, the used approach enables not only a correct identification of parameters of thermodynamic equilibrium but also an analytical description of a nonequilibrium process leading to the mentioned equilibrium.

Along with exact integral formulae, approximate asymptotic formulae are developed for the Lagrangian at a low and high stiffness of the substrate. From properties of the Bessel function it follows that the amplitude of the asymptotic representations decreases as $1/\sqrt{t}$, which is typical for such systems. A similar law of energy decay was previously obtained for the chain without the substrate [32]. The asymptotic behavior, but with the substrate, was obtained by Gendelman et al. for a sinusoidal thermal disturbance (however, at significantly lower frequencies corresponding to slow thermal oscillations) [40]. In contrast to the previous results [32], [40], the present solution reveals two oscillation frequencies $\Omega_1 > \Omega_2$. For the soft substrate (21), they are the doubled upper and lower cutoff frequencies of the chain on the elastic substrate

$$\Omega_1 = 2\omega_0\sqrt{4+\epsilon},\ \Omega_2 = 2\omega_0\sqrt{\epsilon}. \tag{32}$$

For the hard substrate (21), they are the sum and difference of the upper and lower cutoff frequencies

$$\Omega_1 = \omega_0(\sqrt{4+\epsilon}+\sqrt{\epsilon}),\ \Omega_2 = \omega_0(\sqrt{4+\epsilon}-\sqrt{\epsilon}). \tag{33}$$

For the soft substrate, the solution presents high-frequency oscillations typical of a free crystal, which are superimposed on slow oscillations associated with the elastic substrate (Fig. 1). The situation is reversed for the hard substrate: the system demonstrates beats that have high carrier frequency associated with the elastic substrate and a low frequency envelope determined by properties of both the crystal and substrate (Fig. 2). At close stiffness values, the situation is intermediate and can be well described by approximate solutions derived both at low and high ratios of stiffnesses (Fig. 3). The constructed solutions are used to estimate the time of decay of the transient process, which is shown to increase with a rise in the substrate stiffness. The transient process ends with the achievement of the thermodynamic equilibrium state, in which heat transfer implies a macroscopic description. For the chain without the substrate, such description was given elsewhere [33, 34]; with the substrate, it can be similarly developed using the results of this work.

APPENDIX

A1. Lagrangian Representation Derived by Convolution

Consider Lagrangian (16)

$$L = \frac{E}{\pi}\int_0^\pi \cos(2\sqrt{4\sin^2 p + \epsilon}\,\omega_0 t)\,\mathrm{d}p. \tag{A1}$$

The Laplace time transform yields

$$\hat{L} = \frac{E}{\pi}\int_0^\pi \frac{s\,\mathrm{d}p}{s^2 + 4\epsilon\omega_0^2 + 16\omega_0^2\sin^2 p}. \tag{A2}$$

After integration, we derive

$$\hat{L} = Es\,\hat{f}_1(s)\,\hat{f}_2(s), \tag{A3}$$

where

$$\hat{f}_1(s) \overset{\text{def}}{=} \frac{1}{\sqrt{s^2 + 4\omega_0^2(4+\epsilon)}},$$
$$\hat{f}_2(s) \overset{\text{def}}{=} \frac{1}{\sqrt{s^2 + 4\omega_0^2\epsilon}}. \tag{A4}$$

The inverse Laplace transform for (A3) gives

$$L = E\frac{\mathrm{d}}{\mathrm{d}t}\int_0^t f_1(t-\tau)\,f_2(\tau)\,\mathrm{d}\tau. \tag{A5}$$

A substitution of the original functions

$$f_1(t) = J_0(2\sqrt{4+\epsilon}\,\omega_0 t),$$
$$f_2(t) = J_0(2\sqrt{\epsilon}\,\omega_0 t) \tag{A6}$$

into the derived formula provides required formula (19).

A2. Asymptotic Development for the Soft Substrate

Derive asymptotics (21) of the Lagrangian at low ϵ. The integral convolution in formula (20) in the first ap-

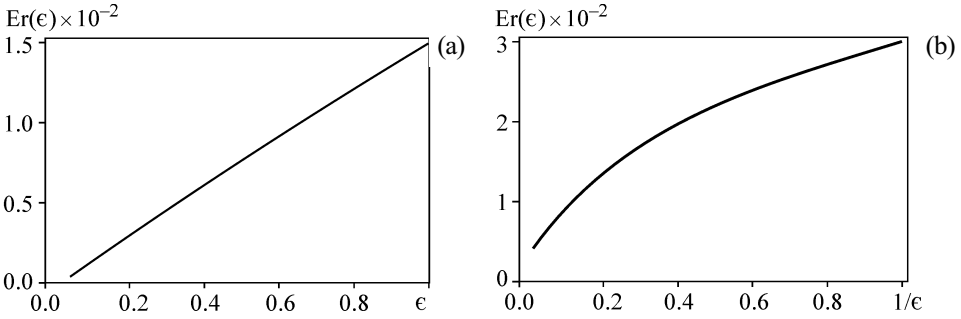

Fig. A1. Integral error of asymptotic representations against ϵ. The error in formulae (21) (a) and (29) (b).

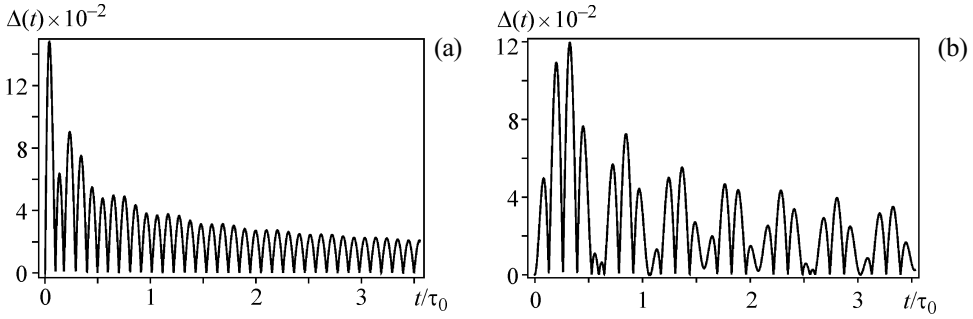

Fig. A2. Discrepancy against time at $\epsilon = 1$ for formulae (21) (a) and (29) (b).

proximation of low ϵ can be represented as

$$S = \int_0^T J_0\left(\frac{2}{\varepsilon}(T-\theta)\right) J_1(\theta)\mathrm{d}\theta, \qquad \text{(A7)}$$

$$\theta \overset{\text{def}}{=} 2\varepsilon\omega_0\tau,\ T \overset{\text{def}}{=} 2\varepsilon\omega_0 t,\ \varepsilon \overset{\text{def}}{=} \sqrt{\epsilon}. \qquad \text{(A8)}$$

It can be shown that the expression $J_0((2/\varepsilon)(T-\theta))$ in (A7) can be asymptotically replaced by $\varepsilon\delta(T-\theta)$ at low ε, where δ is the Dirac delta-function. Then

$$S \approx \varepsilon\int_0^T \delta(T-\theta)J_1(\theta)\mathrm{d}\theta = \frac{\varepsilon}{2}J_1(t) = \frac{1}{2}\sqrt{\epsilon}J_1(2\sqrt{\epsilon}\,\omega_0 t). \qquad \text{(A9)}$$

A substitution of the derived expression into (20) provides sought-for formula (21):

$$\frac{L}{E} = J_0(2\sqrt{4+\epsilon}\,\omega_0 t) - \frac{1}{2}\sqrt{\epsilon}J_1(2\sqrt{\epsilon}\,\omega_0 t). \qquad \text{(A10)}$$

A3. Numerical Estimation of the Error of Asymptotic Formulae

Prior to the estimation of the error of asymptotic expressions (21) and (29), we calculate the integral error

$$\mathrm{Er}(\epsilon) = \sqrt{\frac{1}{t_{\text{er}}}\int_0^{t_{\text{er}}} \Delta^2(t)\mathrm{d}t}, \qquad \text{(A11)}$$

$$\Delta(t) \overset{\text{def}}{=} \frac{|L_{\text{ex}}(t) - L_{\text{ap}}(t)|}{E},$$

where L_{ex} is the exact Lagrangian value, L_{ap} is its approximate representation (21) or (29), and t_{er} is the interval of integration. The calculated dependence of the integral error on the parameter ϵ is exhibited in Fig. A1. According to the derived diagrams, the error of the appropriate formulae tends to zero at low and high ϵ, which bears evidence to their asymptotic accuracy. The error of both formulae is minute up to $\epsilon = 1$. Consequently, a solution can be described by approximate formula (21) at $\epsilon \le 1$ and by approximate formula (29) at $\epsilon \ge 1$. According to Fig. A2, the maximum error does not exceed 1.5% for formula (21) and 3% for formula (29).

In the calculations represented in Fig. A1, we use $t_{\text{er}} = 3.5\tau_0$, i.e. the integration interval is chosen so as to cover first several periods of oscillations. As shown in Fig. A2, the error of asymptotic representations decreases with time, which allows for a relatively small interval of integration for the approximate estimate.

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