

# Ballistic resonance and thermalization in the Fermi-Pasta-Ulam-Tsingou chain at finite temperature

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We study conversion of thermal energy to mechanical energy and vice versa in an  $\alpha$ -Fermi-Pasta-Ulam-Tsingou (FPUT) chain with a spatially sinusoidal profile of initial temperature. We show analytically that coupling between macroscopic dynamics and quasiballistic heat transport gives rise to mechanical vibrations with growing amplitude. This phenomenon is referred to as ballistic resonance. At large times, these mechanical vibrations decay monotonically, and therefore the well-known FPUT recurrence paradox occurring at zero temperature is eliminated at finite temperatures.

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## I. INTRODUCTION

Conversion of mechanical energy in solids to thermal energy results in damping of mechanical vibrations, whereas thermal expansion and heat transport lead to the opposite conversion of thermal energy to mechanical. In macroscopic continuum theories, the conversions are modeled by coupling between the equations of momentum balance and of energy balance (linear thermoviscoelasticity being an example [1]). However, at micro- and nanoscales conventional macroscopic constitutive relations may be inapplicable. For example, recent theoretical [2–4] and experimental [5–9] studies show that the Fourier law of heat conduction may be violated. In particular, the ballistic regime of heat transport is observed [10,11].

A well-known model of thermomechanical processes at micro- and nanoscales is the Fermi-Pasta-Ulam-Tsingou (FPUT) chain [12]. Despite the apparent simplicity of the model, analytical description of macroscopic thermoelasticity, heat transport, and energy conversion in the FPUT chain remains a serious challenge for theoreticians.

Several anomalies of thermomechanical behavior have been observed for the FPUT chain. The heat transport in it is anomalous, i.e., the Fourier law is violated [13–15]. The Maxwell-Cattaneo-Vernotte law also fails to describe the heat transport in FPUT chains [16,17]. Harmonic approximation allows one to derive equations [18,19] and closed-form solutions [20,21] describing heat transport in chains. However, the question arises whether the temperature field, obtained in harmonic approximation, can be used for estimation of thermoelastic effects, e.g., excitation of mechanical vibrations due to thermal expansion. We address this issue below.

Conversion of mechanical energy to thermal energy is an even more challenging issue. Studies of the conversion have a long history, starting from the pioneering work of Fermi, Pasta, Ulam, and Tsingou [12], where initial conditions, corresponding to excitation of the first normal mode of the chain, were considered. It was shown numerically that the energy of this mode demonstrates almost periodic behavior, i.e., the system does not reach thermal equilibrium. In the

literature this phenomenon is referred to as the Fermi-Pasta-Ulam-Tsingou recurrence paradox (see, e.g., [22]). Recent advances in understanding of the paradox are summarized, e.g., in Refs. [22–24]. We note that in the original statement of the FPUT problem the chain has zero initial temperature. The conversion of mechanical energy to thermal energy at finite temperature has not been studied systematically. Thus, in spite of significant progress in the understanding of some particular thermomechanical phenomena in the FPUT chain [12–17,22–25], a comprehensive theory of macroscopic coupled thermoviscoelasticity for this system is yet to be developed.

In this paper we report thermomechanical phenomena observed in the  $\alpha$ -FPUT chain with a spatially sinusoidal profile of initial temperature. First, we show analytically that temperature oscillations, caused by quasiballistic heat transport, and thermal expansion give rise to mechanical vibrations with growing amplitude. This phenomenon is referred to as ballistic resonance. Second, we show numerically that mechanical vibrations, excited by the ballistic resonance, decay monotonically in time. Therefore, at finite temperatures the FPUT recurrence paradox is eliminated.

## II. EQUATIONS OF MOTION AND INITIAL CONDITIONS

We consider the  $\alpha$ -FPUT chain [12] consisting of  $N$  identical particles of mass  $m$ , connected by nonlinear springs. The dynamics of the chain is governed by the equation

$$m\dot{v}_n = C(u_{n+1} - 2u_n + u_{n-1}) + \alpha[(u_{n+1} - u_n)^2 - (u_n - u_{n-1})^2], \quad (1)$$

where  $u_n$  and  $v_n$  are, respectively, the displacement and velocity of the particle  $n$ ,  $C$  is the stiffness, and  $\alpha$  is a parameter characterizing nonlinearity. Periodic boundary conditions  $u_n = u_{n+N}$  are used.

We separate mechanical and thermal displacements of particles as follows [26]. By definition, mechanical motion is associated with the time evolution of the mathematical expectation of particle displacement. The macroscopic displacement field  $u(x, t)$ , corresponding to mechanical motion,

is such that

$$u(na, t) = \langle u_n \rangle, \quad (2)$$

where  $a$  is the lattice constant and  $\langle \dots \rangle$  stands for mathematical expectation (in computer simulations it is replaced by the average over realizations with different initial condition). Macroscopic mechanical energy is calculated using the displacement field  $u(x, t)$  [see formula (13)].

The thermal motion is defined as the difference between the total displacement and the mechanical one. Then thermal displacements  $\tilde{u}_n$  are calculated as

$$\tilde{u}_n = u_n - \langle u_n \rangle. \quad (3)$$

Note that, in contrast to mechanical displacements, the thermal displacements are random. Similar separation is carried out for particle velocities. Then the kinetic temperature  $T_n$  of particle  $n$  is defined as

$$k_B T_n = m \langle \tilde{v}_n^2 \rangle, \quad (4)$$

where  $k_B$  is the Boltzmann constant. Note that the proper choice of a definition for temperature in nonequilibrium systems remains an open question. We use the definition (4), because it has a clear physical meaning (kinetic energy per particle) and it is easy to compute. A comprehensive discussion of various definitions of temperature is presented, e.g., in Ref. [27].

Using the definitions (2)–(4), we introduce the initial conditions, corresponding to the spatially sinusoidal kinetic temperature profile, zero initial fluxes, and no macroscopic mechanical motion

$$\begin{aligned} u_n &= 0, & v_n &= \xi_n \sqrt{\frac{2k_B}{m} \left( T_b + \Delta T \sin \frac{2\pi n}{N} \right)}, \\ \langle \xi_n \rangle &= 0, & \langle \xi_n \xi_m \rangle &= \delta_{nm}, \end{aligned} \quad (5)$$

where  $\xi_n$  are uncorrelated random numbers with zero mean and unit variance,  $\delta_{nm}$  is the Kronecker delta,  $T_b$  is the average (background) temperature, and  $\Delta T$  is the amplitude of the initial temperature profile. Note that in real experiments, similar initial conditions can be realized in the framework of the transient thermal grating technique [7–9].

Heat transfer in harmonic,  $\alpha\beta$ -FPUT, and  $\beta$ -FPUT chains with initial conditions (5) was investigated in Refs. [16, 17, 28]. However, in these works thermoelastic effects and thermalization were not considered.

Note that the initial conditions used in the original FPUT problem [12] significantly differ from the initial conditions in (5). In Ref. [12], deterministic initial conditions, corresponding to excitation of the first mode of mechanical vibrations at zero temperature, were considered. In contrast, initial conditions (5) are stochastic. The temperature and thermal energy of the chain are finite, while initial mechanical motion is absent. The consequences of this difference in initial conditions are discussed in Sec. V.

### III. THEORY OF BALLISTIC RESONANCE

We present a continuum model, describing the macroscopic linear thermoelasticity of the  $\alpha$ -FPUT chain (1).

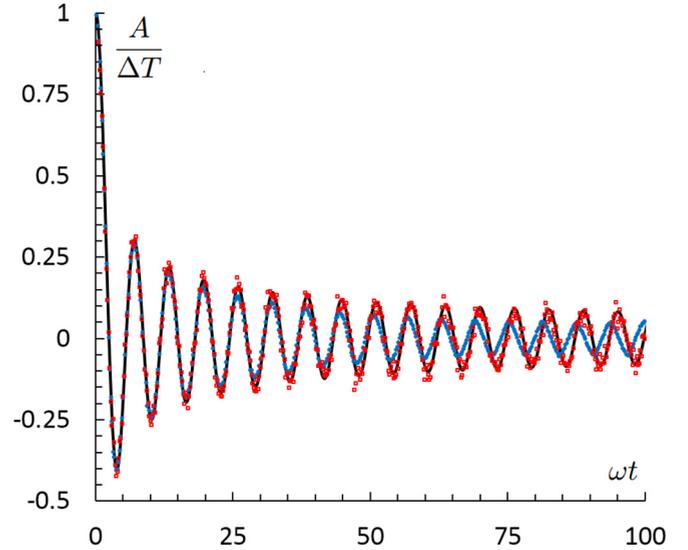


FIG. 1. Oscillations of temperature caused by quasiballistic heat transport from the analytical solution (9) (line) and results of numerical integration of equations of motion (1) for  $\alpha a/C = -0.25$  (red squares) and  $-1$  (blue circles).

Using the model, we describe an unexpected resonance phenomenon.

#### A. Sinusoidal initial temperature profile

We assume that macroscopic mechanical motion of the chain is described by the equation of linear thermoelasticity [26], while the behavior of temperature (heat transfer) is described by the ballistic heat equation [18, 19]. Conversion of mechanical energy to thermal energy is neglected. Then the macroscopic behavior of the chain in the continuum limit is described by the equations

$$\ddot{u} = c_s^2 (u'' - \beta T'), \quad (6)$$

$$\ddot{T} + \frac{1}{t} \dot{T} = c_s^2 T''. \quad (7)$$

Here  $u(x, t)$  is the displacement field,  $T(x, t)$  is the temperature field, the prime stands for the spatial derivative,  $c_s = \sqrt{E/\rho}$  is the speed of sound,  $E$  is Young's modulus,  $\rho$  is the density, and  $\beta$  is the thermal expansion coefficient. The relation between macroscopic and microscopic parameters of the chain is given by formulas (2), (4), and (16).

We note that both macroscopic equations (6) and (7) are derived from the equations of motion (1). Anharmonic effects are taken into account only in Eq. (6). Equation (7) is derived using harmonic approximation [18, 19] and therefore it corresponds to the purely ballistic heat transport regime. However, it is shown below that this equation describes the evolution of temperature with acceptable accuracy, at least for some time, depending on the nonlinearity parameter  $\alpha a/C$  (see, e.g., Fig. 1).

Periodic boundary conditions and the initial conditions

$$T = T_b + \Delta T \sin(\lambda x), \quad \dot{T} = 0, \quad u = 0, \quad v = 0, \quad (8)$$

corresponding to microscopic conditions (5)<sup>1</sup>, are used, where  $\lambda = 2\pi/L$  and  $L$  is the chain length. The solution of the ballistic heat equation (7) with initial conditions (8) has the form [18]

$$T = T_b + A(t) \sin(\lambda x), \quad A(t) = \Delta T J_0(\omega t), \quad (9)$$

where  $\omega = \lambda c_s$  and  $J_0$  is the Bessel function of the first kind. Formula (9) shows that temperature oscillates in time (see Fig. 1).

Substituting the expression (9) into the dynamics equation (6), we obtain

$$\ddot{u} = c_s^2 u'' - \lambda c_s^2 \beta \Delta T J_0(\omega t) \cos(\lambda x). \quad (10)$$

It can be seen that the temperature acts as an external force, exciting the first normal mode of mechanical vibrations. From properties of the Bessel function  $J_0$  it follows that the external force oscillates with frequency  $\omega$  and decays as  $1/\sqrt{t}$ . Note that the frequency coincides with the first eigenfrequency of mechanical vibrations.

The solution of Eq. (10) yields an exact expression for displacements

$$u(x, t) = z(t) \cos(\lambda x), \quad z(t) = -\beta \Delta T \omega t J_1(\omega t) / \lambda. \quad (11)$$

At large times ( $\omega t \rightarrow \infty$ ), the amplitude of displacement  $z$  has the asymptotic behavior

$$z(t) \approx -\sqrt{\frac{2}{\pi}} \frac{\beta \Delta T}{\lambda} \sqrt{\omega t} \cos(\omega t - 3\pi/4). \quad (12)$$

Formula (12) shows that the amplitude grows in time as  $\sqrt{t}$ . The corresponding mechanical energy  $\mathcal{E}$  is calculated via

$$\mathcal{E} = \frac{1}{2L} \int_0^L (\rho v^2 + E u^2) dx = \mathcal{E}_* \omega^2 t^2 [J_0^2(\omega t) + J_1^2(\omega t)], \quad (13)$$

where  $\mathcal{E}_* = E \beta^2 \Delta T^2 / 4$  is proportional to the potential energy of the system due to thermal expansion in the case of uniform temperature profile  $\Delta T$ . At large times, the energy grows linearly, i.e.,  $\mathcal{E} \approx 2\mathcal{E}_* \omega t / \pi$ .

Thus the coincidence of a frequency of temperature oscillations with the first eigenfrequency of the chain leads to excitation of mechanical vibrations with growing amplitude. This phenomenon is referred to as ballistic resonance.

### B. Periodic initial temperature profile

We generalize the presented results for the case of an arbitrary periodic initial temperature profile  $T_0(x) = T_0(x + L)$ .

Fourier series expansion of the profile yields

$$\begin{aligned} T_0 &= \frac{a_0}{2} + \sum_{k=1}^{\infty} [a_k \cos(\lambda_k x) + b_k \sin(\lambda_k x)], \quad \lambda_k = k\lambda, \\ a_k &= \frac{2}{L} \int_0^L T_0(x) \cos(\lambda_k x) dx, \\ b_k &= \frac{2}{L} \int_0^L T_0(x) \sin(\lambda_k x) dx. \end{aligned} \quad (14)$$

The solution of Eqs. (6) and (7), corresponding to the temperature profile (14), is derived using formula (11) and the superposition principle

$$u = \beta c_s t \sum_{k=1}^{\infty} J_1(\omega_k t) [a_k \sin(\lambda_k x) - b_k \cos(\lambda_k x)], \quad (15)$$

where  $\omega_k = k\omega = k\lambda c_s$ . Formula (15) shows that all eigenmodes, included in the expansion of the function  $T_0$ , resonate. The amplitudes of these modes grow in time as  $\sqrt{t}$ . However, since the Fourier coefficients  $a_k$  and  $b_k$  decay with increasing  $k$ ,<sup>2</sup> the main contribution to growth of displacements is given by long-wavelength harmonics (small  $k$ ). Thus the ballistic resonance occurs for any periodic distribution of the initial temperature.

## IV. NUMERICAL RESULTS FOR BALLISTIC RESONANCE

We compare the predictions of the presented continuum theory with the results of the numerical solution of the discrete equations of motion (1). The macroscopic length, density, Young modulus, speed of sound, and thermal expansion coefficient are related to the microparameters of the chain as [26]

$$\begin{aligned} L &= Na, \quad \rho = \frac{m}{a}, \quad E = Ca, \\ c_s &= a \sqrt{\frac{C}{m}}, \quad \beta = -\frac{\alpha k_B}{aC^2}. \end{aligned} \quad (16)$$

Here the thermal expansion coefficient is calculated as  $\beta = \gamma k_B / Ea$ , where  $\gamma = -\alpha a / C$  is the Grüneisen parameter (see, e.g., [26,29]).

To compute macroscopic mechanical characteristics, e.g.,  $z$  and  $\mathcal{E}$ , we consider  $N_r$  realizations of the chain (1) with random initial conditions (5). For each realization, the equations of motion are solved numerically using the fourth-order symplectic integrator [30] with optimized parameters [31]. In our simulations the total energy is conserved with an accuracy of order of 0.001%.

The amplitudes of mechanical vibrations  $z$  and mechanical energy  $\mathcal{E}$  were computed via

$$\begin{aligned} z &\approx -\frac{1}{\pi} \sum_{n=0}^{N-2} \langle u_{n+1} - u_n \rangle_r \sin \frac{2\pi n}{N}, \\ \dot{z} &\approx \frac{2}{N-1} \sum_{n=0}^{N-1} \langle v_n \rangle_r \cos \frac{2\pi n}{N}, \quad \mathcal{E} = \frac{m}{4a} (\dot{z}^2 + \omega^2 z^2). \end{aligned} \quad (17)$$

Here  $\langle \dots \rangle_r$  represents averaging over the realizations.

<sup>2</sup>This statement holds at least for all differentiable functions.

<sup>1</sup>Note that initial temperature in (8) is twice smaller than in (5). This is due to the fact that a half of kinetic energy of the chain is converted to potential energy. This fast transient process, occurring at short times, is disregarded by formula (7). See Refs. [18–21] for further discussions.

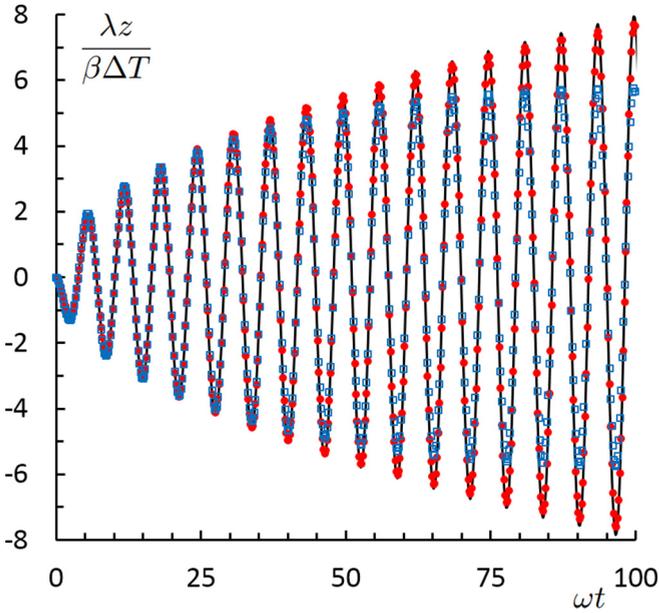


FIG. 2. Growth of amplitude of mechanical vibrations due to ballistic resonance for the analytical solution (11) (solid line) and numerical results for  $\alpha a/C = -0.25$  (circles) and  $-1$  (squares).

To investigate the influence of anharmonic effects, we fix the background temperature  $T_b$  and change the parameter of nonlinearity  $\alpha a/C$  in the interval  $[-1; 0]$ . For the remaining parameters, the following values were used:

$$\begin{aligned} \Delta t &= 0.05\tau_*, & t_{\max} &= 1.4 \times 10^4 \tau_*, & \tau_* &= 2\pi\sqrt{m/C}, \\ \Delta T &= 0.5T_b, & v_0 &= 0.1c_s, & N &= 10^3, & N_r &= 10^4. \end{aligned} \quad (18)$$

Here  $v_0$  is the amplitude of random initial velocities, corresponding to background temperature  $2T_b$ .

We consider the behavior of the kinetic temperature of the chain. The analytical solution (9) suggests that the temperature profile remains sinusoidal. Using this information, we compute the amplitude  $A(t)$  of the temperature profile [see formula (9)]. In numerical simulations, the temperature is calculated by the definition (4). It can be shown that the contribution of  $\langle v_n \rangle$  to the amplitude  $A$  is negligible. Therefore, in formula (4) the total particle velocity  $v_n$  is used instead of  $\tilde{v}_n$ . The amplitudes for  $\alpha a/C = -0.25$  and  $-1$  are shown in Fig. 1. For both values of  $\alpha$  the temperature oscillates in time. These oscillations are responsible for the ballistic resonance. For  $\alpha a/C = -0.25$  the oscillations are described by the analytical solution (9) with high accuracy. Deviations from the analytical solution for  $\alpha a/C = -1$  are caused by anharmonic effects, neglected in the derivation of the ballistic heat equation (7).

The time dependence of the amplitude of mechanical vibrations  $z(t)$  is presented in Fig. 2. It can be seen that the amplitude grows in time. The initial growth is accurately described by the analytical solution (11). Over time, an analytical solution deviates from the numerical solution. The rate of deviation increases with increasing absolute value of the nonlinearity coefficient  $\alpha a/C$ .

The growth of amplitude of mechanical vibrations is due to the partial conversion of thermal energy to mechanical energy.

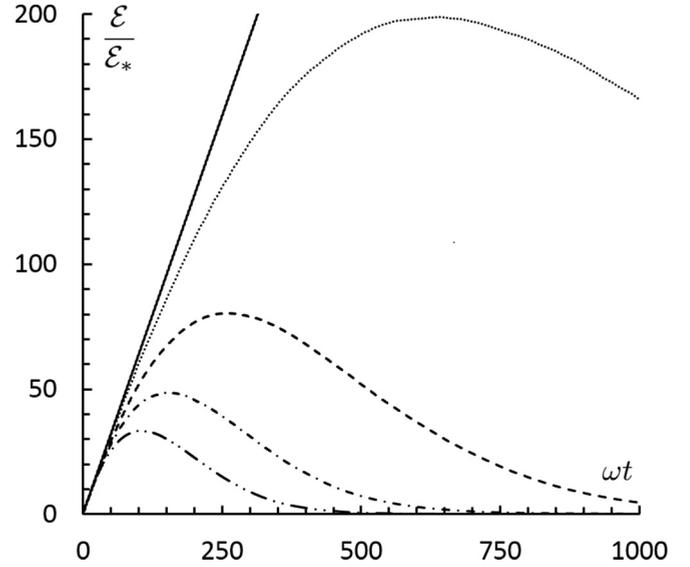


FIG. 3. Time dependence of mechanical energy  $\mathcal{E}$  for the analytical solution (13) (solid line) and numerical results for  $\alpha a/C = -0.25$  (dotted line),  $-0.5$  (dashed line),  $-0.75$  (dash-dotted line), and  $-1$  (dash-double-dotted line).

The conversion can be clearly seen in Fig. 3. The figure shows that initially the mechanical energy grows with time as predicted by the analytical solution (13). Since the total energy of the system is conserved, the growth of mechanical energy is associated with a decrease of thermal energy. Thus the phenomenon of ballistic resonance, predicted by continuum theory [Eqs. (6) and (7)], is observed in direct numerical simulations.

## V. THERMALIZATION

Numerical simulations show that mechanical vibrations, excited by the ballistic resonance, decay in time (see Fig. 4).

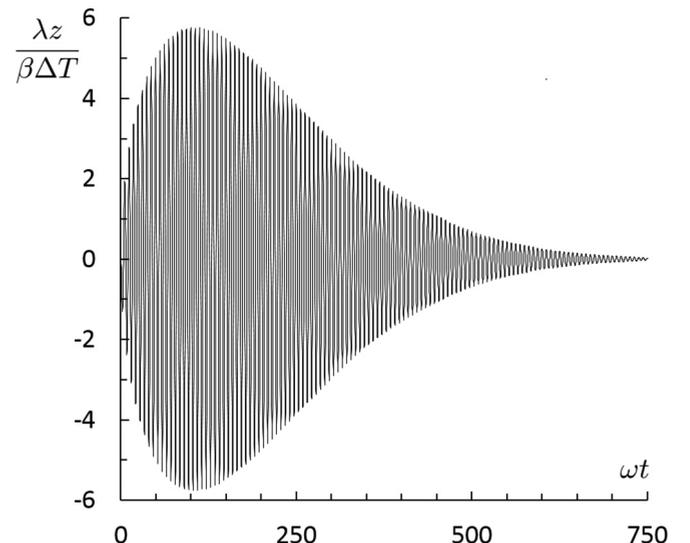


FIG. 4. Decay of amplitude of mechanical vibrations for long times (numerical results for  $\alpha a/C = -1$ ).

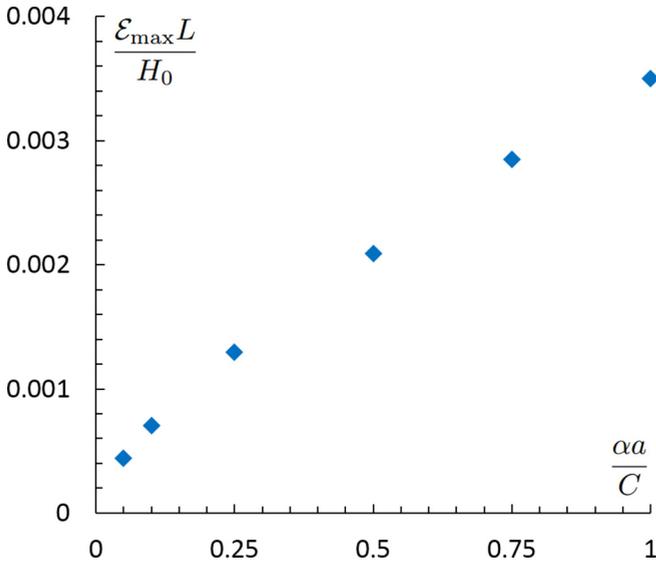


FIG. 5. Maximum mechanical energy  $\mathcal{E}_{\max}$  excited by the ballistic resonance for different values of the nonlinearity coefficient  $\alpha a/C$ . Here  $H_0$  is the total energy of the chain.

The decay is caused by thermalization, i.e., conversion of mechanical energy to thermal energy. This process is not covered by our continuum model (6) and (7). Decay of mechanical energy can be clearly seen in Fig. 3. The energy reaches the maximum value, depending on nonlinearity coefficient  $\alpha a/C$ , and then monotonically tends to zero.

The maximum mechanical energy  $\mathcal{E}_{\max}$  excited by the ballistic resonance, normalized by the total energy of the chain  $H_0$ , is shown in Fig. 5. Here  $\mathcal{E}_{\max}$  increases with increasing absolute value of the nonlinearity coefficient  $\alpha a/C$ . For all considered values of  $\alpha a/C$ , the maximum mechanical energy is several orders of magnitude less than the thermal energy. We note that in the original FPUT problem [12] the situation is the opposite, because thermal energy is equal to zero, while the mechanical energy is finite.

<sup>3</sup>Reference [32] considered decay of the first normal mode of mechanical vibrations at finite background temperature.

Thus, under the considered initial conditions, the mechanical energy of the chain is monotonically converted into thermal energy. This fact is in agreement with the results of numerical simulations carried out in Ref. [32] with different initial conditions.<sup>3</sup> Therefore, the FPUT recurrence paradox is eliminated by finite thermal motion.

## VI. CONCLUSION

We have shown that excitation of a periodic, e.g., sinusoidal, initial temperature profile in the  $\alpha$ -FPUT chain leads to mechanical resonance. The temperature of the chain oscillates in time due to the quasiballistic (wave) nature of heat transport. Nonuniform distribution of temperature causes thermal expansion, which plays the role of a periodic force, exciting macroscopic mechanical vibration. The frequency of this “force” coincides with the eigenfrequency of mechanical vibrations leading to the resonance.

A continuum model of the ballistic resonance has been developed. It was shown that the predictions of the model are in good agreement with the results of numerical simulations. Note that, in contrast to the conventional mechanical resonance, the ballistic resonance occurs in the closed system without any external excitation.

We expect that ballistic resonance may be observed in two- and three-dimensional crystals. However, since in the  $d$ -dimensional case the sinusoidal temperature profile decays as  $1/t^{d/2}$  [21], the effect of ballistic resonance will be weaker.

It was shown that mechanical vibrations, caused by the ballistic resonance, decay monotonically. Therefore, the well-known FPUT recurrence paradox is eliminated by adding a finite thermal motion. In our simulations the energy of mechanical vibrations is much smaller than the thermal energy. This fact appears to be a necessary condition for monotonic decay of mechanical vibrations. However, further work is needed to prove this statement rigorously.

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