ENERGY DISTRIBUTION IN ONE-DIMENSIONAL CRYSTAL

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Summary Reversible transfer between mechanical and thermal energy is considered for α-Fermi-Pasta-Ulam (FPU) crystal. Numeric study for long enough periods of time demonstrate numerous transitions between mechanical and thermal degrees of freedom. Influence of initial velocity fluctuations on the energy transfer process is analyzed.

INTRODUCTION

Nowadays, one of the most rapidly developing areas of modern mechanics is the mechanics of nanostructures [1, 2, 3]. Thanks to nanotechnologies it is possible to obtain almost ideal, defectfree materials. Therefore, prediction of the properties and behavior of this materials is a topical problem. Understanding of heat transfer at microlevel is significant to obtain link between microscopic and macroscopic description of solids [4, 5]. Development of computer technology allows to simulate large enough pieces of material, and to investigate their behavior on the required time interval.

The important close topic is Zermelo's Paradox, resulting from the Poincare recurrence theorem [6, 7], which can be effectively studied using finite one-dimensional crystals. We study the celebrated α-Fermi-Pasta-Ulam (FPU) system [8, 9], for which some questions still remain open.

In this regard, in this paper we consider the process of converting the mechanical energy of a nonlinear one-dimensional crystal into heat and back over time. We also study the times much greater then the system return time.

PROBLEM DEFINITION

A chain of identical particles of mass m, connected by the same nonlinear springs with stiffness C is considered.

The dynamic equations have the form: $\ddot{u}_k = \omega_0^2(u_{k-1} - 2u_k + u_{k+1})(1 + u_{k+1} - u_{k-1}), \quad \omega_0 \stackrel{\text{def}}{=} \sqrt{\frac{C}{m}}$, where u_k — displacement of kth particle; k — index that is arbitrary integer. The boundary conditions are periodical: $u_{k+N} = u_k$, where $N \gg 1$ — number of independent particles. Two cases are considered: deterministic and stochastic problem.

DETERMINISTIC PROBLEM

Initial conditions

Initial displacement is zero. Initial velocity in the crystal is defined as follows: $v(x)|_{t=0} = A \sin\left(\frac{2\pi x}{L}\right)$, where A — amplitude, L — crystal length, $x \in [0, L]$.

The crystal shape determining method

For small time velocity distribution along the length of the crystal clearly has a sinus form. However, over the time the chain distribution loses its shape and motion of particles indistinguishable from the heat. This happens due to the nonlinear interaction between the particles. However, over the time the chain takes the form of a sine again but curved by thermal motion. To determine how the chain shape is close to a sine more accurately, we calculate the parameter E^* — ratio of the total mechanical energy E to the total initial mechanical energy E_0.$E^* \in [0, 1]$. The larger the parameter E^*, the greater the crystal shape is similar to a sine.

Analysis of the solution of the problem for a long period of time

Time in this section is measured in the number of oscillations of the sinus. According to the graph $T(t)$ (Fig. 1a) you can see that after some time system returns to a state close to the original. This means that the velocity distribution regains the sine shape. It also shows that the system does not return to the initial state perfectly, but with some deviations. Fig. 1b shows the same graph, but for a longer period of time. It is seen that the peak height isn't constantly decreasing, but varying according to a certain law.

STOCHASTIC PROBLEM

Initial conditions

Initial displacement in the crystal is zero. Initial velocity is defined as follows (Fig. 2a): $v(x)|_{t=0} = A\left(\sqrt{2}\sin\left(\frac{2\pi x}{L}\right) + \sqrt{3\sigma}\rho\right)$, where A — amplitude, L — crystal length, $x \in [0, L]$, σ — dispersion, ρ — random variable, $\rho \in [-1, 1]$.

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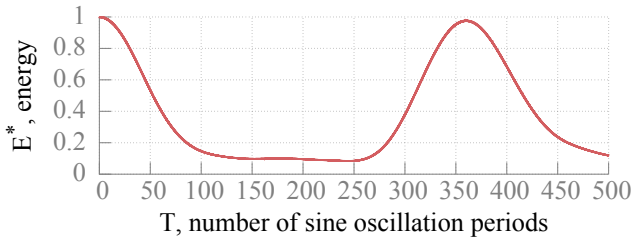
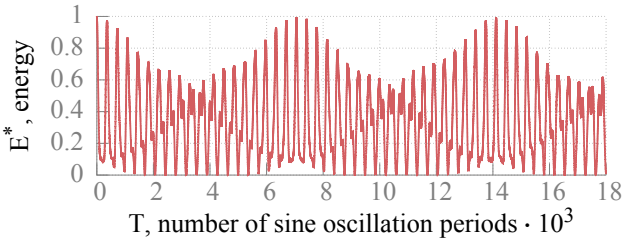
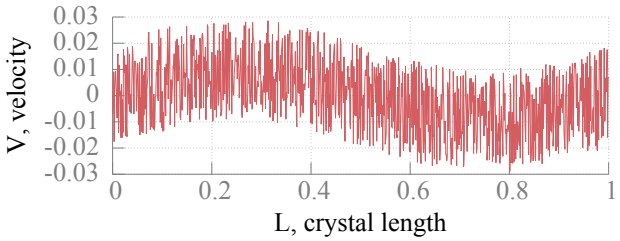


a) For small T

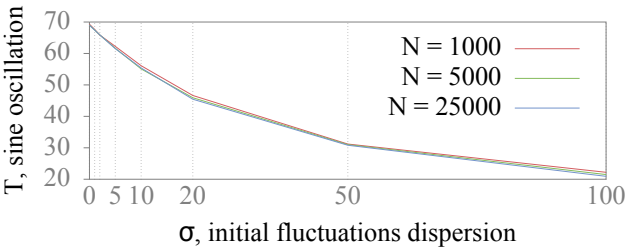


b) For big T

Figure 1: Results



a) Initial conditions



b) Results

Figure 2: Stochastic problem

Results

Time T_α, for which the function $E^*(T)$ falls below a certain value α, depending on the initial fluctuations dispersion σ, was determined. $\alpha = 0.1$, so we get the time value, for which 90% of the mechanical energy is converted into heat. Amplitude $A = 0.01 \cdot \sqrt{2} \approx 0.0141$.

Three cases are calculated for the following amount of particles: $N = 1000$, $N = 5000$ and $N = 25000$ giving almost the same results. In each case, the time T_α calculated for the variance $\sigma = 0; 1; 2; 5; 10; 20; 50; 100$. The results are shown in Fig. 2b. This graph shows that the addition of thermal energy to mechanical at the initial time leads to the fact that the mechanical energy converting into thermal energy becomes faster. It is also seen that the decay rate function $E^*(T)$ for the initial dispersion of the investigated fluctuation range is practically independent from the number of particles.

CONCLUSIONS

The problem of converting of the mechanical energy into thermal energy and back over the time in one-dimensional non-linear crystal is studied. If the crystal is short enough, after some time part of the thermal energy converts back into mechanical energy. The longer is the crystal, the longer one needs to wait for the reverse transformation of the energy and the less thermal energy goes back into mechanical energy. Time to reverse energy transformation is inversely proportional to the amplitude of the velocity fluctuations. The addition of thermal energy to mechanical at the initial time leads to the fact that the mechanical energy converts into thermal energy faster. By adding thermal energy 100 times greater than mechanical energy, the transformation rate of the mechanical energy into thermal energy increases by about 3.5 times. For the investigated range of the particles in the crystal (1000–25000), the rate of the mechanical energy conversion into thermal energy is practically independent from the particle number in the crystal.

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