Thermalization in Feedback Controlled Fermi-Pasta-Ulam Lattice

Egor Usik,* Natalia Amelina,† and Alexander Fradkov‡
Saint-Petersburg State University
Saint-Petersburg, Russia
(Dated: April 17, 2015)

A controlled version of the celebrated Fermi-Pasta-Ulam problem is studied. The speed-gradient control algorithm is analyzed by computer simulation. Approximation of the system Hamiltonian prespecified value is proposed as the control goal. It is demonstrated that the control goal is achieved in the controlled system. It is shown that the controlled system tends to approximate equipartition state much faster than it happens in the open loop (classical) system. Such a phenomenon is observed under control with sufficiently small intensity: less than 0.5% of the total system energy.

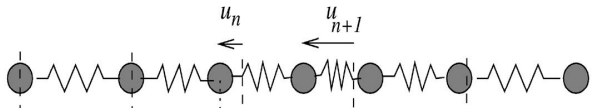

FIG. 1. Schematic picture of the FPU model: masses that can move only in one dimension are coupled by nonlinear springs. u_n is the relative displacement with respect to the equilibrium position of the nth mass. The two ends of the chain were assumed to be fixed, i.e., $u_0 = u_N = 0$

I. INTRODUCTION

The celebrated Fermi-Pasta-Ulam problem bears the name of the three scientists who were looking for a theoretical physics problem suitable for an investigation using one of the very first computers, the Maniac. They decided to study the thermalization process of a solid. The Fermi-Pasta-Ulam (FPU) problem was first introduced in a Los Alamos report in May 1955 [5]. It marked the beginning of both a new field, nonlinear physics (this problem is of central importance in the theories of solitons and chaos), and the age of computer simulations of scientific problems.

The original idea proposed by Enrico Fermi was to simulate the one-dimensional analogue of atoms in a crystal: a long chain of particles linked by springs that obey Hooke's law (a linear interaction), but with a weak nonlinear correction (quadratic for the FPU-α model or cubic for the FPU-β model), see Figure 1.

The authors were interested in a studying a possibility of approaching the statistical equilibrium by simulation. However they got some unexpected and counter intuitive observations that triggered development of the whole new area of physics surveyed in many papers, see e.g. [2, 9]. After more than 50 years there still no unified understanding of the phenomenon. More or less common opinion is that there exist two time scales corresponding to different behavior of the system [1, 4].

In a relatively short time, the system reaches a state different from the initial one several modes, in addition to the initially excited ones, enter the game but still very far from energy equipartition. This is the problematic state observed at low energy in the original FPU paper.

Such a state, however, is only apparently stationary, in fact it is not: similarly to a metastable state of statistical mechanics, on a much longer time scale it does evolve towards statistical equilibrium.

In the spirit of general cybernetical physics approach [7] in our research the following two problems were posed.

1. How significantly the system behavior can be altered by a small controlling action influencing the right hand sides of the system model?

2. Can a control action speed up or slow down the transient process of the approaching to the statistical equilibrium?

The present paper is a continuation of [8]. It contains further examination results providing some evidences that both questions have positive answer. The key point for evaluation of an appropriate control action (design of the control algorithm) providing the desired change in the system behavior is use of the so called speed-gradient (SG) method [7] allowing one to find a concise formula for the control of the nonlinear system energy. The SG-method will be exposed briefly in the next Section.

Section 3 is devoted to description of the FPU system (FPU-α model) in both uncontrolled and controlled versions. Simulation results for controlled system are presented in Section 4. The last section contains some conclusions.

*egor.usik@gmail.com
†n.amelina@spbu.ru
‡Also at Institute of Problems in Mechanical Engineering, Saint-Petersburg State University, Saint-Petersburg, Russia; fradkov@mail.ru

II. PRELIMINARIES

A. Speed-gradient method

Consider the continuous nonstationary system $\dot{x} = F(x,u,t)$. A number of feedback design methods are based on reduction of the current value of some goal (objective) function $Q\big(x(t),t\big)$. The current value $Q\big(x(t),t\big)$ may reflect the distance between the current state $x(t)$ and the current point of the goal trajectory $x_*(t)$, such as $Q(x,t) = \big|x - x_*(t)\big|^2$, or the distance between the current state and the goal surface $h(x) = 0$, such as $Q(x) = \big|h(x)|^2$, or the value of some characteristic of the system dynamics that is desirable to diminish. For continuous-time systems the value $Q(x)$ does not depend directly on control u and decreasing the value of the speed $\dot{Q}(x) = \partial Q/\partial x F(x,u)$ can be posed as immediate control goal instead of decreasing $Q(x)$. This is the basic idea of the speed-gradient (SG) method, proposed by [6], where a change in the control u occurs along the gradient in u of the speed $\dot{Q}(x)$. The general SG algorithm has the form

$$u = -\Psi\big(\nabla_u \dot{Q}(x,u)\big) \tag{1}$$

where $\Psi(z)$ is vector-function forming acute angle with its argument z. For affine controlled systems $\dot{x} = f(x) + g(x)u$ algorithm (1) is simplified to:

$$u = -\Psi\big(g(x)^T \nabla Q(x)\big) \tag{2}$$

Special cases of (1) are the proportional SG-algorithm

$$u = -\Gamma \nabla_u \dot{Q}(x,u), \tag{3}$$

where Γ is a positive-definite matrix, and the relay SG-algorithm

$$u = -\Gamma \operatorname{sign}\Big(\nabla_u \dot{Q}(x,u)\Big). \tag{4}$$

B. Speed-gradient control of energy

One of the most important quantities in physics is energy, which is not only the main invariant of a system and the key to a description of a system on the basis of the Hamiltonian formalism but also a measure of interaction between different systems. The equations of dynamics in the Hamiltonian form are used to describe quite different physical systems and phenomena, from celestial bodies to molecular ensembles. Hence, it is only natural to begin the study of the fundamental laws of transformation of the properties of systems via control with the energy transformation laws. In this section, it is assumed that the investigated system is conservative, i.e., we ignore losses and dissipation. Then, in free motion (i.e., in the absence of external forces), the system energy is an invariant. Hence, the statement of the problem of transfer- ring the system from one energy level to another by weak (ideally, arbitrarily weak) control makes sense. For brevity, we limit ourselves to examination of the control problems in which the mathematical model of the system is given in the Hamiltonian form,

$$\begin{aligned} &\dot{q}_i = \frac{\partial H(q,p,u)}{\partial p_i}, \quad \dot{p}_i = -\frac{\partial H(q,p,u)}{\partial q_i}, \\ &i = 1,\dots,n, \end{aligned} \tag{5}$$

where n – is the number of the degrees of freedom; $q = \operatorname{col}(q_1,\dots,q_n)$, $p = \operatorname{col}(p_1,\dots,p_n)$ – are vectors of generalized coordinates and generalized momenta, which form the state vector of the system, $x = \operatorname{col}(q,p)$; $H = H(q,p,u)$ – is the Hamiltonian of the controlled system; and $u(t) \in \mathbb{R}^m$ – is the dimensionless input (the vector of external generalized forces). In the vector form, model (5) an be written as

$$\dot{q} = \nabla_p H(q,p,u), \dot{p} = -\nabla_q H(q,p,u). \tag{6}$$

We examine the problem of approaching a given energy level H_* of a free (uncontrolled) system, i.e., specify the control goal as

$$\lim_{t\to\infty} H_0(q(t),p(t)) \;=\; H_*, \tag{7}$$

where $H_0(q,p) = H(q,p,0)$ is the Hamiltonian of the free system described by Eqn. (5) with $u = 0$. we assume that the Hamiltonian is linear in control, $H(q,p,u) = H_0(q,p) + H_1(q,p)^T u$, where $H_0(q,p)$ is the Hamiltonian of the free system and $H_1(q,p)$ is m-dimensional vector whose components are the so-called interaction Hamiltonians.

To solve the problem, the SG-method (see Section II A, [7]) is used. We introduce the goal function

$$Q(x) = \frac{1}{2}\left(H_0(q,p) - H_*\right)^2, \tag{8}$$

with $x = \operatorname{col}(q,p)$. The control goal in (7) then becomes

$$\lim_{t\to\infty} Q(x(t)) \;=\; 0. \tag{9}$$

To apply the SG method, we calculate the speed (rate) of variation of the goal function caused by the control of the system,

$$\begin{aligned} \dot{Q} = (H_0 - H_*)\left(\frac{\partial H_0}{\partial q}\dot{q} + \frac{\partial H_0}{\partial p}\dot{p}\right) = \\ = (H_0 - H_*)\{H_0, H_1\}u, \end{aligned} \tag{10}$$

and then calculate the speed gradient in u: $\nabla_u \dot{Q} = (H - H_*)\{H_0,H_1\}^T$, where $\{H_0,H_1\}$ is the Poisson bracket [**?**] of the Hamiltonians H_0, H_1. We can write the SG-algorithm in the finite form, e.g., in the linear and relay variants:

$$u = -\gamma(H_0 - H_*)\{H_0,H_1\}^T, \tag{11}$$

$$u = -\gamma \operatorname{sign}\left((H_0 - H_*)\{H_0,H_1\}^T\right), \tag{12}$$

where $\gamma > 0$ is the control gain.

III. FERMI-PASTA-ULAM SYSTEM

A. FPU equations of motion

Consider the Hamiltonian of FPU-α model:

$$H = \sum_{i=0}^{N} \frac{1}{2} p_i^2 + \sum_{i=0}^{N} \frac{1}{2}(u_{i+1} - u_i)^2 + \sum_{i=0}^{N} \frac{\alpha}{3}(u_{i+1} - u_i)^3, \tag{13}$$

where u_i is the displacement of atom i, along the chain, with respect to its equilibrium position, and p_i is its momentum. The coefficient $\alpha \ll 1$ measures the strength of the nonlinear contribution to the interaction potential. The two ends of the chain were assumed to be fixed, i.e., $u_0 = u_{N+1} = 0$.

The FPU equations of motion [3], derived from Hamiltonian (13) are as follows

$$\begin{cases} \dot{u}_i = p_i, \\ \dot{p}_i = (u_{i+1} + u_{i-1} - 2u_i) + \\ \qquad + \alpha[(u_{i+1} - u_i)^2 - (u_i - u_{i-1})^2]. \end{cases} \tag{14}$$

The common approach in physics is to think in terms of the normal modes, related to the displacements through $A_k = \sqrt{2/(N+1)} \sum_{i=1}^{N} u_i \sin(ik\pi/N+1)$ with the frequencies $\omega_k^2 = 4\sin^2(k\pi/2(N+1))$. Energy equipartition means that the time average of E_k up to time T , namely

$$\bar{E}_k(T) = \frac{1}{T} \int_0^T E_k(P(t), Q(t))dt, \tag{15}$$

for large T converges (up to minor nonlinear contributions) to the energy per degree of freedom $\varepsilon = E/N$, E denoting the total energy.

Let's rewrite Hamiltonian (13) as

$$H = \frac{1}{2} \sum_{k=1}^{N} (\dot{A}_k^2 + \omega_k^2 A_k^2) + \\ + \frac{\alpha}{3} \sum_{k,l,m=1}^{N} c_{klm} A_k A_m A_l \omega_k \omega_m \omega_l, \tag{16}$$

where the coefficients c_{klm} are given, for example, in [10]. The last term, generated by the nonlinear contribution to the potential, leads to a coupling between the modes, and scales as $N^{3/2}$.

Fermi, Pasta and Ulam thought that, due to this term, the energy introduced into a single mode, mode $k = 1$ in their simulation, should slowly drift to the other modes, until the equipartition of energy predicted by statistical physics is reached. The beginning of the calculation indeed suggested that this would be the case. Modes $2, 3, ...,$ were successively excited. However, one day they let the program run long after the steady state had been reached. When they realized their oversight and came back to the room, they noticed that the system, after remaining in a steady state for a while, had then departed from it. To their great surprise, after 157 periods of the mode $k = 1$, almost all the energy (all but 3%) was back to the lowest frequency mode, as shown in figure **??** where the identical picture obtained in our numerical experiments is shown.

Note that in order to obtain reliable numerical results a specific numerical integration method is used, the so called symplectic or geometrical integration. Particularly the MATLAB package GniCodes was used.

B. Control of FPU system

To apply the control let us consider the Hamiltonian of the system with control:

$$H_{control} = \sum_{i=0}^{N} \frac{1}{2} p_i^2 + \sum_{i=0}^{N} \frac{1}{2}(u_{i+1} - u_i)^2 \\ + \sum_{i=0}^{N} \frac{\alpha}{3}(u_{i+1} - u_i)^3 + u_N \omega, \tag{17}$$

where ω is the control.

The FPU equations of motion, derived from Hamiltonian (17) is

$$\begin{cases} \dot{u}_i = p_i, \\ \dot{p}_i = (u_{i+1} + u_{i-1} - 2u_i) \\ \qquad + \alpha[(u_{i+1} - u_i)^2 - (u_i - u_{i-1})^2] + \mu_i \omega_i, \end{cases} \tag{18}$$

where $\omega_i = -\gamma(H - H_*)p_i$, $\gamma > 0$, $i = 1, \ldots, N$.

To apply the SG-method one needs to choose an appropriate goal function. For control of Hamiltonian system a natural goal function corresponding to the goal equivalent to energy control is as follows: $Q(p, u) = \frac{1}{2}(H - H_*)^2$, where H is Hamiltonian (13) and $H*$ is the goal (desired) value of the energy.

IV. SIMULATION RESULTS

Simulation of the controlled FPU lattice was carried out with the following parameters: $t_{fin} = 8000, H^* = 3, N = 32$. The following cases were studied:

1.) $i = 32 \quad \mu_{32} = 1, \quad i < 32 \quad \mu_i = 0;$

2.) $i = 31 \quad \mu_{31} = 1, \quad i \neq 31 \quad \mu_i = 0;$

3.) $i = 30 \quad \mu_{30} = 1, \quad i \neq 30 \quad \mu_i = 0.$

Consider the case 1) when apply the control algorithm (18) to last mode $i = 32$. Fig. 3 presents typical results of simulation in this case. We could see that the controlled system tends to approximate equipartition

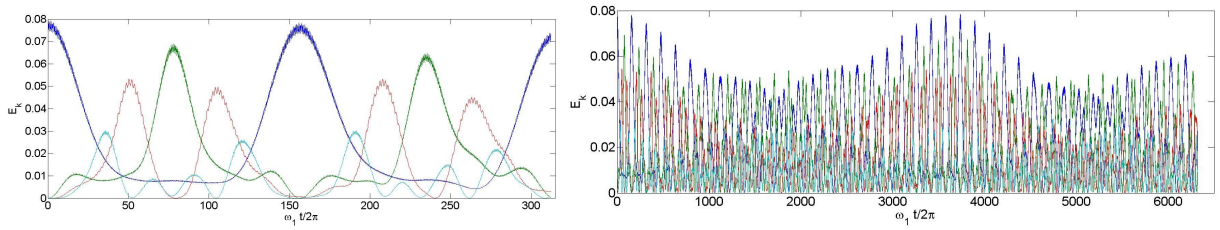

FIG. 2. FPU recurrence: the plot shows the time evolution of the sum of kinetic and potential energies $E_k = \frac{1}{2}(\dot{A}_k^2 + \omega_k^2 A_k^2)$ of each of the four lowest modes with $t_{fin} = 8000, H^* = 3, \gamma = 0$. Initially, only mode 1(blue) was excited.

TABLE I. Numerical analysis of the transient time.

γ	t_{pp}	L	d	t_p
0.01	13000	0.3	130	12500
0.012	10000	0.5	120	10417
0.015	7000	0.31	105	8333
0.02	6000	0.22	120	6250
0.05	3000	0.25	150	2500

state with a reasonable accuracy depending on the control gain γ. For example, if we consider two cases when $\gamma = 0.05$ and $\gamma = 0.01$ we could see that with $\gamma = 0.01$ the transient time has increased from 2500 to 10000 (see Fig. 3(a, d)). Table I presents numerical results that are based on simulations. Here $d = \gamma t_{pp}$, L is the amplitude of the steady-state oscillations, t_p is the transient time. Based on this 5 experiments we could calculate the mathematical expectation, which equals to 125 and standard deviation equals to 15.

Fig. 4(a) depicts the transition time for range of $\gamma = 0.01$ – 0.5 is presented. The control strength $\max u(t)$ could be seen on Fig. 4(b) for various γ. For example, for $\gamma = 0.01$ $\max u(t) = 0.0060$. Under sufficiently small control a tendency to the energy equipartition (thermalization) of FPU Lattice is observed.

The Fig. 5(a) refers to an uncontrolled α model, with $N = 32, \alpha = 0.25$, at rather small value of $\varepsilon = 10^{-3}$, and shows the averaged energy spectrum, i.e. $\bar{E}_k(T)$ vs. k (see equation 15), at different times T. The energy was initially equidistributed among the lower 10% of modes (the rectangular profile in the figure). Quite soon, already at $T \simeq 10^4$, a well defined profile is formed, in which only some low frequency modes effectively take part to energy sharing, the energies of the remaining ones decaying exponentially with k. The Fig. 5(b) refers to controlled model, with control gain $\gamma = 0.5$.

Now consider the cases 2) and 3) when we apply the control algorithm (18) to mode $i = 31$ and $i = 30$. Fig. 6 shows typical results of simulation in the case $i = 31$, and Fig. 7 — for the case $i = 30$.

V. CONCLUSION

In the paper a controlled version of the celebrated Fermi-Pasta-Ulam problem introduced in [8] is further analyzed. The algorithm for control of the system energy based on Speed-gradient approach is proposed and analyzed by computer simulation. It is demonstrated that the control goal is achieved in the controlled system with a reasonable accuracy depending on the control gain γ. It is shown that the controlled system tends to approximate equipartition state much faster than it happens in the open loop (classical) system. Such a phenomenon is observed under control with sufficiently small strength: less than 0.5% of the total system energy. The transient time (time till approximate equipartition is achieved) is of order 10^4 while for classical FPU-system it has order about 10^8–10^9, see [1].

Based on simulation results it was shown that the thermalization occurs faster if the control action is applied to the last mode and the degree of thermalization decreases if we control further from the edge.

ACKNOWLEDGMENTS

The authors acknowledge the support of RFBR (grants 14-08-01015, 15-08-02640).

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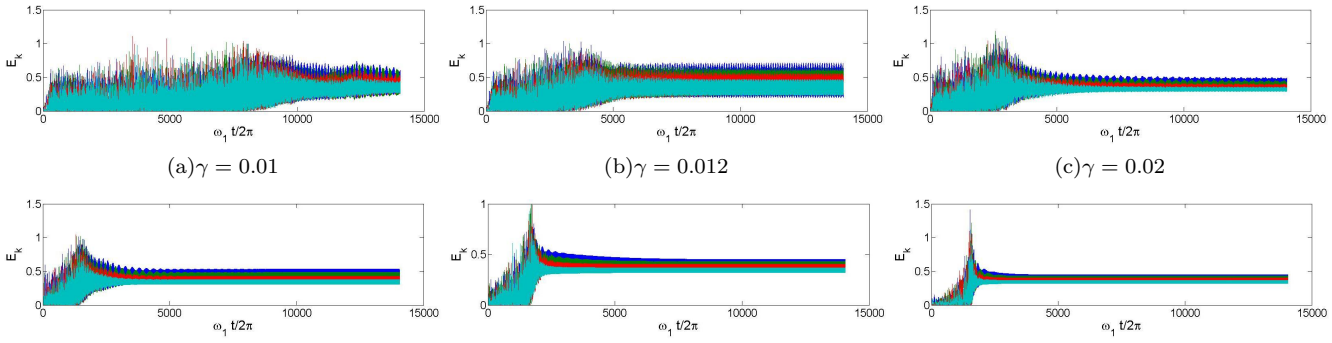

(a)$\gamma = 0.01$ (b)$\gamma = 0.012$ (c)$\gamma = 0.02$

(d)$\gamma = 0.05$ (e)$\gamma = 0.1$ (f)$\gamma = 0.2$

FIG. 3. Controlled FPU system evolution (last mode $i = 32$): the plot shows the time evolution of the sum of kinetic and potential energies $E_k = \frac{1}{2}(\dot{A}_k^2 + \omega_k^2 A_k^2)$ of each of the four lowest modes with $t_{fin} = 8000, H^* = 3$ for different control gains γ.

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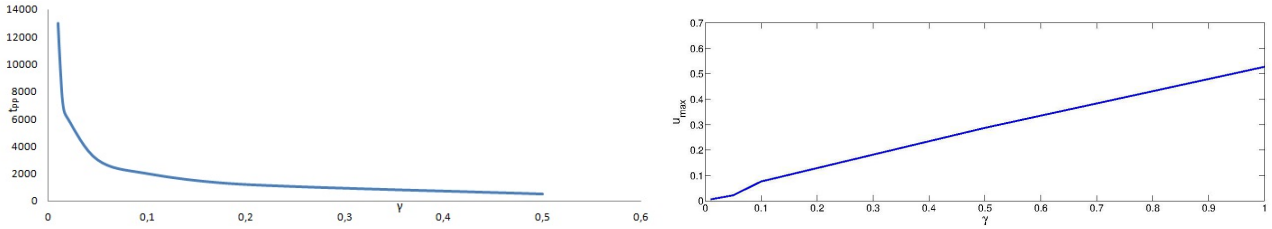
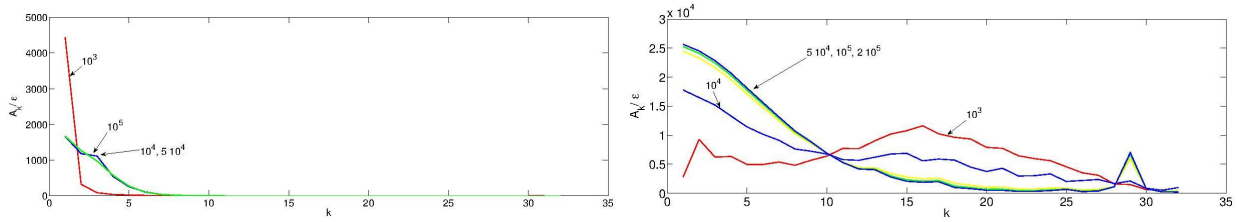


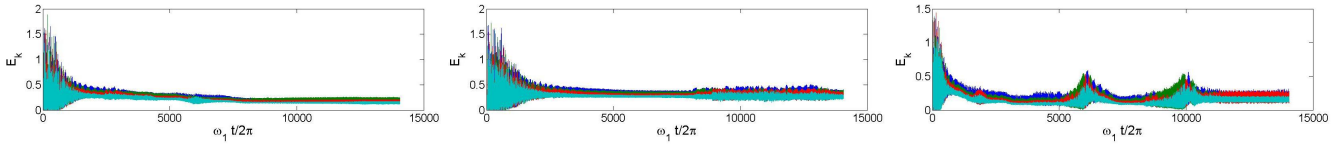
(a)The transient time for controlled FPU system $\gamma = 0.01 \ldots 1$. (b)Control strength u_{max} for $\gamma = 0.01 \ldots 1$.

FIG. 4. The transient time and the control strength



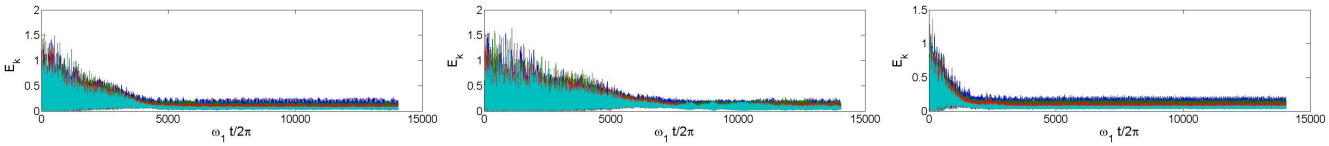
(a)α-model; $N = 32, \varepsilon = 10^{-3}$. (b)Controlled α-model; $N = 32, \varepsilon = 10^{-3}, \gamma = 0.5$.

FIG. 5. The averaged energy spectrum at different times T



(a)$\gamma = 0.05$ (b)$\gamma = 0.03$ (c)$\gamma = 0.1$

FIG. 6. Controlled FPU system evolution (mode $i = 31$): the plot shows the time evolution of the sum of kinetic and potential energies $E_k = \frac{1}{2}(\dot{A}_k^2 + \omega_k^2 A_k^2)$ of each of the four lowest modes with $t_{fin} = 8000, H^* = 3$ for different control gains γ.



(a)$\gamma = 0.05$ (b)$\gamma = 0.03$ (c)$\gamma = 0.1$

FIG. 7. Controlled FPU system evolution (mode $i = 30$): the plot shows the time evolution of the sum of kinetic and potential energies $E_k = \frac{1}{2}(\dot{A}_k^2 + \omega_k^2 A_k^2)$ of each of the four lowest modes with $t_{fin} = 8000, H^* = 3$ for different control gains γ.