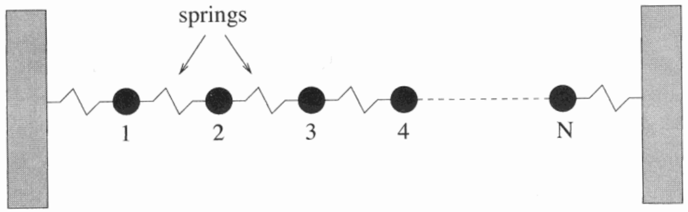
	Lectures	Exercises	Home work problems
Ordinary differential equations	Linear dynamics	E1	
	Non-linear dynamics	E2	
	Molecular dynamics		H1a/H1b
Stochastic methods	Monte Carlo integration	E3	
	Metropolis algorithm		H2a/H2b
	Brownian dynamics	E4	
Partial differential equations	Quantum structure	E5	H3a
	Quantum dynamics		H3b

Fermi-Pasta-Ulam model

One-dimensional chain of masses connected with non-linear springs.



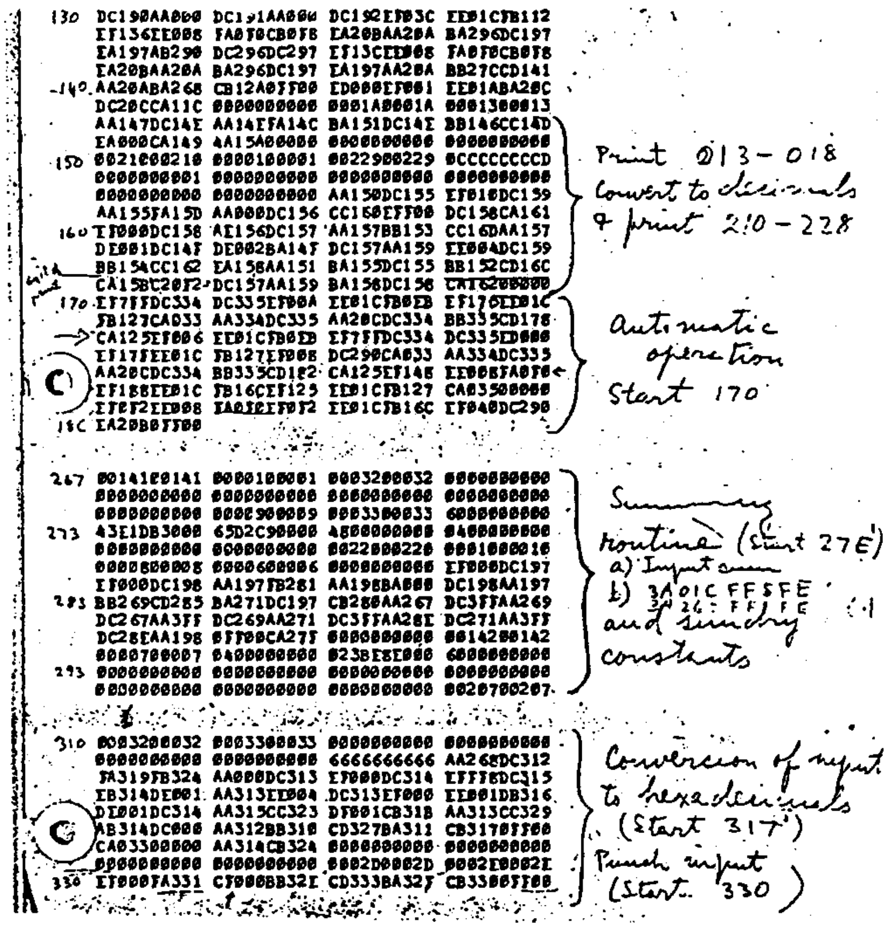
α-model

$$H = \sum_{i=1}^{N} \frac{p_i^2}{2m} + \sum_{i=0}^{N} \left[\frac{\kappa}{2}(u_{i+1} - u_i)^2 + \frac{\alpha}{3}(u_{i+1} - u_i)^3 \right]$$

Fermi-Pasta-Ulam problem

After the second world war Fermi *et al*. became interested in using the newly developed computing machines to test physical ideas, to perform ”computer experiments” or ”computer simulations”.

They wanted to check the prediction of statistical mechanics on the thermalization of solids, which relies on the ergodic hypothesis.



Printout of Fermi’s program. It is written in machine language.
from H. L. Anderson, J. Stat. Phys. **43**, 731 (1986)

Ergodic hypothesis

Time average = Ensemble average

Consider a closed system

Classical mechanics

The system follows a deterministic time-evolution where the energy is conserved. The time-evolution is reversible with no direction in time.

Statistical mechanics

The system will move to a state of thermal equilibrium, where the entropy is maximized. The time-evolution is irreversible with a clear direction of time.

Equipartition theorem

In classical statistical mechanics the mean value of each independent quadratic term in the energy is equal to $\frac{k_B T}{2}$.

Mean value

$$\langle A \rangle = \frac{\int dx_1 \ldots dp_N \;\; A(x_1, \ldots, p_N) \;\; \exp\left[-E(x_1, \ldots, dp_N)/k_B T\right]}{\int dx_1 \ldots dp_N \;\; \exp\left[-E(x_1, \ldots, dp_N)/k_B T\right]}$$

Consider

$$E(x_1, \ldots, p_N) = a x_i^2 + E'(x_1, \ldots, x_{i-1}, x_{i+1}, \ldots, p_N)$$

which implies that

$$\left\langle a x_i^2 \right\rangle = \frac{k_B T}{2}$$

Equipartition theorem

In classical statistical mechanics the mean value of each independent quadratic term in the energy is equal to $\frac{k_BT}{2}$.

Energy of an ideal gas particle

$$E = \frac{\boldsymbol{p}^2}{2m} = \frac{p_x^2}{2m} + \frac{p_y^2}{2m} + \frac{p_z^2}{2m}$$

$$\langle E \rangle = \frac{3k_BT}{2}$$

System of interacting particles

$$E = \sum_{i=1}^{N} \frac{\boldsymbol{p}_i^2}{2m} + V(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_N)$$

$$\langle E_{kin} \rangle = N\frac{3k_BT}{2}$$

Harmonic oscillator in 1 dim

$$E = \frac{p^2}{2m} + \frac{k}{2}x^2$$

$$\langle E \rangle = \frac{k_BT}{2} + \frac{k_BT}{2} = k_BT$$

System of independent harmonic oscillators in 1 dim

$$E = \sum_{i=1}^{N} E_i = \sum_{i=1}^{N} \left[\frac{p_i^2}{2m} + m\frac{k}{2}x_i^2\right]$$

$$\langle E_i \rangle = \left\langle \frac{p_i^2}{2m} + \frac{k}{2}x_i^2 \right\rangle = k_BT \quad \forall i$$

$$\langle E \rangle = Nk_BT$$

Harmonic system

Hamiltonian

$$H = \sum_{i=1}^{N} \frac{p_i^2}{2m} + \sum_{i=0}^{N} \frac{\kappa}{2}(u_{i+1} - u_i)^2$$

Modal representation - normal modes

$$Q_k = \sqrt{\frac{2}{N+1}} \sum_{i=1}^{N} \sqrt{m} u_i \sin\left(\frac{ik\pi}{N+1}\right)$$

$$u_i = \sqrt{\frac{2}{N+1}} \sum_{k=1}^{N} \frac{Q_k}{\sqrt{m}} \sin\left(\frac{ik\pi}{N+1}\right)$$

and

$$P_k = \sqrt{\frac{2}{N+1}} \sum_{i=1}^{N} \sqrt{m} v_i \sin\left(\frac{ik\pi}{N+1}\right)$$

$$v_i = \sqrt{\frac{2}{N+1}} \sum_{k=1}^{N} \frac{P_k}{\sqrt{m}} \sin\left(\frac{ik\pi}{N+1}\right)$$

for $k = 1, \ldots, N$ and $i = 1, \ldots, N$.

Hamiltonian

$$H = \frac{1}{2} \sum_{k=1}^{N} \left[P_k^2 + \omega_k^2 Q_k^2\right]$$

with

$$\omega_k = 2\sqrt{\frac{\kappa}{m}} \sin \frac{k\pi}{2(N+1)}$$

i.e. independent harmonic oscillators.

Assuming equipartition

$$\left\langle \frac{1}{2} P_k^2 \right\rangle = \frac{k_B T}{2} \quad \forall k$$

$$\left\langle \frac{1}{2} \omega_k^2 Q_k^2 \right\rangle = \frac{k_B T}{2} \quad \forall k$$

and

$$\langle E_k \rangle = \left\langle \frac{1}{2}(P_k^2 + \omega_k^2 Q_k^2) \right\rangle = k_B T \quad \forall k$$

Fermi-Pasta-Ulam model

$$H = \sum_{i=1}^{N} \frac{p_i^2}{2m} + \sum_{i=0}^{N} \left[\frac{\kappa}{2}(u_{i+1} - u_i)^2 + \frac{\alpha}{3}(u_{i+1} - u_i)^3 \right]$$

$\alpha = 0$

Linear system.

can be described by normal modes

no energy exchange between the modes

no equipartition of the energy among the normal modes

$\alpha \neq 0$

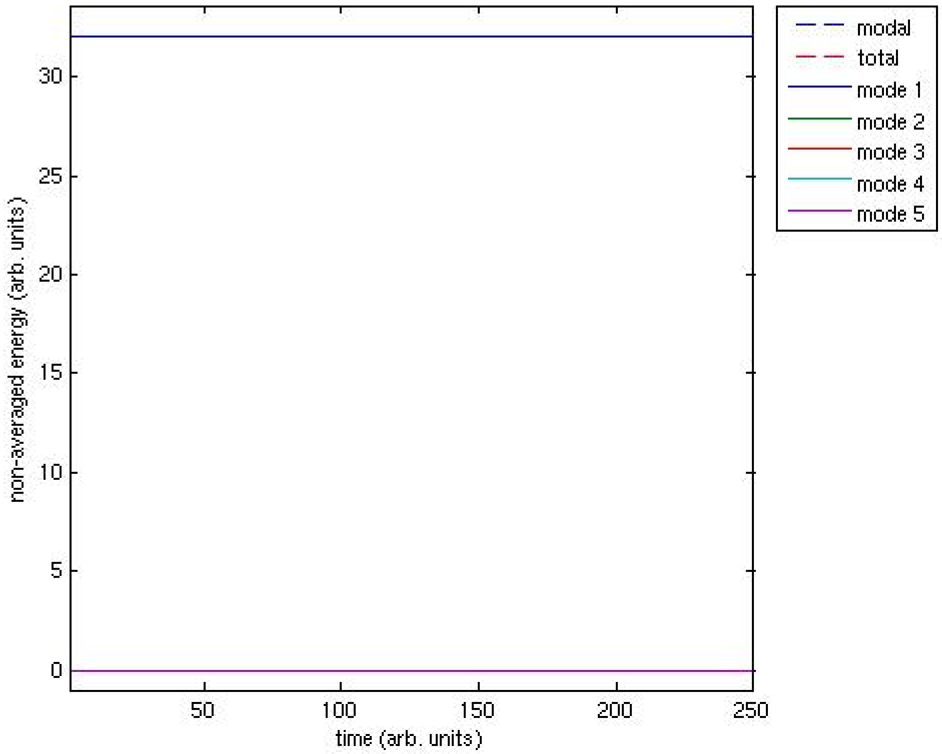
Non-linear system

can approximately be described by normal modes (weak non-linearity)

energy exchange between the modes

equipartition of the energy among the normal modes **?**

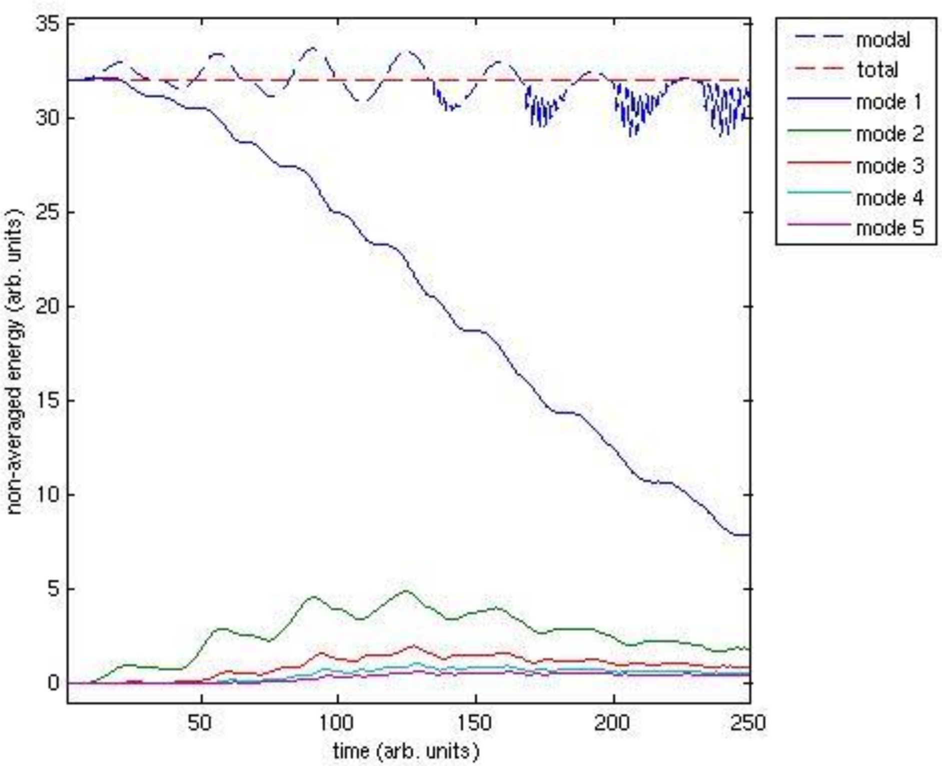
Harmonic system – numerical result



No equipartition of the energy

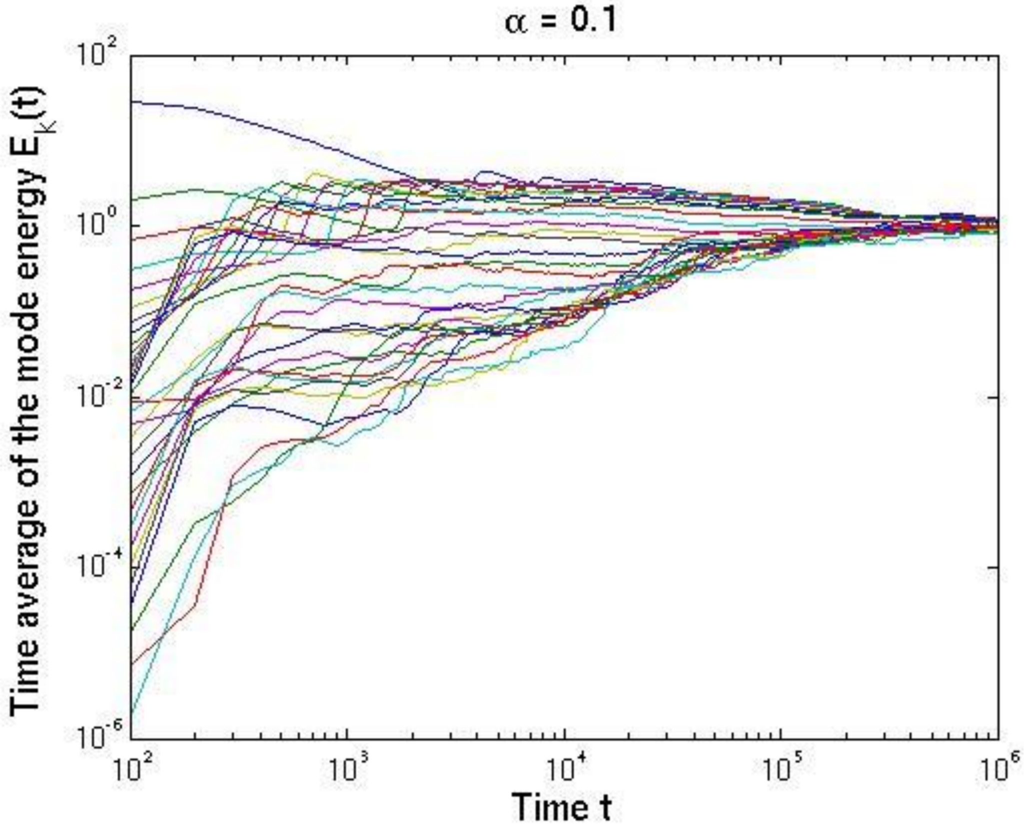
Anharmonic system – numerical result

$$\alpha = 0.1$$



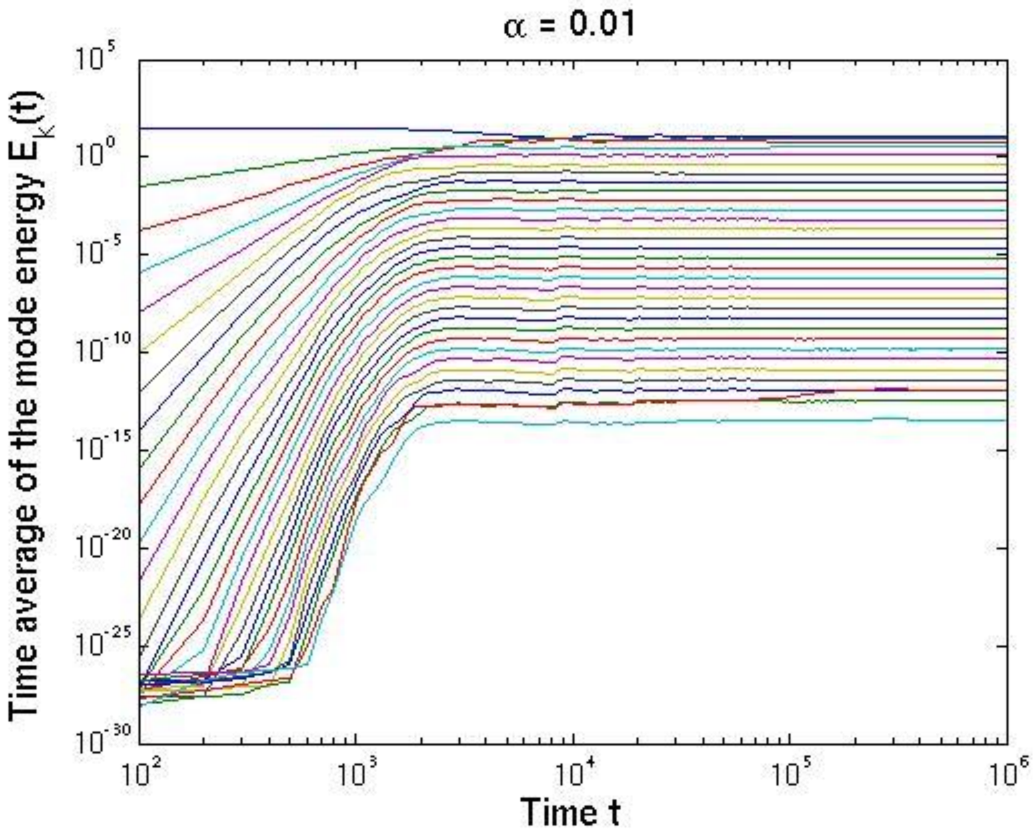
Equipartition of the energy ?

Anharmonic system – numerical result

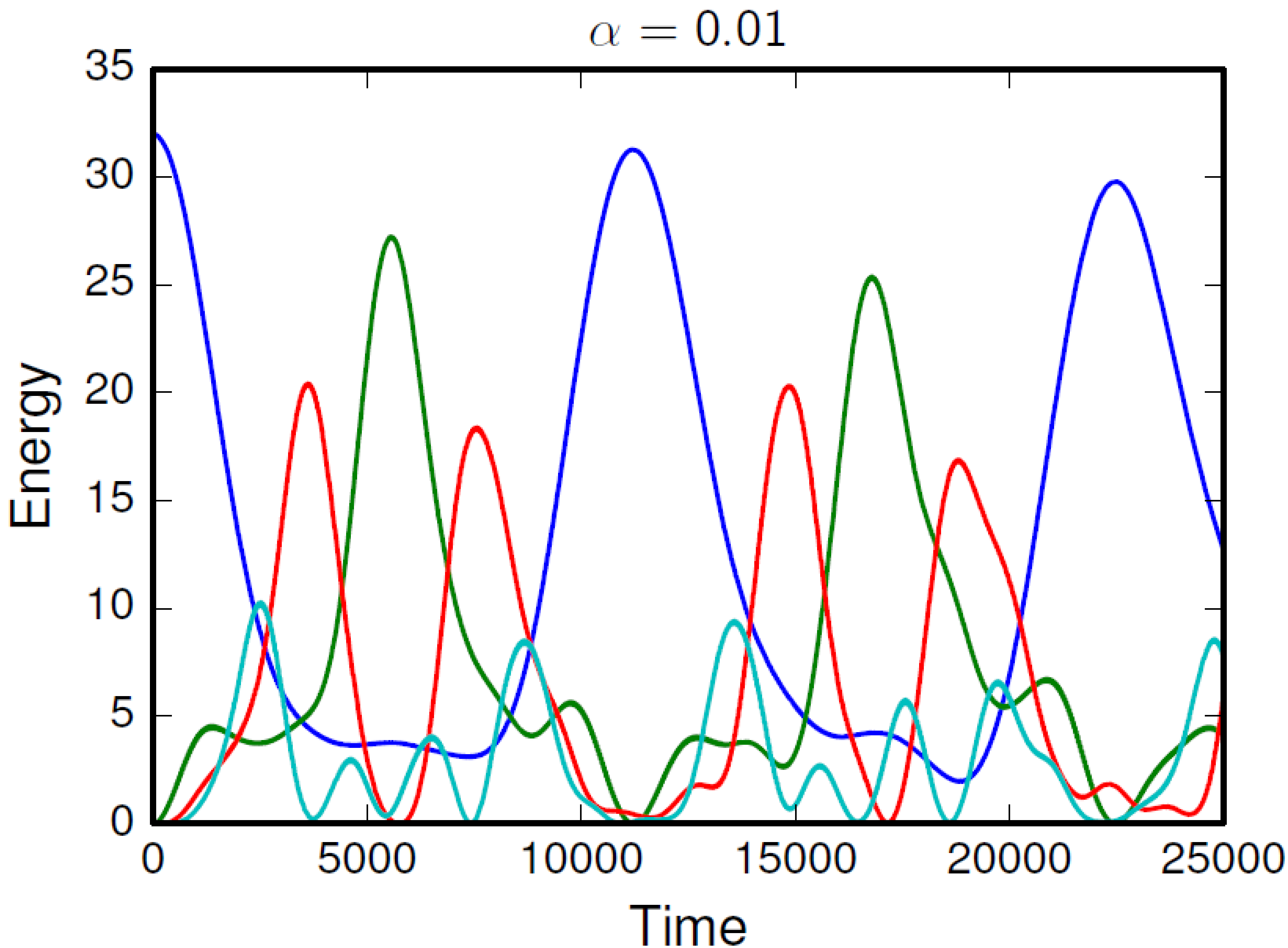


Equipartition of the energy !

Anharmonic system – numerical result



No equipartition of the energy !


$\alpha = 0.01$
35
30
25
20
15
10
5
0
Energy
0
5000
10000
15000
20000
25000
Time

Fermi-Pasta-Ulam model

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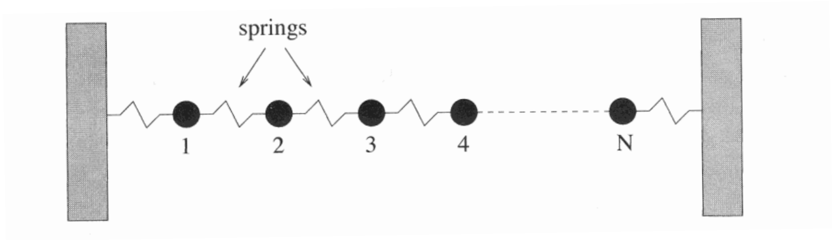

α-model

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Report written by Fermi, Pasta, and Ulam
Work done by Fermi, Pasta, Ulam, and Tsingou