Practical Assignment 5

Fermi-Pasta-Ulam and **Tsingou** Problem

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Computational Physics IV

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General Instructions

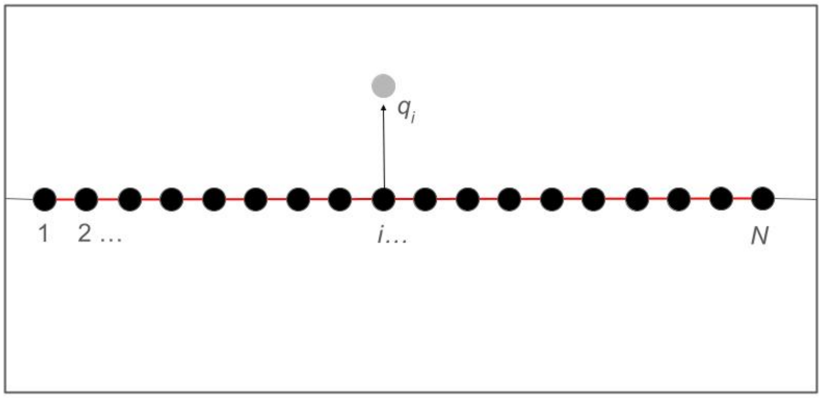
- Use any language you like. I recommend `FORTRAN` or C++.
- While writing a report include 3 sections.
- In section 1 describe your algorithm in natural language (not in programming language).
- In section 2 paste your code.
- In section 3 include your output figures, answer the questions in the last section, and describe what you learned in ≤ 250 words.
- Include axis labels, legends, and short comments on figures.
- Answer to the bonus question is not compulsory (nothing is) but would be desirable. You can find the relevant resources for yourself.

Question

The Fermi-Pasta-Ulam-Tsingou (FPU) problem studies a chain of coupled oscillators with weak nonlinear coupling. Consider the α–FPUT model discussed in Fermi et al. (1955)[1], with $N = 32$ oscillators of unit mass and fixed ends. Consider the following schematic which represents the system, black dots indicate the oscillators (1 through N). Each of these oscillators is connected to the adjacent oscillator with a nonlinear spring. Let q_i be the arbitrary displacement of the i^{th} oscillator. The Hamiltonian of such a system is naturally

$$H = \sum_{j=1}^{N} \frac{p_j^2}{2} + \frac{1}{2}\sum_{j=0}^{N}(q_{j+1} - q_j)^2 + \frac{\alpha}{3}\sum_{j=0}^{N}(q_{j+1} - q_j)^3.$$

[1] This is a report of a numerical experiment performed at the Los Alamos National Laboratory of the USA by scientists working on the Manhattan Project. The report was initially classified, but its counterintuitive result had already become a public knowledge before it eventually got declassified.



The equations of motion are

$$\ddot{q}_j = (q_{j+1} - 2q_j + q_{j-1}) + \alpha\Big[(q_{j+1} - q_j)^2 - (q_j - q_{j-1})^2\Big], \quad j = 1, \ldots, N.$$

With the fixed boundary conditions (i.e. $q_0 = q_{N+1} = 0$), the solution of above equations is a linear combination of normal modes which are [2][3]

$$\phi_{j,k} = \sqrt{\frac{2}{N+1}}\,\sin\Big(\frac{\pi k j}{N+1}\Big), \qquad k = 1, \ldots, N.$$

Project the displacements and momenta onto these basis functions:

$$Q_k(t) = \sum_{j=1}^{N} \phi_{j,k}\, q_j(t), \qquad P_k(t) = \sum_{j=1}^{N} \phi_{j,k}\, p_j(t).$$

The linear frequency of mode k is

$$\omega_k = 2\sin\Big(\frac{\pi k}{2(N+1)}\Big).$$

The (linear) modal energy is then

$$E_k(t) = \tfrac{1}{2}\Big(P_k(t)^2 + \omega_k^2 Q_k(t)^2\Big).$$

- Write a code that integrates the the equations of motion using any symplectic method (e.g., you can use Velocity Verlet algorithm Schloss (Schloss)).

[2] You can convince yourself of this statement by considering a system of only 2 oscillators, which also has two normal modes; the symmetric and antisymmetric mode. Any linear combination of these normal modes is a solution of this system.

[3] Although the list of authors in this paper only contains Enrico Fermi, John Pasta and Stanislav Ulam, much of the computational work was done by one Mary Tsingou who is acknowledged as merely a footnote in this paper. In several modern texts on the the problem Miss. Tsingou has been acknowledged duly.

- Initialize the system by exciting only the first mode:

$$q_j(0) = A\sin\left(\frac{\pi j}{N+1}\right), \quad p_j(0) = 0,$$

  with $A = 0.1$.

- Output 1: Compute the energy in each linear mode $E_k(t)$, and plot $E_1(t), E_2(t), E_3(t)$ versus time.

- Output 2: Produce a heatmap of normalized mode energies $E_k(t)/\sum_j E_j(t)$ with time on the X axis and mode index k on the Y axis.

- Output 3: Define the recurrence measure

$$R(t) = \frac{\sum_{k=1}^{N}\left(Q_k(t)Q_k(0) + P_k(t)P_k(0)\right)}{\sum_{k=1}^{N}\left(Q_k(0)^2 + P_k(0)^2\right)},$$

  where (Q_k, P_k) are modal coordinates. Plot $R(t)$ versus time, and estimate the recurrence time T_R.

Questions

1. How does the recurrence time T_R depend on the nonlinearity α?

2. If you start this system from some initial mode, does the energy dissipate to all available normal modes of the system irreversibly?

3. How is the behavior exhibited by the system paradoxical?

Bonus Question

How does KAM (Kolmogorove-Arnold-Moser) theorem resolves this paradox?

References

Fermi E., Pasta P., Ulam S., Tsingou M., 1955, Technical report, Studies of the nonlinear problems. Los Alamos National Laboratory (LANL), Los Alamos, NM (United States)

Schloss J., , Verlet Integration, https://www.algorithm-archive.org/contents/verlet_integration/verlet_integration.html