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E2 Nonlinear lattice oscillations

You will here consider the Fermi-Pasta-Ulam-Tsingou problem, or formely the Fermi-Pasta-Ulam problem. It was one of the first non-trivial problems that was studied using computers. Fermi and coworkers wanted to check the predictions of statistical mechanics on the thermalization of solids.

You will implement the model and study some of its behavior. You should solve the problems using the `C` language. For your convenience you can find a file, `E2code.c`, on the homepage to help you get started. You can adapt some of the files from E1 to help you here as well.

1 The Fermi-Pasta-Ulam-Tsingou problem

After the second world war Enrico Fermi and coworkers at Los Alamos 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. Fermi, Pasta, Ulam and Mary Tsingou [1] considered a vibrating string that included a non-linear term. To their surprise they found that the behavior of the system was quite different from what intuition would have led them to expect. Fermi thought that after many iterations, the system would exhibit thermalization, an ergodic behavior in which the influence of the initial modes of vibration fade and the system becomes more or less random with all modes excited more or less equally. Instead, the system exhibited a very complicated quasi-periodic behavior [2].

The *Fermi-Pasta-Ulam-Tsingou* (FPUT) experiment was important both in showing the complexity of nonlinear system behavior and the value of computer simulation in analyzing systems. It is also central in the theory of solitons. When considering the FPUT problem Zabusky and Kruskal [3] were able to explain the the periodic behavior in terms of the dynamics of localized excitations. They introduced the notion "solitons" for these waves with particle type of properties.

The FPUT model consists of a one-dimensional chain of masses connected with non-linear springs.

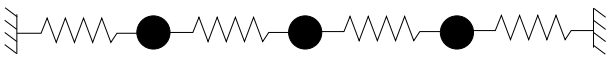

Figure 1: System of three coupled harmonic oscillators with fixed boundary conditions.

The so called α-model is defined by the Hamiltonian

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

where m is the mass of the particles, u_i the displacement of particle i from its equilibrium position, and p_i the corresponding momentum. The harmonic force constant is denoted by κ and α is a measure of the anharmonic coupling strength. The boundary conditions are $u_0 = u_{N+1} = 0$.

Task

1. Derive the corresponding equation of motion for $u_i(t)$. (0p)

For the Fermi-Pasta-Ulam-Tsingou problem it is convenient to put $m = \kappa = 1$, which then defines the dimensionless units that are used.

2 Harmonic case

In the harmonic case, with linear springs only ($\alpha = 0$), the problem can be solved analytically. The solution can then be expressed in terms of *normal modes*, the eigenvectors, according to

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

$$P_k = \sqrt{\frac{2}{N+1}} \sum_{i=1}^{N} \frac{p_i}{\sqrt{m}} \sin\left(\frac{ik\pi}{N+1}\right), \quad k = 1, \ldots, N$$

where the corresponding eigenfrequencies are given by

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

The inverse transforms are

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

$$p_i = \sqrt{\frac{2}{N+1}} \sum_{k=1}^{N} \sqrt{m} P_k \sin\left(\frac{ik\pi}{N+1}\right), \quad i = 1, \ldots, N$$

The Hamiltonian for the system

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

is then transformed to

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

which shows that the system can be described by N independent modes with energy

$$E_k = \frac{1}{2} \left[P_k^2 + \omega_k^2 Q_k^2 \right] \quad k = 1, \ldots, N$$

Task

2. Consider the harmonic case, $\alpha = 0$. Write a `C` program that solves the equation of motion and determines $u_i(t)$ and $p_i(t)$. This is similar to task 4 of E1.

   Implement the transformation between the ordinary coordinates u_i and p_i and the normal coordinates Q_k and P_k. On the homepage you find a `C` program (E2.c) that gives some hints regarding the transformation.

   Assume initial conditions $u_i(0)$ and $p_i(0)$ such that that all energy is initially localized in mode $k = 1$, i.e. $E_k(t = 0) = E_0\ \delta_{1k}$, and only kinetic, i.e. $P_k = \sqrt{2E_0}\ \delta_{1k}$ and $Q_k = 0\ \forall k$. Consider the case $N = 32$ and assume $E_0 = N$.

   Perform a simulation with time-step Δt=0.1 for the time span t_{max}=25 000. Plot $E_k(t)$, k=1,2,...,5. Verify that $E_k(t) = E_k(0)$, i.e. no energy transfer takes place among the normal modes. (1p)

3 Equipartition

The *equipartition theorem* in classical statistical mechanics states the *mean value of each independent quadratic term in the Hamiltonian is equal to* $k_B T/2$, where T is the temperature for the system [4]. This is derived using ensemble averaging. This implies that for the harmonic case above we have

$$\left\langle \frac{1}{2} P_k^2 \right\rangle_{ens} = \left\langle \frac{1}{2} \omega_k^2 Q_k^2 \right\rangle_{ens} = \frac{k_B T}{2} \ , \quad \forall k$$

and that the energy in each mode should be equal

$$\langle E_k \rangle_{ens} = k_B T \ , \quad \forall k$$

The *ergodic hypothesis* states that the ensemble average $\langle \ldots \rangle_{ens}$ and time average $\langle \ldots \rangle_{time}$ are equal and the ensemble average could then be obtained by performing a time average, by computing the time evolution of the system. This is obviously not true for the harmonic system above, the initial

distribution of the energy over the different modes will be kept for ever, no equipartition of the energy. It was then believed that any weak anharmonicity would introduce energy transfer between the modes and eventually equipartition the energy. This was precisely what Fermi and coworkers wanted to test using the FPUT model.

4 Anharmonic case

In the non-linear case, $\alpha \neq 0$, with the Hamiltonian

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

the solution is not known and the use of computer simulations becomes indispensable, as realized by Fermi and coworkers. The Hamiltonian can be transformed using the normal coordinates as

$$\mathcal{H} = \frac{1}{2} \sum_{k=1}^{N} \left[P_k^2 + \omega_k^2 Q_k^2 \right] + \frac{\alpha}{3} \sum_{k,l,m=1}^{N} c_{klm} Q_k Q_l Q_m \omega_k \omega_l \omega_m$$

The total energy is no longer exactly given by the sum of the energies in the different modes. However, Fermi *et al.* argued that for weak anharmonicity one expects to get equipartition of the energy among the different normal modes.

Task

3. Consider now the anharmonic case, $\alpha \neq 0$, and the two cases $\alpha = 0.01$ and $\alpha = 0.1$. Use the same setup as in Task 2 and present your results in the same way. In this case you should obtain energy exchange between the different modes. (1p)

4. Consider again the anharmonic case with $\alpha = 0.01$ and $\alpha = 0.1$, but now consider a considerably longer timespan, $t_{max} = 10^6$. In this case it becomes time-consuming to evaluate and save the energy in the various normal modes at each time-step and the output file becomes very large. Modify therefore your program so that the normal mode energies are calculated and saved only once for each 1000 time-steps. Determine the normal mode energies $E_k(t)$ at the corresponding times, i.e. at

   $$t_n = 1000\ n\ \Delta t\ , \qquad n = 1, 2, \ldots$$

   Compute the time-average of the normal mode energies

   $$\langle E_k \rangle_{time}(t) = \frac{1}{t} \int_0^t dt'\ E_k(t')$$

Plot your results for $\langle E_k \rangle_{time}(t)$ for all normal modes with logarithmic scale for both axis. Do you obtain equipartition of the energy? (2p)

Despite the fact that more than 60 years have passed since the Fermi-Pasta-Ulam-Tsingou problem was presented, it has not yet been fully understood [5].

A Code

```c
/*
 * Help routines for E2
 *
 * E2code.c
 */

#include <stdio.h>
#include <math.h>
#include <stdlib.h>
#define N_PARTICLES 32
#define PI 3.141592653589


/*
 * trans_matrix[N_PARTICLES][N_PARTICLES]: empty allocated array which
 * will be filled with sine transformation matrix
 * N_PARTICLES: number of particles in system
 */
void construct_transformation_matrix(
    double trans_matrix[N_PARTICLES][N_PARTICLES], int n_particles)
{
    double factor = 1 / ((double)n_particles + 1);
    for(int i = 0; i < n_particles; i++){
    for(int j = 0; j < n_particles; j++){
        trans_matrix[i][j] = sqrt(2 * factor)
                * sin((j + 1) * (i + 1) * PI * factor);
    }
    }
}

/*
 * Transformation matrix constucted in above function
 * q cartesian coordinate of paricles
 * Q output normal modes coordinate
 * N_PARTICLES is number of particles in system
 */
void transform_to_normal_modes(double trans_matrix[N_PARTICLES][N_PARTICLES],
                  int n_particles,
                  double *q, double *Q)
{
    for(int i = 0; i < n_particles; i++){
    double sum = 0;
    for(int j = 0; j < n_particles; j++){
        sum += q[j] * trans_matrix[i][j];
    }
    Q[i] = sum;
    }
}

int main()
{
    double trans_matrix[N_PARTICLES][N_PARTICLES];
    double q[N_PARTICLES];
    double Q[N_PARTICLES];

    construct_transformation_matrix(trans_matrix, N_PARTICLES);

    // Evolove system in time

    transform_to_normal_modes(trans_matrix, N_PARTICLES, q, Q);
    return 0;
}
```

References

[1] T. Dauxois, Physics Today **6**, 55 (2008).

[2] E. Fermi, J. Pasta, and S. Ulam, "Studies of Nonlinear Problems". Document LA-1940 (1955).
See also: http://en.wikipedia.org/wiki/Fermi-Pasta-Ulam_problem

[3] N. J. Zabusky and M. D. Kruskal, Phys. Rev. Lett. **15** 240 (1965).

[4] F. Reif, *Fundamental of Statistical and Thermal Physics* (McGraw-Hill, 1965).

[5] M. Onorato, L. Vozella, D. Proment, and Y. Lvov, PNAS **112** 4208 (2015).