Identifying Thermalization in Nonlinear Oscillating Systems with Chaotic Motion

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Introduction
The Fermi-Pasta-Ulam-Tsingou Problem

In 1955, E. Fermi, J. Pasta, S. Ulam, and M. Tsingou found that a multi-particle dynamic system with nonlinear forces does not reach thermal equilibrium [1,2].

To the side we illustrate an example of such a system, represented by masses and springs, attached to fixed ends.

\[ F = k \times x \]
\[ m\ddot{x}_j = k\left( x_{j+1}(t) + x_{j-1}(t) - 2x_j(t) \right) \]
7 masses in this sample trial oscillate due to coupled forces across a long period of time.
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Finding Thermalization
Lack of Thermalization through Fourier Analysis

In the absence of the nonlinear term ($\alpha = 0$), the energy of each Fourier mode is conserved [1,2], resulting in no thermalization. Perturbations do not break this integrable structure for long times.

In terms of the Fourier modes

$$Q_k(t) = \sqrt{\frac{2}{N}} \sum_{n=1}^{N} x_n(t) \sin \frac{\pi kn}{N}$$

the equations of motion may be written as

$$\ddot{Q}_k + \omega_k^2 Q_k = \alpha \sum_{i,j=1}^{N} C_{ij} Q_i Q_j$$

with the energy of each Fourier mode equaling

$$E_k = \frac{1}{2}(\dot{Q}_k^2 + \omega_k^2 Q_k^2)$$
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Lack of Thermalization through Energy Distribution Analysis

For an initial sine wave configuration of the masses, the lack of thermalization in a weakly nonlinear system ($\alpha \ll 1$) is evident through computation of the kinetic and potential energies (lack of equipartition).

\[
E = \frac{1}{2} m \dot{x}_i^2 + \frac{(x_{i+1} - x_i)^2}{2} + \frac{(x_i - x_{i-1})^2}{2}
\]
Numerical Computation
The quantity plotted is the energy (kinetic plus potential in each of the first five modes). The units for energy are arbitrary. \( N = 32 \); \( a = 1/4 \); \( 8t^2 = 1/8 \). The initial form of the string was a single sine wave. The higher modes never exceeded in energy 20 of our units. About 30,000 computation cycles were calculated.
10,000,000

Time points needed to be computed to find evidence of thermalization in small systems (Number of Masses < 200).
Updates—Trials and Distributions
Lack of Thermalization in Extended Trials with No Starting Velocity

Apparent thermalization at $10^{13}$ time units.

Some Error!
Lack of Thermalization in Extended Trials with *Added Starting Velocity*

- Apparent thermalization at $10^{10}$ time units.

[Graph showing energy distribution vs. time with high error noted.]
Fourier Energy Mode Comparisons—Without Velocity vs. With Velocity
Thermalization Behavior in Gases

The FPUT problem may be compared to the behavior of gases in a chaotic state, which follows these principles:

- Dispersed across a large area
- Not affected by potential or binding forces
- The average kinetic energy stays constant while the particles experience different velocity through collision.
- *Can be modeled with a Maxwell-Boltzman distribution*
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An early model of the velocity (kinetic energy) FPUT distribution shows that the Maxwell-Boltmann curve is not present.
The single-dimension FPUT problem does not carry gas-like thermalization properties.
Ideas to Further Project

- Calculate area under graph of velocity frequency distribution to find energy.
- Compute difference between two distributions, such as least squares difference.
- Create a velocity space map to analyse whether chaos is truly evident.
- Are the particles’ energy bounded, or do they vary with the system?
References

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