The Metastable State of the FPUT Problem

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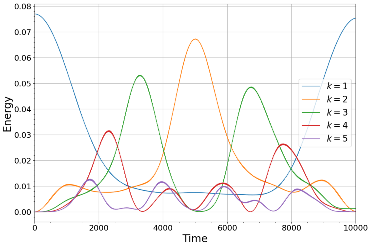
Introduction

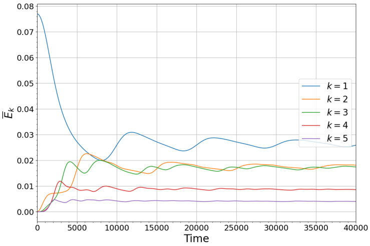
- The ergodic hypothesis has been a point of debate in physics for a long time.
- Regardless of the initial state of the system, we expect ergodic systems to achieve "thermal equilibrium": occupy the macro-state which has the highest amount of micro-states.
- These assumptions were challenged when in 1953 Enrico Fermi, John Pasta, Stanislaw Ulam, and Mary Tsingou (FPUT) numerically studied a chain of oscillators interacting non-linearly with each other.
- It is expected that if one mode of the system is initially excited, then the energy would flow to other modes over time and global equipartition would be achieved.

Introduction

- Surprisingly, the system exhibited near-periodic behavior; almost all the energy returns to the original mode.



(a) Original FPUT data for a system with 32 particles.



(b) Time averaged mode energies as a function of time.

Introduction

- The system seems to get locked in a state different than what is expected at thermal equilibrium. This "metastable" state relaxes to equilibrium over a much bigger timescale.
- Our goal is to study the metastable state and to understand its route to thermal equilibrium. We would like to understand how the timescale over which the metastable state breaks down depends on the system parameters.
- Another interesting question is whether there exists a critical energy below which the system does not thermalize. It is expected that in the thermodynamic limit, $N \to \infty$, this threshold should vanish, implying that all systems eventually reach equilibrium.

The (α and β) FPUT Model

- Consider a chain of oscillators with non-linear interactions:

$$H = \sum_{n=0}^{N} \frac{p_n^2}{2} + \frac{1}{2}(q_n - q_{n+1})^2 + \frac{1}{3}\alpha(q_n - q_{n+1})^3 + \frac{1}{4}\beta(q_n - q_{n+1})^4. \tag{1}$$

- This Hamiltonian can be transformed to the normal mode space $\begin{pmatrix} Q_k \\ P_k \end{pmatrix} = \sqrt{\frac{2}{N+1}} \sum_{n=0}^{N} \sin\left(\frac{nk\pi}{N+1}\right) \begin{pmatrix} q_n \\ p_n \end{pmatrix}$, to get:

$$H = \sum_{k=0}^{N} \frac{P_k^2 + \omega_k^2 Q_k^2}{2} + \frac{1}{3}\alpha \sum_{j,k,l=0}^{N} A_{jkl} Q_j Q_k Q_l + \frac{1}{4}\beta \sum_{j,k,l,m=0}^{N} B_{jklm} Q_j Q_k Q_l Q_m. \tag{2}$$

The (α and β) FPUT Model

- Energies $E_k = \frac{P_k^2+\omega_k^2 Q_k^2}{2}$ of individual modes are conserved in the linear system ($\alpha = \beta = 0$). Introduction of non-linear terms allows the energy to flow between different modes.
- The spectral entropy is a good measure to characterize how close the FPUT system is to equilibrium:

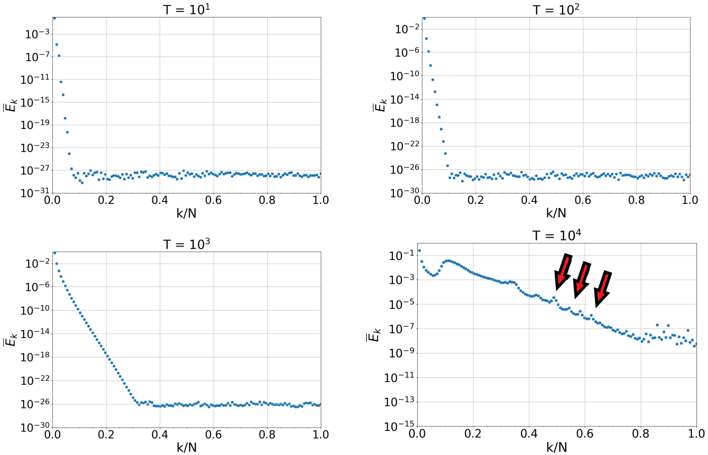
$$S(t) = -\sum_{k=1}^{N} e_k(t)\ln(e_k(t)), \quad e_k = \frac{E_k}{\sum_{k=1}^{N} E_k}. \qquad (3)$$

- This entropy goes from 0, when only one mode is excited, to $S_{\max}$ ($= \ln N$ for the α model) when equipartition is achieved. We therefore introduce the rescaled entropy which takes values between 0 and 1:

$$\eta(t) = \frac{S(t) - S_{\max}}{S(0) - S_{\max}}. \qquad (4)$$

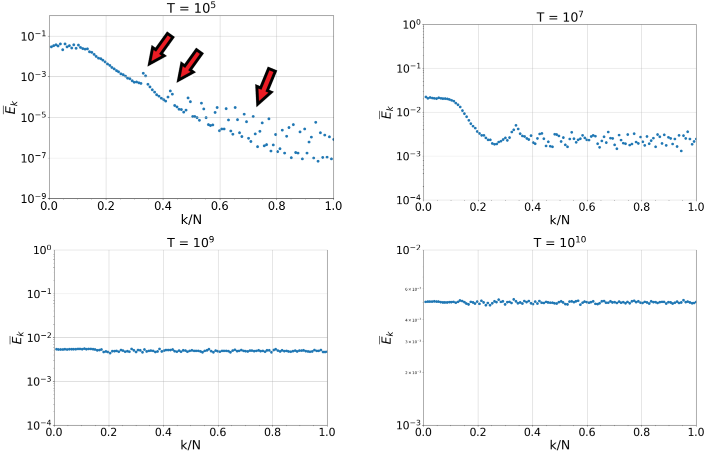
The Metastable State

- We study an FPUT system at two different energies.
- Spectral plots for $N = 127$, $\alpha = \beta = 0.25$, $E = 0.635$. The system quickly relaxes to a metastable state.



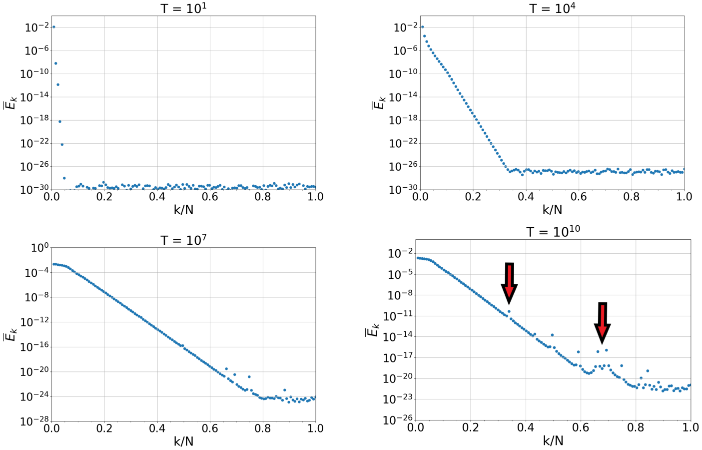
The Metastable State

- Note the "near-resonance" peaks. They lift the spectrum and allow the metastable state to relax to equilibrium over a larger time-scale.



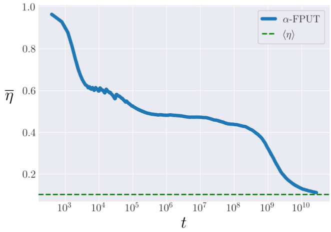
The Metastable State

- If we initialize the system with a smaller energy $E = 0.0127$, the system is locked in the metastable state for the whole time.

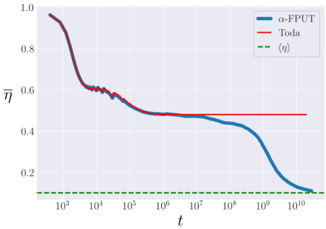


The Metastable State

- Plotting the spectral entropy as a function of time, it is clear when the metastable state starts to break down. This allows us to estimate the lifetime of a metastable state.



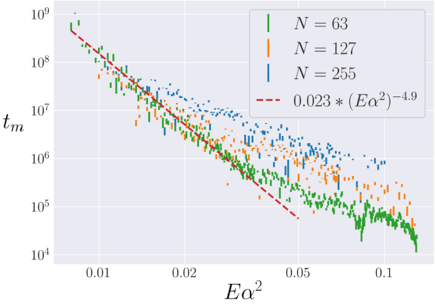
(a) Rescaled spectral entropy as a function of time for a 63 particle system with $E\alpha^2 = 0.02$.



(b) Comparison with the Toda model, which is an integralable approximation to the α-FPUT model.

The Metastable State

- The lifetimes of the metastable state in various systems are plotted as a function of $E\alpha^2$. For small $E\alpha^2$ (small energies, small non-linearities), the lifetime is independent of the system size. In this limit, the data is observed to follow a power law.



- It is hard to say whether this graph follows the power law below the energies plotted above, since these energies cannot be studied with current computational capabilities.

Conclusions and Further Questions

- FPUT systems have two timescales over which they relax to equilibrium. The system quickly gets locked into a metastable state, which then slowly moves towards equipartition.
- Resonances give rise to local peaks in the FPUT spectrum. These resonances then diffuse energy to near-by modes, resulting in the spectrum being lifted. Could be explained by the 4 and 6 wave resonances proposed by Lvov [BHLO19].
- Lifetime of the metastable state was measured by comparing it with the Toda model. Increasing energy/non-linearity hastens the breakdown of the metastable state. At small energies the lifetime is independent of system size. Cannot say whether there exists a critical energy threshold.
- Flach, et al [FIK06] have shown the existence of q-breathers in FPUT systems, which are special periodic states. We would like to understand how they affect the evolution of the metastable state.

Acknowledgments

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