Behavior and Breakdown of Higher-Order FPUT Recurrences

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Abstract

Using computer-based simulations, we investigate the existence and behavior of higher-order recurrences (HoR)s in two Fermi Pasta Ulam Tsingou (FPUT) models (called "alpha" and "beta"). These HoRs include the previously known super-recurrences [2] but also involve others, such as "super-super-recurrences". We find that the HoR periods scale non-trivially with energy due to apparent singularities (points where the period blows up). We study these singularities and their subtle differences in the two models. As the initial energy is increased, the breakdown mechanisms of the super-recurrences are found to differ in the two models. In the beta-FPUT model, the breakdown of super-recurrences is associated with the system's approaching equilibrium. In the alpha-FPUT model, the super-recurrences breakdown by losing their shape until they no longer form, while the system is still not at equilibrium.

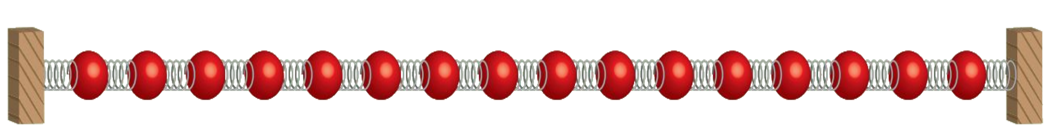


Fig 1: FPUT model, consisting of N masses connected with *nonlinear* springs

Source: Porter, Mason A., et al. "Fermi, Pasta, Ulam and the Birth of Experimental Mathematics, " *American Scientist* 97.3 (2009): 214-221, figure 2

Introduction

In 1953, Fermi, Pasta, Ulam, and Tsingou (FPUT) considered models consisting of masses connected by nonlinear springs, shown in figure 1. For low energies, contrary to the equipartition theorem of statistical mechanics, the energy was shared among only a few normal modes, and there were remarkable near-recurrences to the initial state [2]. Longer computer-time runs later showed the existence of super-recurrences, in which a still greater proportion of the initial energy returned to the initial state [1]. Furthermore, FPUT-like recurrences and super-recurrences have been studied in numerous other models. They have been experimentally observed and studied in deep water-waves, optical fibers, and feedback ring systems. While FPUT recurrences and the questions they raise about how equilibrium is actually approached continue to challenge researchers today, super-recurrences themselves have been the focus of few studies.

The Hamiltonian of the two models ("alpha" and "beta") are

$$\mathcal{H}_\alpha = \sum_{n=1}^{N}\frac{p_n^2}{2} + \sum_{n=0}^{N}\frac{1}{2}(q_{n+1}-q_n)^2 + \frac{\alpha}{3}(q_{n+1}-q_n)^3$$

$$\mathcal{H}_\beta = \sum_{n=1}^{N}\frac{p_n^2}{2} + \sum_{n=0}^{N}\frac{1}{2}(q_{n+1}-q_n)^2 + \frac{\beta}{4}(q_{n+1}-q_n)^4$$

where N is the number of masses, q is the position of mass n, and p is its momentum. To study the normal mode dynamics of the many-body system, we use the canonical transform ,

$$\begin{bmatrix} q_n \\ p_n \end{bmatrix} = \sqrt{\frac{2}{N+1}}\sum_{k=1}^{N}\begin{bmatrix} Q_k \\ P_k \end{bmatrix}\sin\left(\frac{nk\pi}{N+1}\right)$$

Finally, rescaling Q and P allows the model to be studied with

$$\mathcal{H}_{\beta=1}(Q,P) = \beta E$$

$$\mathcal{H}_{\alpha=1}(Q,P) = \alpha^2 E$$

Results

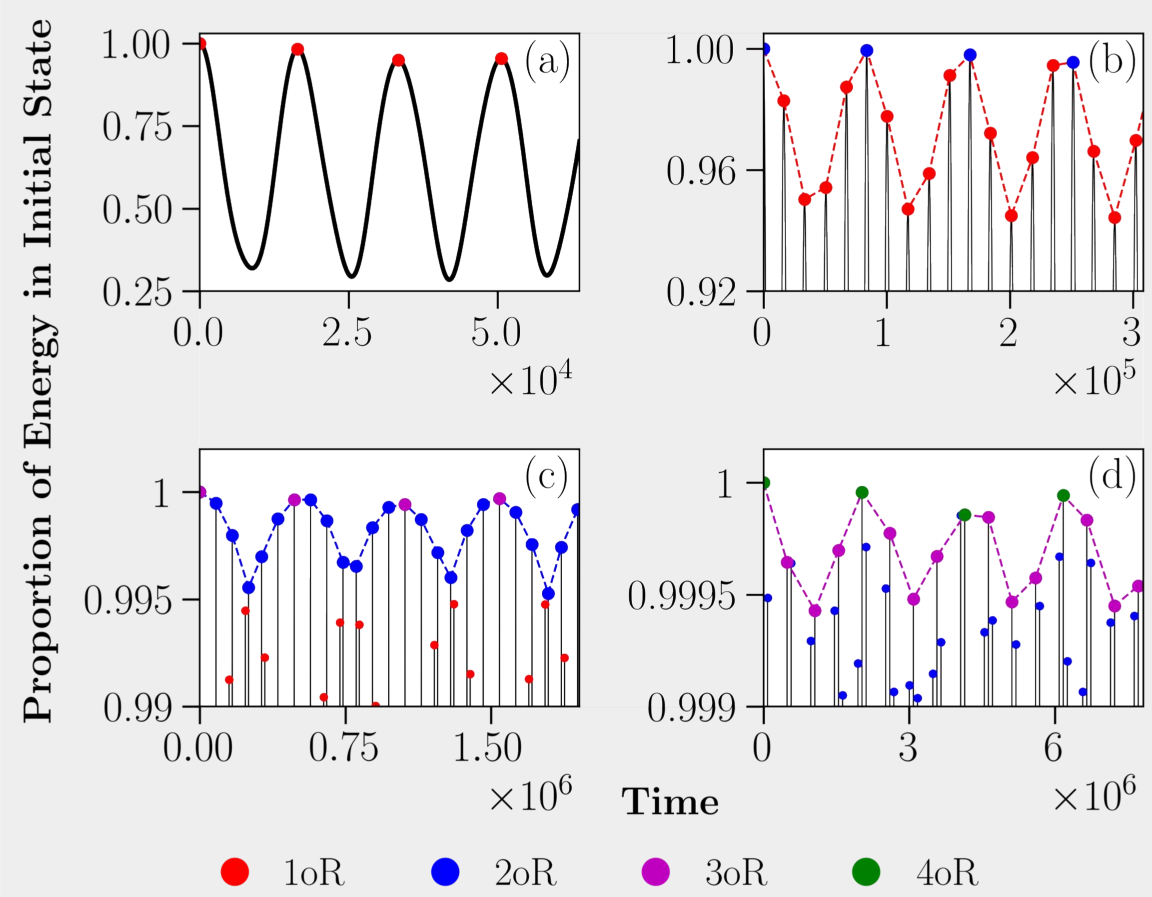


Fig 2. The proportion of energy in the initial state is shown, revealing the HoRs in the alpha FPUT lattice ($E\alpha^2$=4.35x10⁻⁴ and N=31). We call the FPUT recurrences 1oR, super-recurrences 2oR, etc: (a) 1oRs in red, (b) 2oRs in blue, (c) 3oRs in purple, and (d) 4oRs in green. We find similar results for the beta model

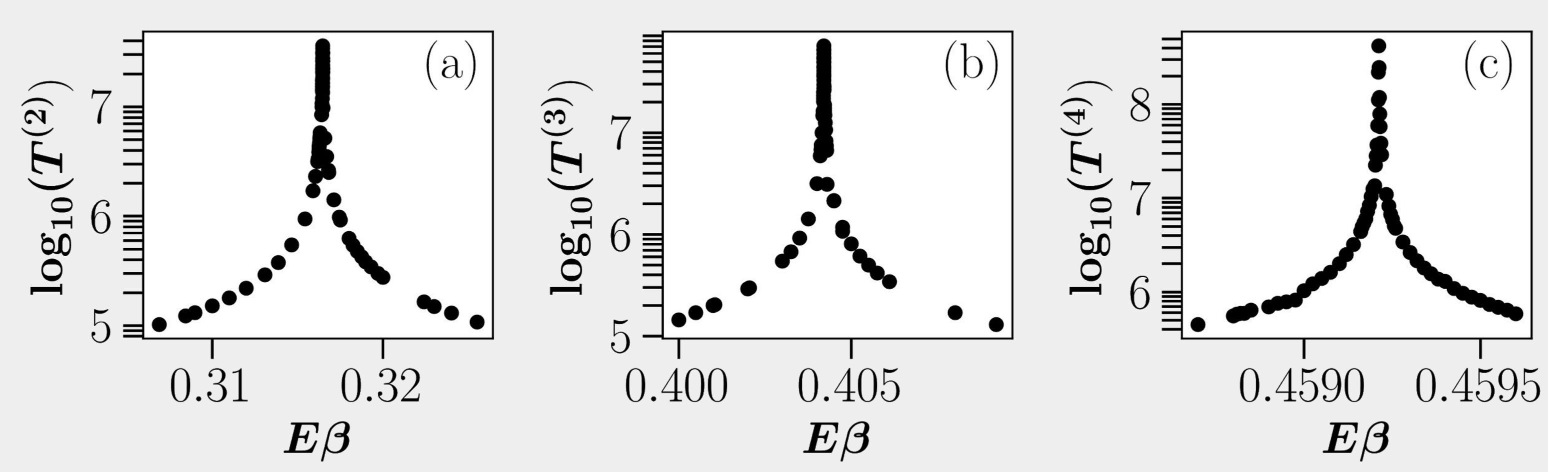


Fig 3. Apparent singularities in the (a) 2oR-period and (b) 3oR-period, and (c) 4oR-period for the beta-FPUT lattice with N=31. Similar results were found in the alpha model, but in the alpha model the 2oRs did not exhibit these singularities

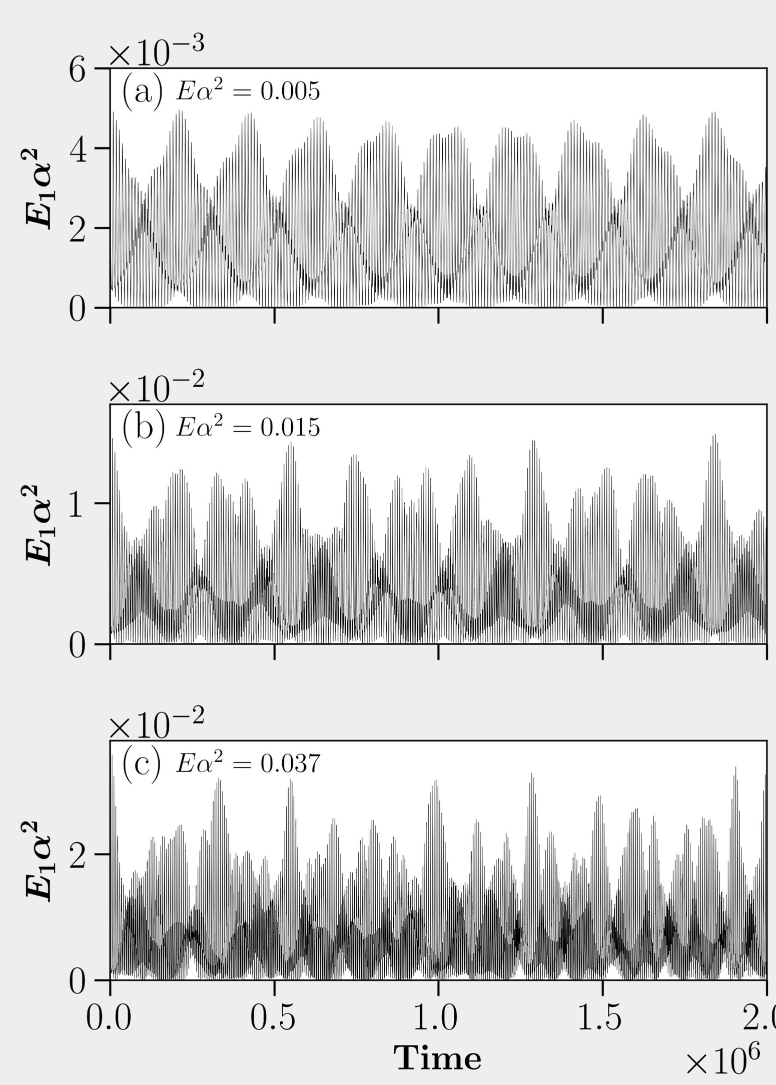


Fig 4. The break down of 2oRs for the alpha-FPUT model. Increasing energy causes the 2oRs to lose their shape on a very short time scale and thus never truly form.

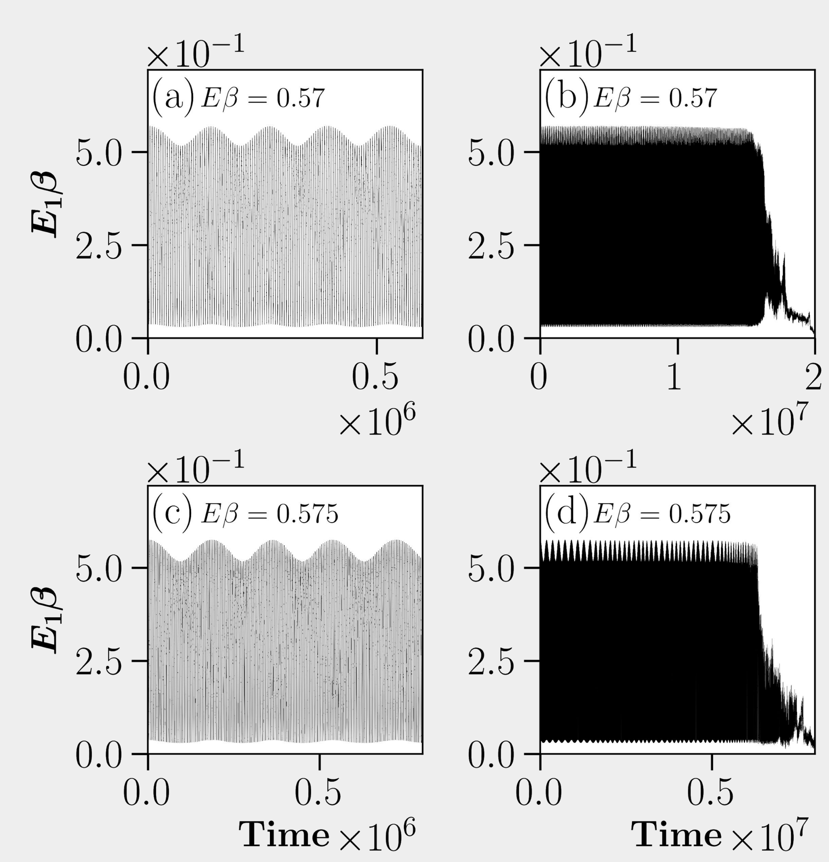
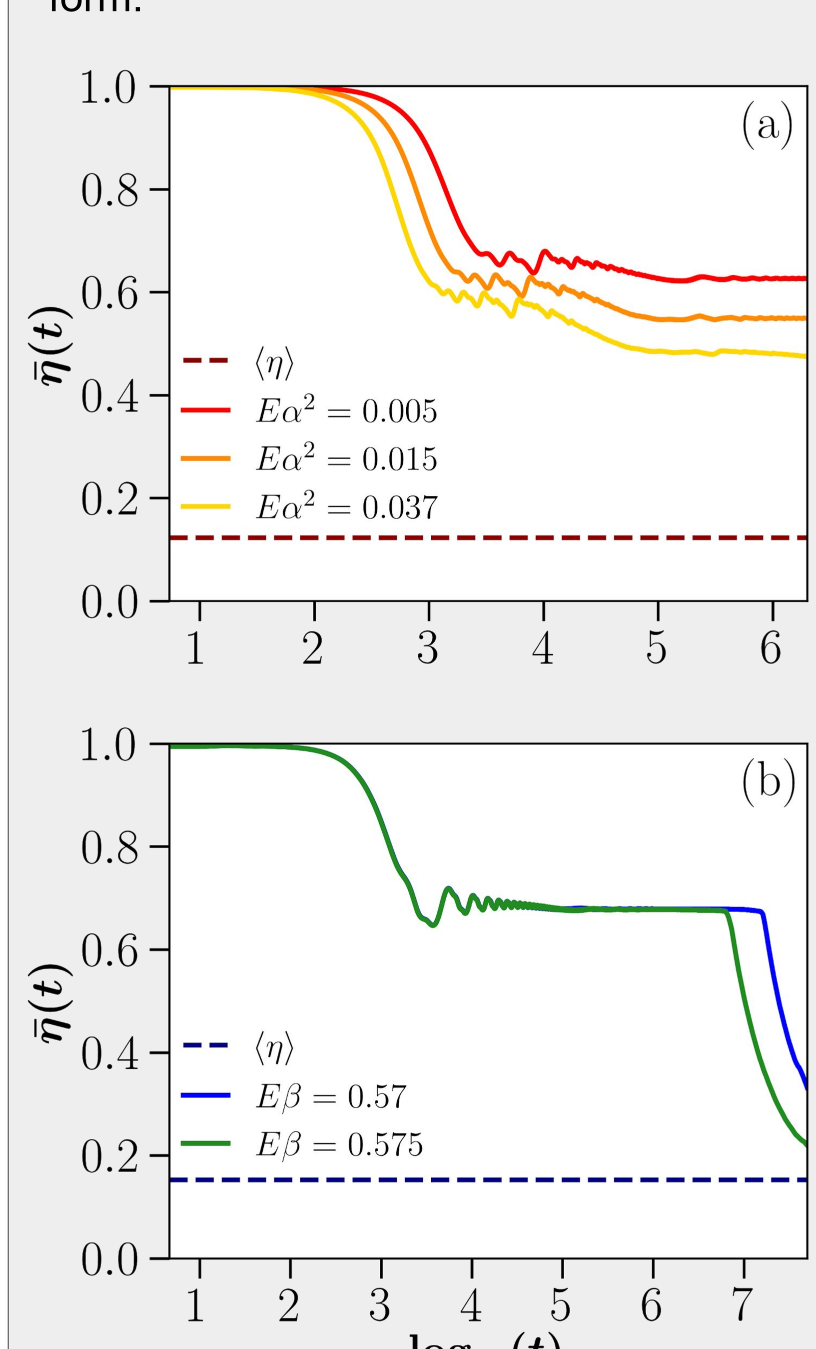


Fig 5. Shows breakdown of 2oRs in the beta-FPUT model. Parts a and c show the 2oRs, while parts b and d show a longer timescale where they break down.



In order to study the relationship between the 2oR breakdown and approach to equilibrium, we utilize what is known as the spectral entropy, which is given by

$$S(t) = -\sum_{k=1}^{N} e_k \ln(e_k)$$

where

$$e_k(t) = E_k(t)/\sum_k E_k(0)$$

Then, it is common to rescale it and study,

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

Fig 6. The time averaged, rescaled spectral entropy for the parameters considered in Figs 4 and 5. The breakdown of 2oRs in the (a) alpha-FPUT model is not associated with an approach to equilibrium, while it is for the (b) beta-FPUT lattice. The plateau exhibited in the graphs shows what is called the "metastable" state, which prevents reaching equilibrium, which is shown by the dashed line.

Numerical Methods

We solved Hamilton's equations, which describe how the system changes in time, numerically using the SABA2C integrator [3]. This is a symplectic integrator, which means it conserves energy, which is essential for Hamiltonian mechanics. We wrote these computer-based simulations in Fortran 90, computed them on the Shared Computer Cluster (SCC), and created the graphics using Matplotlib in Python. This integration scheme introduced a relative error in the energy of about 10^{-9}, ensuring numerical energy conservation. Furthermore, to test the time-reversal symmetry of classical mechanics, we ran the codes backwards in time to ensure that energy was properly returned to the initial state.

Conclusion

While FPUT recurrences and the questions they raise about the approach to equilibrium continue to be an active area of research today, the nature of super-recurrences themselves have been the focus of few studies. Using computer-based simulations, this study represents a considerable extension of the pioneering work of Tuck and Menzel on super-recurrences [1]. We found that the HoR periods to scale non-monotonically and non-trivially due to the existence of apparent singularities, which we conjecture are caused by nonlinear resonances. These apparent singularities have been observed in both models, but we have not observed any in the alpha model's super-recurrences.

Furthermore, for the system to thermalize, there must have been a breakdown of FPUT recurrences and therefore any other HoRs beforehand. Increasing the energy to see this breakdown, we found that the breakdown mechanisms of 2oRs differ between the two models. The breakdown in the beta- model occurs abruptly, while for the alpha model, the 2oRs lose their shape until they no longer form. Also, using the spectral entropy, we showed that the breakdown of 2oRs in the beta model is associated with the system's approaching equilibrium, while in the alpha model, the degrading of the 2oRs shape does not lead to immediate thermalization.The interesting differences between the alpha and beta models provide further evidence of the subtleties involved in the approach to equilibrium in classical many-body systems.

In this study, the initial state was fixed to include only the first mode. An interesting extension would be to see if one observes the same phenomena observed in this study in other long-wavelength initial states, such as initial involving only even normal mode states in the beta-FPUT model and linear combinations of even and odd normal mode states.

References

[1] Tuck, J. L., and M. T. Menzel. "The superperiod of the nonlinear weighted string (FPU) problem." Advances in Mathematics 9.3 (1972): 399-407.

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[3] Laskar, Jacques, and Philippe Robutel. "High order symplectic integrators for perturbed Hamiltonian systems." Celestial Mechanics and Dynamical Astronomy 80.1 (2001): 39-62.