Behavior and Breakdown of Higher-Order FPUT Recurrences

Salvatore Pace

(Work in collaboration with David Campbell)

The Ergodic Hypothesis

- Boltzmann [1] stated the ergodic hypothesis: over a long period of time, a trajectory will cover all of phase space. Thus, for an ergodic system, statistical mechanics weighted averages over phase space should converge to time averages of the observable.
- In the 1950s, Fermi, Pasta, Ulam and Tsingou (FPUT) wanted to study how ergodicity would be approached for a system with far from equilibrium with a small nonlinearity allowing weak energy sharing between degrees of freedom.

[1] Boltzmann, Ludwig. "Ueber die mechanischen Analogien des zweiten Hauptsatzes der Thermodynamik." *Journal für die reine und angewandte Mathematik* 100 (1887): 201-212.

FPUT Lattice

Canonical coordinate and momenta Hamiltonian:

- α-model: $H_\alpha(\boldsymbol{q},\boldsymbol{p}) = \sum_{n=1}^{N} \frac{p_n^2}{2} + \sum_{n=0}^{N} \frac{1}{2}\left(q_{n+1}-q_n\right)^2 + \frac{\alpha}{3}\left(q_{n+1}-q_n\right)^3$
- β-model: $H_\beta(\boldsymbol{q},\boldsymbol{p}) = \sum_{n=1}^{N} \frac{p_n^2}{2} + \sum_{n=0}^{N} \frac{1}{2}\left(q_{n+1}-q_n\right)^2 + \frac{\beta}{4}\left(q_{n+1}-q_n\right)^4$

Boundary Conditions

$$q_0 = q_{N+1} = 0$$

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Normal mode coordinate and momenta Hamiltonian:

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Canonical Transformation

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

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

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Rescale phase space:

$$(\boldsymbol{Q},\boldsymbol{P}) \to (\boldsymbol{Q}/\alpha, \boldsymbol{P}/\alpha) \quad \Longrightarrow \quad H_{\alpha=1}(\boldsymbol{Q},\boldsymbol{P}) = \alpha^2 E$$

$$(\boldsymbol{Q},\boldsymbol{P}) \to (\boldsymbol{Q}/\sqrt{\beta}, \boldsymbol{P}/\sqrt{\beta}) \quad \Longrightarrow \quad H_{\beta=1}(\boldsymbol{Q},\boldsymbol{P}) = \beta E$$

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FPUT Problem

STUDIES OF NON LINEAR PROBLEMS

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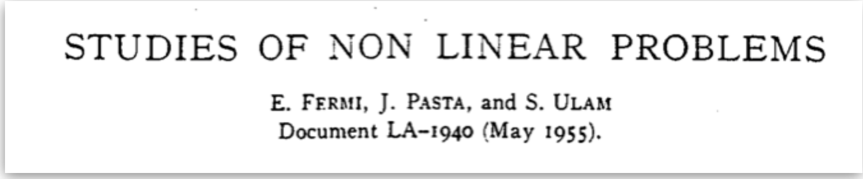
Document LA-1940 (May 1955).

- Expectation: Energy would be equipartioned among normal modes (prediction by equilibrium statistical mechanics).

FPUT Problem



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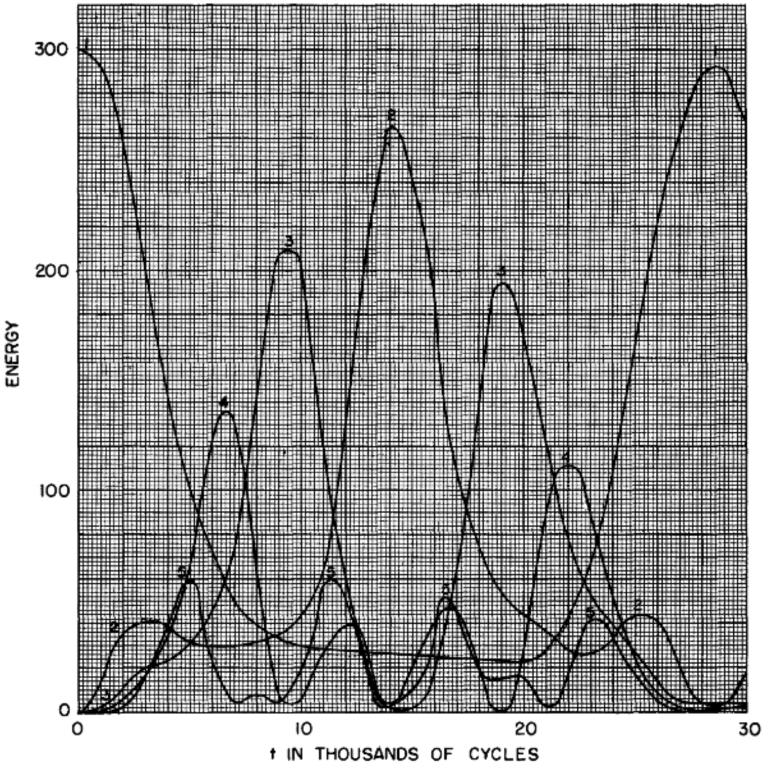
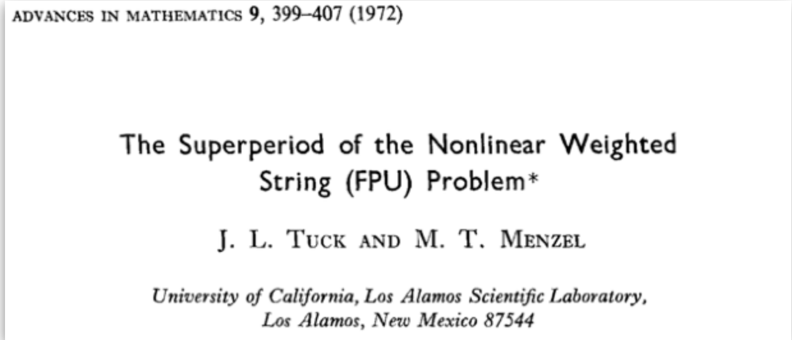
- Numerical Observation: For long-wavelength, low energy initial state, energy shared only among the lowest normal modes and remarkable near-recurrences to the initial state



Fermi, E., Pasta, J. and Ulam, S "Studies of the nonlinear problems," No. LA-1940. Los Alamos Scientific Lab., N. Mex., 1955. Republished in p. 978-98 of The Collected Papers of Enrico Fermi, Vol 2 f E. Segré, Chairman of the Editorial Board, University of Chicago Press, 1965

Super-Recurrences



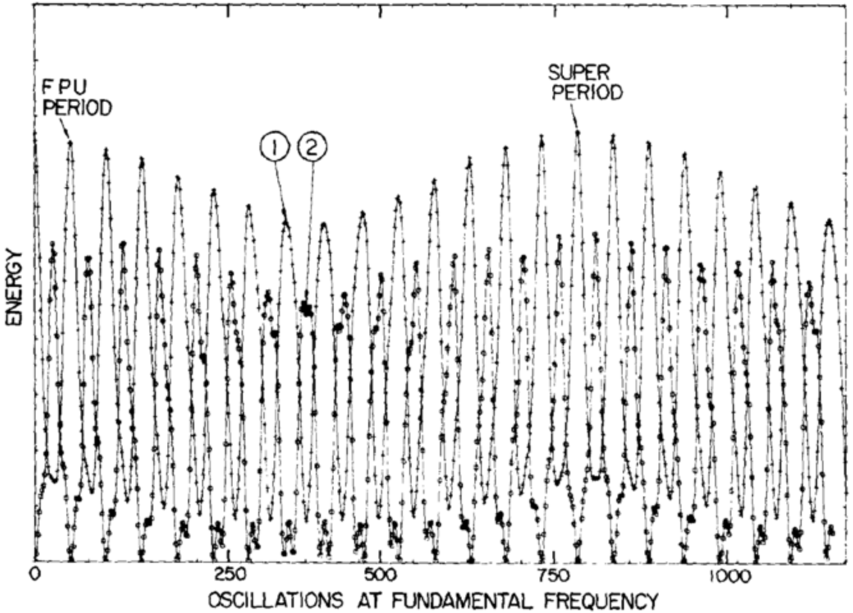
ADVANCES IN MATHEMATICS 9, 399–407 (1972)

The Superperiod of the Nonlinear Weighted String (FPU) Problem*

J. L. Tuck and M. T. Menzel

University of California, Los Alamos Scientific Laboratory, Los Alamos, New Mexico 87544

- First Objection to original FPUT results: Run it longer!
  - Longer numerical integration times showed the existence of *super-recurrences*



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Previous studies on Super-recurrences

SOME MORE OBSERVATIONS ON THE SUPERPERIOD OF THE NON-LINEAR FPU SYSTEM

G.P. DRAGO and S. RIDELLA
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Received 23 October 1986; revised manuscript received 13 March 1987; accepted for publication 9 April 1987
Communicated by A.P. Fordy

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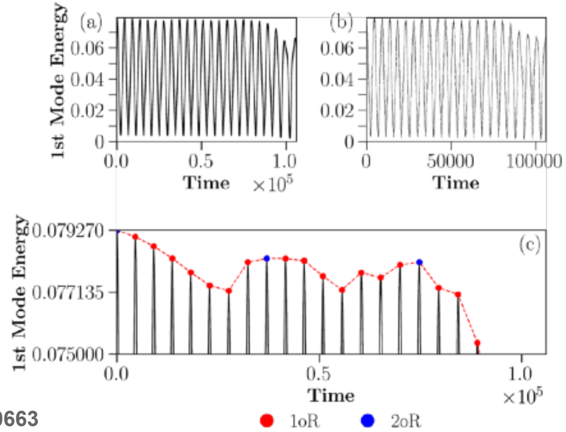

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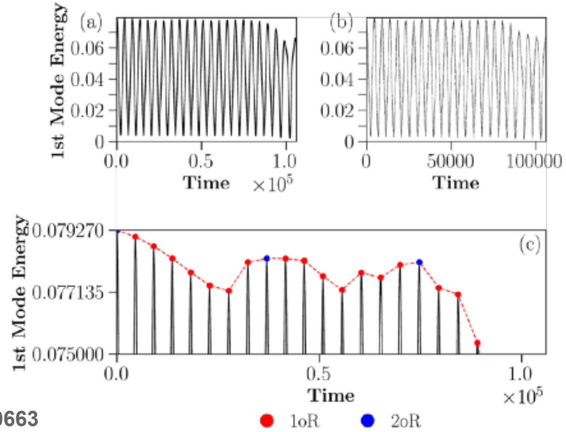

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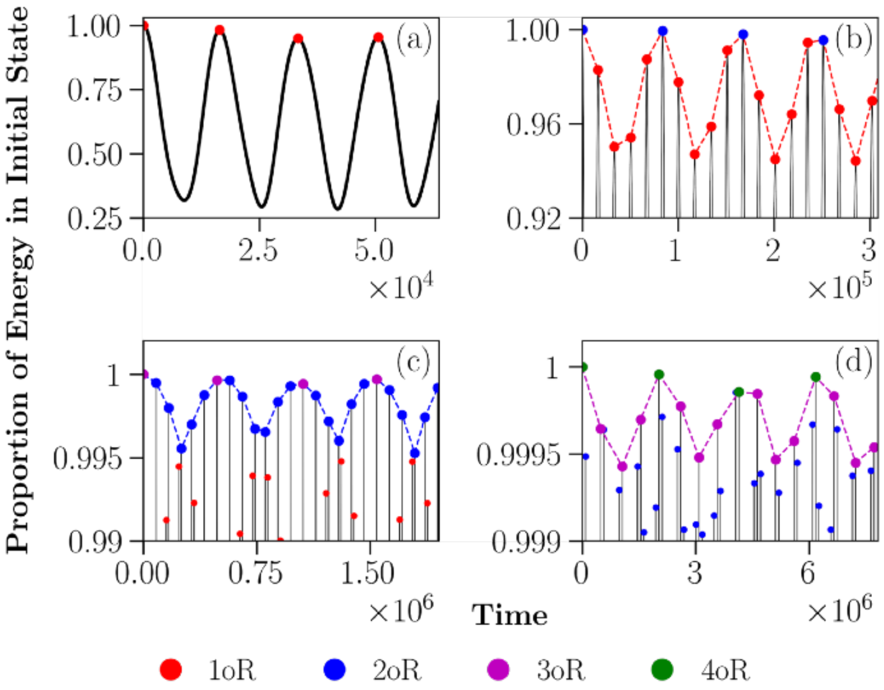
- Shifted perturbation scheme:
  - Expand: $Q_k = \sum_{n=0}^{\infty} Q_{k,n}\alpha^n$
  - Nonlinear Frequency: $\Omega_k^2 = \omega_k^2 + \sum_{n=1}^{\infty} \mu_{k,n}\alpha^n$
- Super-recurrencess in α-model are due to a beat-like mechanism from different resonances among nonlinear frequencies.
- Could not find general explanation for super-recurrence in β-model
- Proposed higher-order recurrences could exist, but they couldn't find any analytically or numerically.

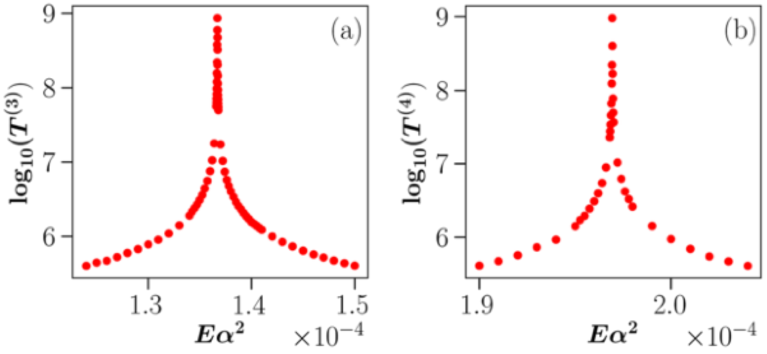
Existence Higher-order recurrences (HoR)s

- Terminology:
    - 1st order recurrence (1oR) - Original FPUT recurrence
    - 2nd order recurrence (2oR) - Tuck and Menzel's super-recurrence
    - 3rd order recurrence (3oR) - "super-super-recurrence"
- Higher-order recurrences are increasingly subtle, but seen in both α and β-model

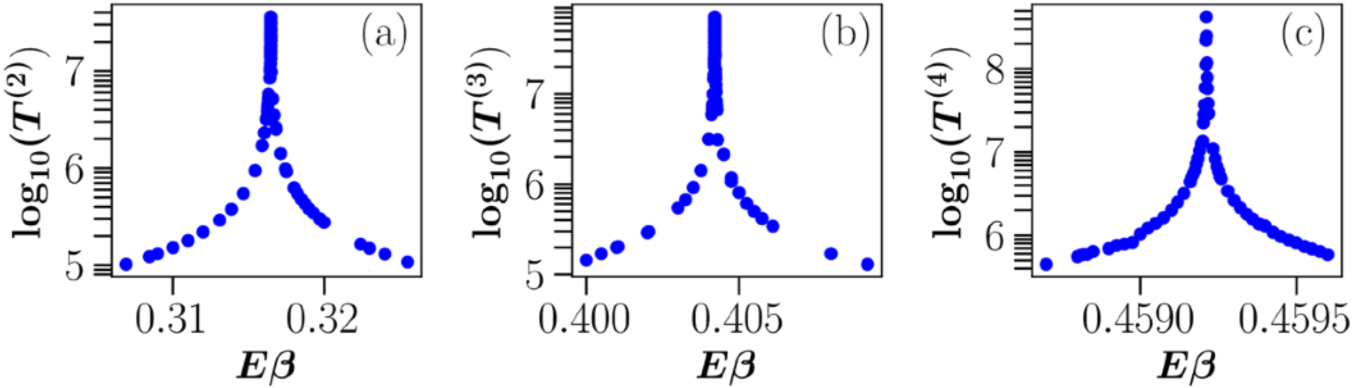


Nontrivial energy scaling of HoR times

- Apparent singularities in HoR times which depend sensitive on energy and nonlinear parameter
  - Thought to be caused by near resonance between nonlinear normal modes.



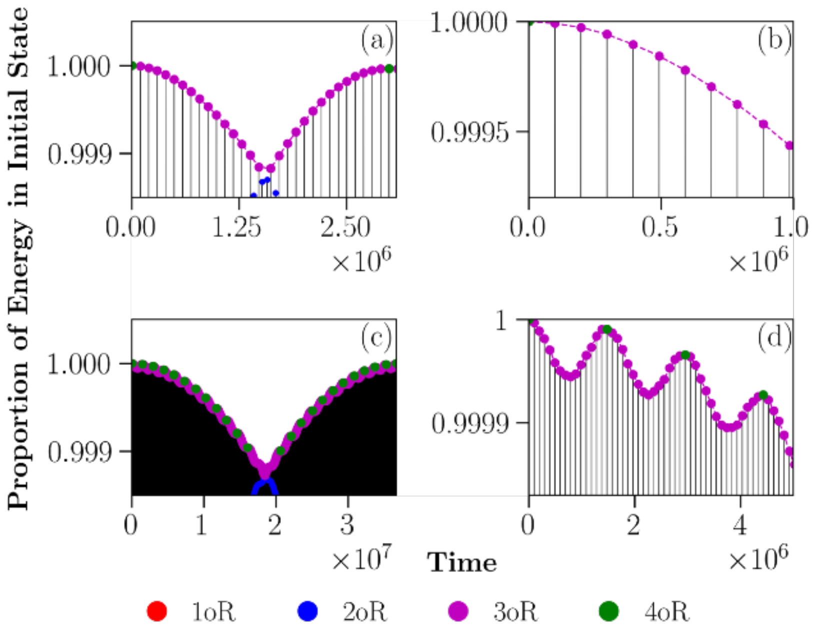
- α-model's 2oRs do not exhibit singularities, while β-model does.



Behavior at singularities

At energies where HoR time blow up, new HoRs are formed

- These “new” HoRs have shorter periods than the HoRs which have their HoR time blowing up.
- Seen in both the α-model and β-model.



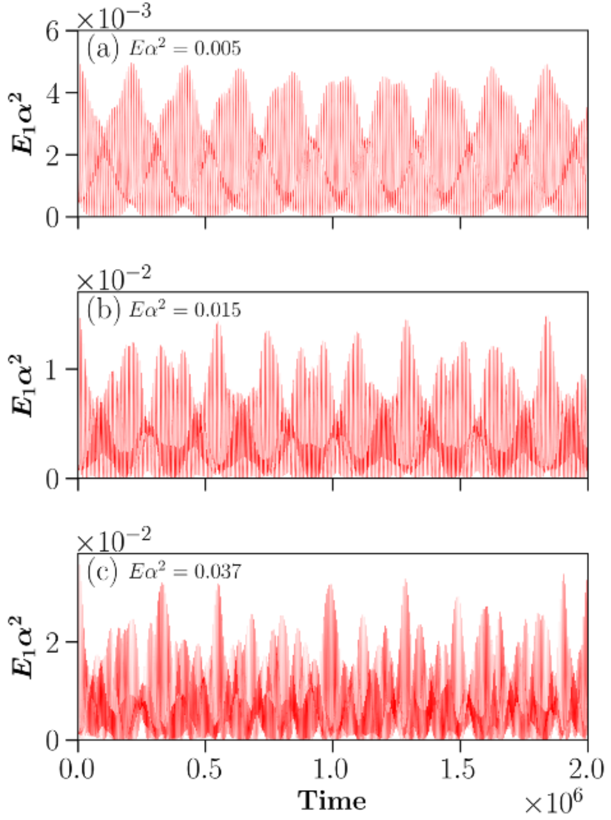
Thermalization time scales and metastability

- For long-wavelength initial conditions, there exists different timescales for the rate of thermalization
  - Strong-stochastic threshold [1]: A threshold between “weak” and “strong” chaos which changes the thermalization timescales
- Metastable state [2]: Below a certain energy, there exists an apparent stationary state that causes the FPUT lattice to thermalize on a much slower timescale.
- Does the breakdown of the HoRs mean the breakdown of this quasi-stationary state?

[1] Benettin, Giancarlo, et al. "The fermi—pasta—ulam problem and the metastability perspective."
[2] Pettini, Marco, et al. "Weak and strong chaos in Fermi–Pasta–Ulam models and beyond."

Breakdown of 2oRs in α-model

- Increasing energy causes 2oRs structure to degrade
  - Larger energy = greater degradation
  - Occurs at very short time scales.



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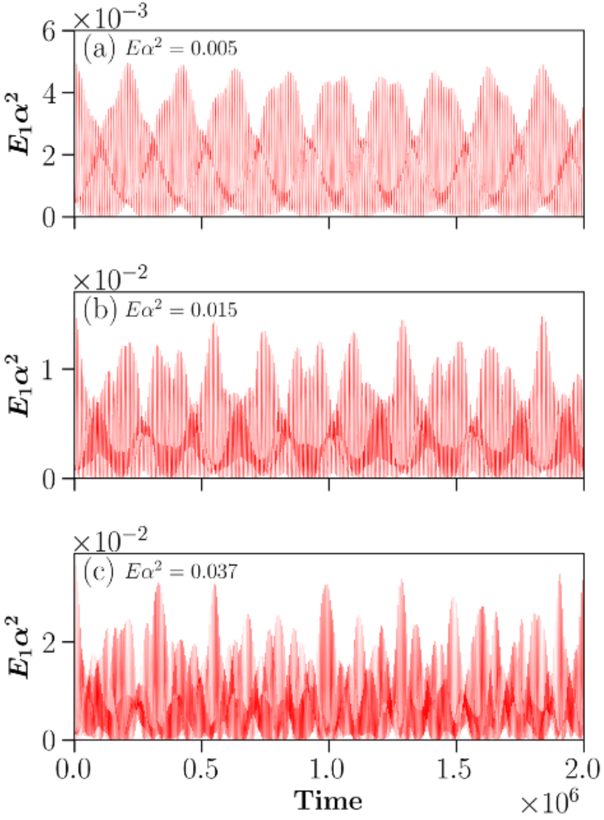
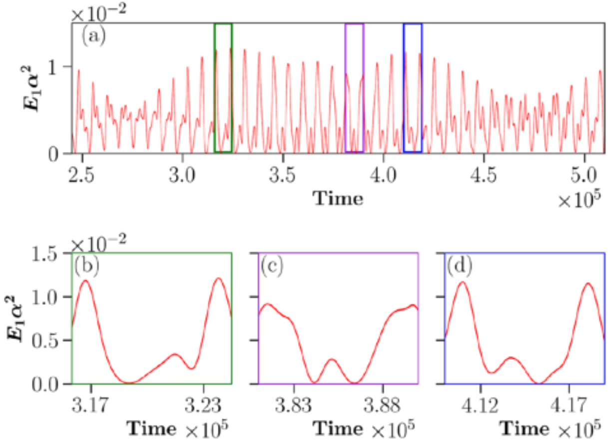
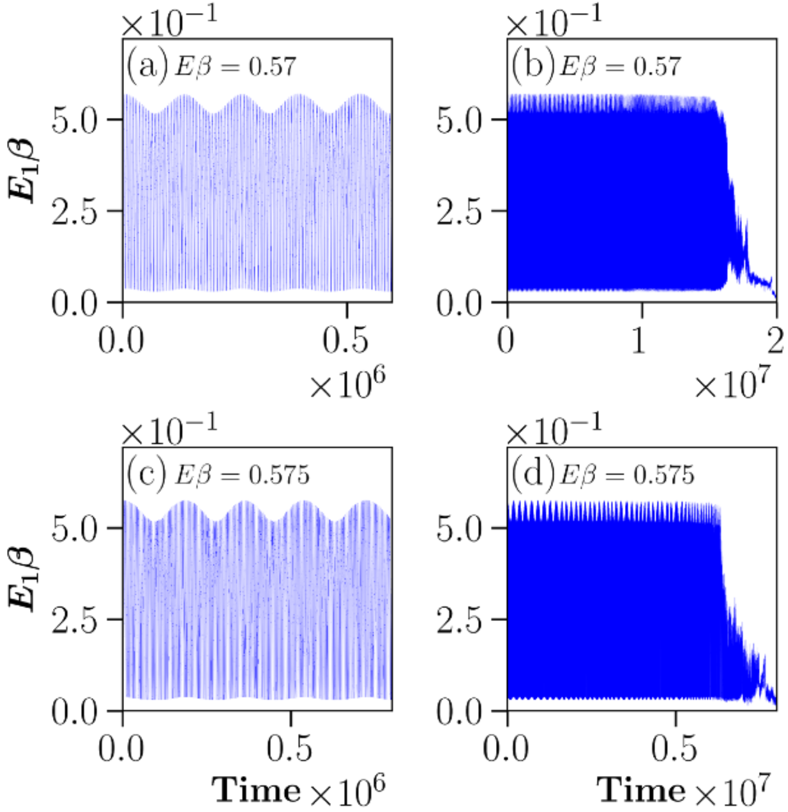


- Degradation of 2oRs due to due to a secondary FPUT recurrence, a “mini recurrence”



Breakdown of 2oRs in β-model

- Increasing energy does not deform 2oRs in β-model and thus no "mini-recurrences" are formed
  - 2oRs break down abruptly
  - Increasing energy, even sensitivity, causes breakdown to happen sooner in time



Indicator of equipartition

- Spectral Entropy: $S(t) = -\sum_{k=1}^{N} e_k \ln(e_k)$, where $e_k(t) = E_k(t) / \sum_k E_k(0)$
    - Rescale: $\eta(t) = \frac{S(t) - S_{\max}}{S(0) - S_{\max}}$

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Euler-Mascheroni constant.

- Ensemble Average: $\langle \eta \rangle = \dfrac{1}{\mathcal{Z}} \int_{\mathbb{R}} \prod_{k=1}^{N} (dQ_k dP_k)\, \eta(\boldsymbol{Q}, \boldsymbol{P}) e^{-\beta H(\boldsymbol{Q}, \boldsymbol{P})} \sim \dfrac{1-\gamma}{S_{\max} - S(0)}$
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➔ Look for when lattice is ergodic ($\bar{\eta}(t) = \langle \eta \rangle$) as a equipartion indicator

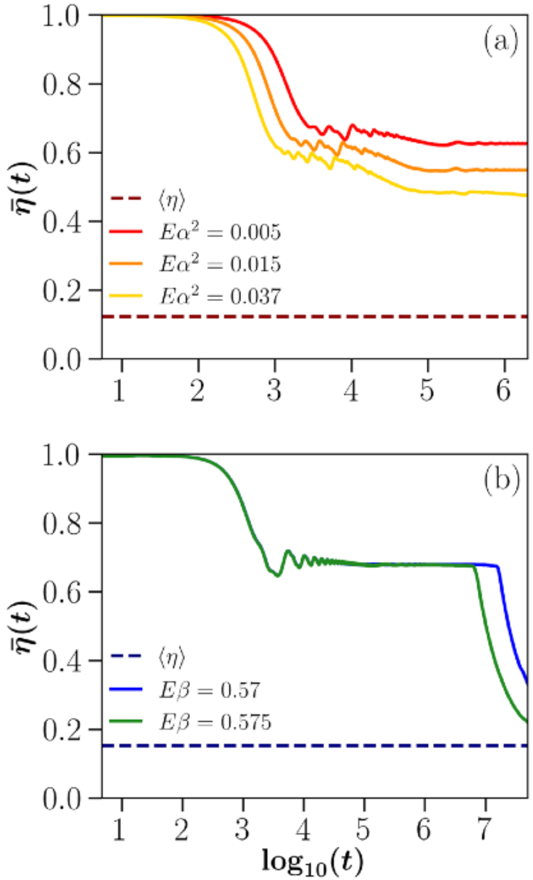
2oRs breakdown and thermalization

Figure (a) shows the α-model

- Breakdown of super-recurrences in the α-FPUT lattice occurs while the lattice is still metastable.

Figure (b) shows the β-model

- Breakdown of super-recurrences in the β-FPUT lattice is associated with the destruction of the so-called metastable state and hence is associated with relaxation towards equilibrium.



Remark on Lattice Size

- Results are general to different lattice sizes.
    - Breakdown mechanisms are the same
    - Apparent singularities (or the lack of) in the two models are the same

[1] Zabusky, N. J. "Nonlinear lattice dynamics and energy sharing."
[2] Toda, Morikazu. "Mechanics and Statistical Mechanics of Nonlinear Chains."

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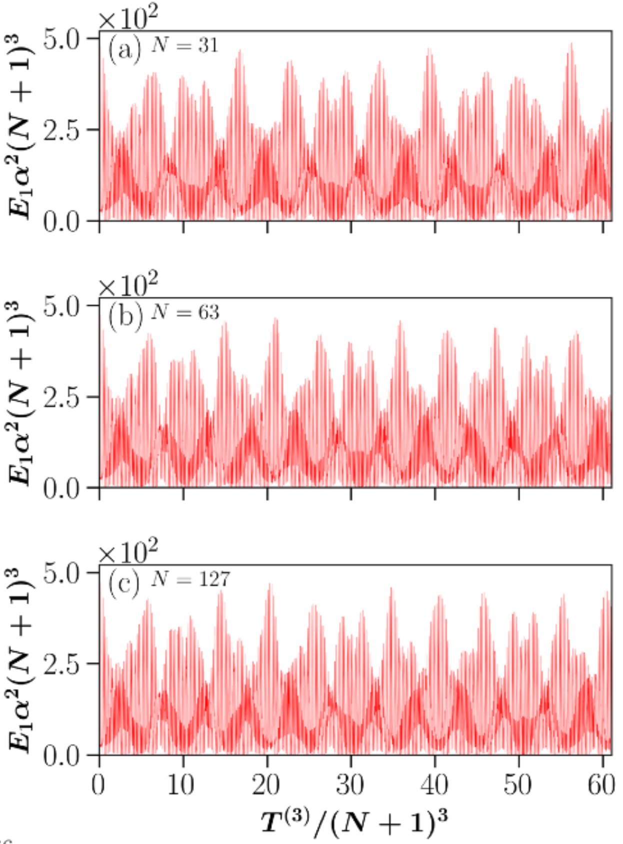
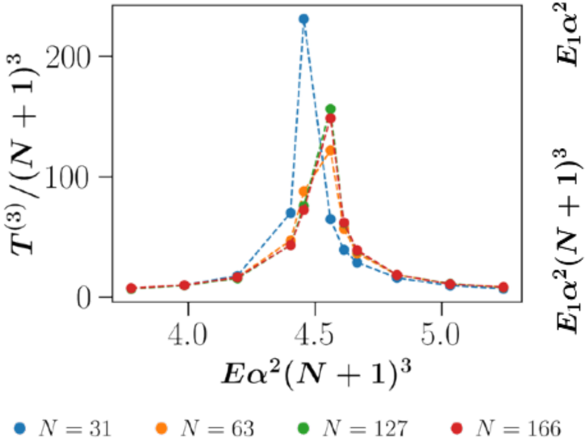


- A rescaling [1,2] of energy and time in the α-model used to study FPUT recurrences is found to work very nicely for HoRs.



$$t \rightarrow \frac{t}{(N+1)^3}$$

$$E\alpha^2 \rightarrow E\alpha^2(N+1)^3$$

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Recap

- HoRs Exist in both the α-model and β-model
- HoR times scale non trivially with energy because of apparent singularities.
  - β-model has singularities for 2oRs and greater
  - α-model has singularities for 3oRs and greater
- HoRs breakdown mechanisms and correspondence to thermalization are different between α-model and β-model
  - β-model 2oRs breakdown abruptly alongside breakdown of metastable state
  - α-model 2oRs breakdown on small timescale while lattice is still metastable
- Results seen general to different lattice sizes