Thermalization and chaos in the classical α-Fermi-Pasta-Ulam-Tsingou problem

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Ref: Ganapa, S., Apte, A. & Dhar, A. (2020). Thermalization of Local Observables in the α-FPUT Chain. J. Stat. Phys 180 (1), 1010–1030 Springer.

-Thermalization is the process of physical bodies reaching thermal equilibrium through mutual interaction.

- Once a system thermalizes we can use the principles of equilibrium statistical physics – necessary if we are dealing with macroscopic systems.

- Impracticality of the Ergodic hypothesis – Look for other ways to explain what causes thermalization.

Equilibration in the α-FPUT chain

$$H(\{p_i, q_i\}) = \sum_{i=0}^{N-1} \left[\frac{p_i^2}{2} + \frac{(q_{i+1} - q_i)^2}{2} + \alpha \frac{(q_{i+1} - q_i)^3}{3} + \beta \frac{(q_{i+1} - q_i)^4}{4} \right]$$

- For $\alpha = \beta = 0$, it becomes a harmonic chain - integrable.
- Description in terms of normal modes.

For PBC

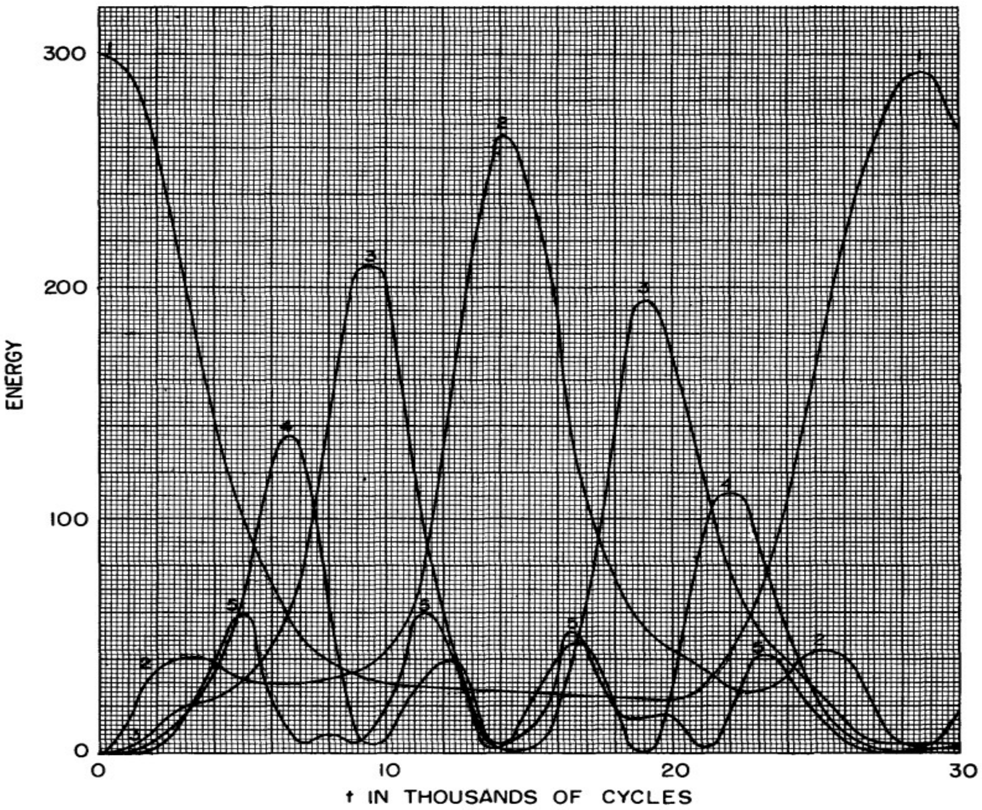
$$H = \sum_{k=0}^{N-1} E_k, \quad \text{where } E_k = \left[\frac{|P_k|^2}{2} + \frac{\Omega_k^2 |Q_k|^2}{2} \right]$$

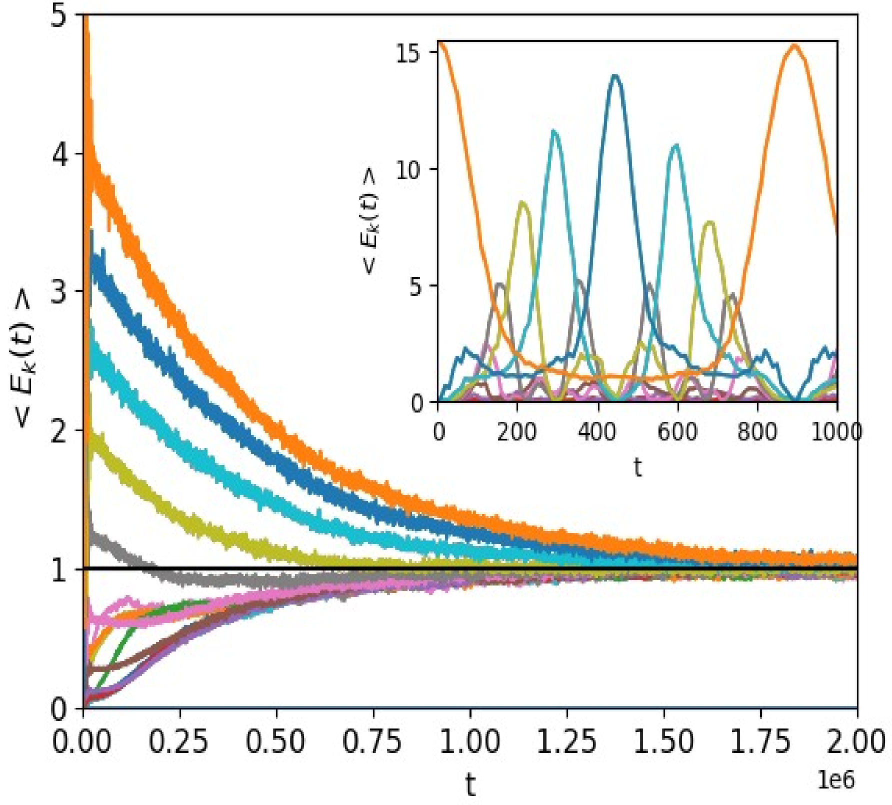
$$q_0 = q_N \ and \ q_1 = q_{N+1}$$

$$\Omega_k = 2\sin(k\pi/N), k = 0, 1, 2, ..., N-1$$

- No energy exchange between different normal modes → most of the phase is not covered by the system → no thermalization is observed.
- For the α-FPUT system, $\beta = 0$ and $\alpha \neq 0$.
- System with a nonlinear spring $F = -x - \alpha x^2$.
- The nonlinearity is quantified by the dimensionless parameter: $\varepsilon = \alpha\sqrt{(E/N)}$.
- **Original problem**: Excite the first normal mode of the harmonic chain and then look at the time evolution of the system. Nonlinearity is expected to be sufficient.
- Observed quasiperiodic behaviour instead of the expected equipartition of energy.

Results of F,P,U,T – 1955(l) and Onorato et al - 2015(r)





Another approach - check equipartition theorem

$$\left\langle q_i \frac{\partial H}{\partial q_j} \right\rangle = \left\langle p_i \frac{\partial H}{\partial p_j} \right\rangle = E_0 \delta_{ij}$$

$\langle \ldots \rangle$: equilibrium ensemble average

E_0: equilibrium equipartitioned energy of the system

- This is exact when compared to the normal modes approach because normal modes of the harmonic chain are only approximately those of the FPUT chain.
- Take a blob of initial conditions and evolve each of them individually. Then take the ensemble averages.

Unique features of our work

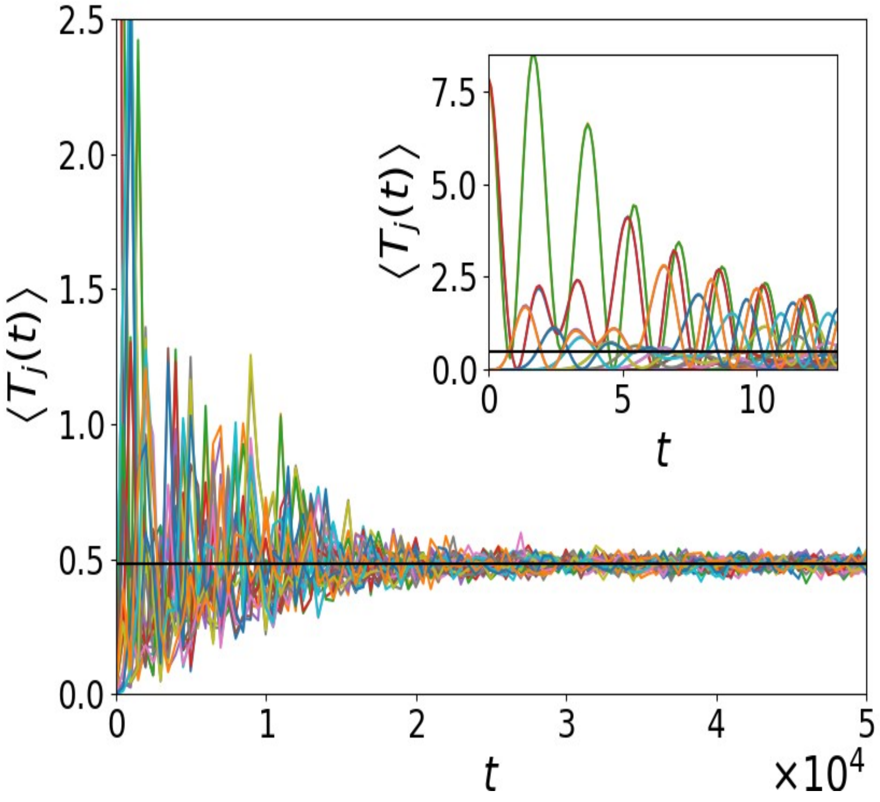
- Thermalization in local observables instead of normal modes.

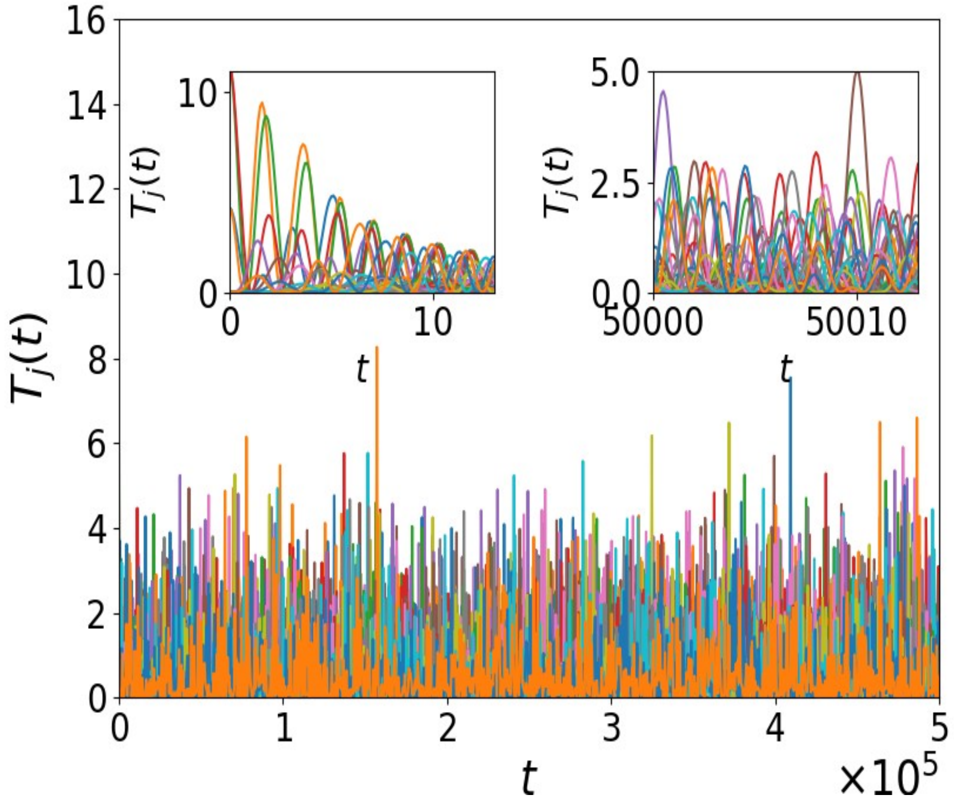
- Initial conditions corresponding to spatially localized energy instead of Normal mode localization.

- Attempt to relate chaos and thermalization in the classical α-FPUT problem.

Results

α-FPUT problem ε = 0.0848, ɣ = 0.9(l) and single realization(r)



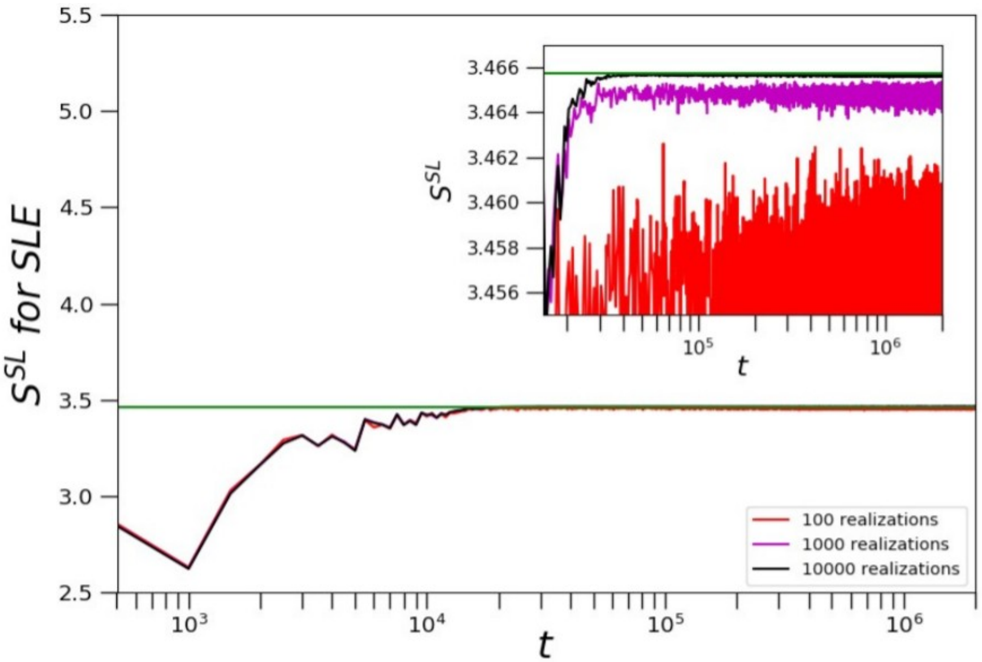


Equilibration time using Entropy

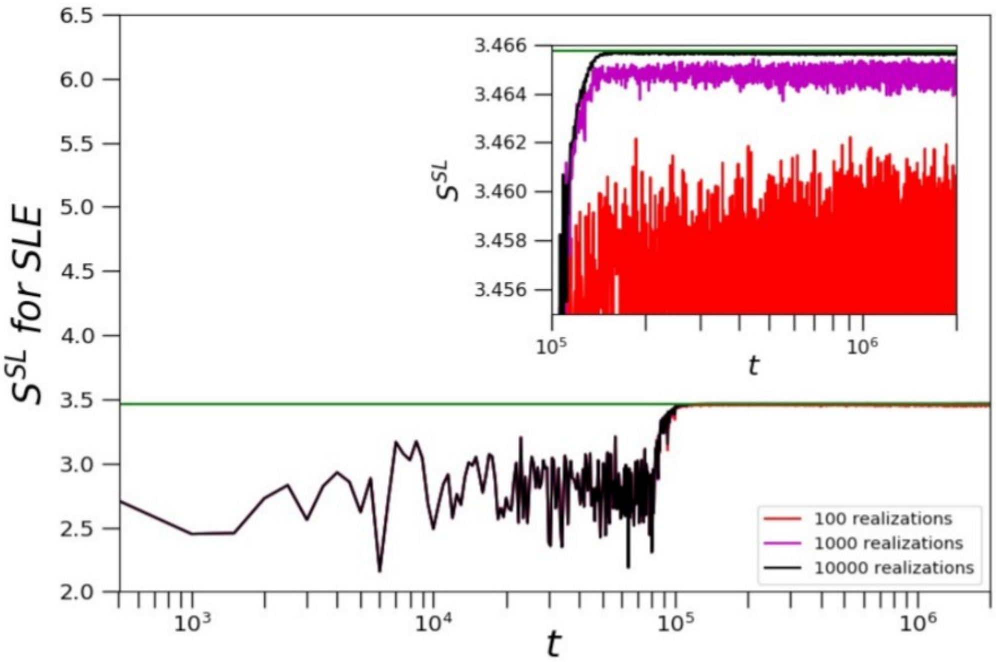
$$S(t) = -\sum_{i=0}^{N-1} f_i(t) \ln f_i(t)$$

$$f_i(t) = \nu_i(t) / \sum_{r=0}^{N-1} \nu_r(t)$$

$\gamma = 0.9$



$\gamma = 10^{-8}$

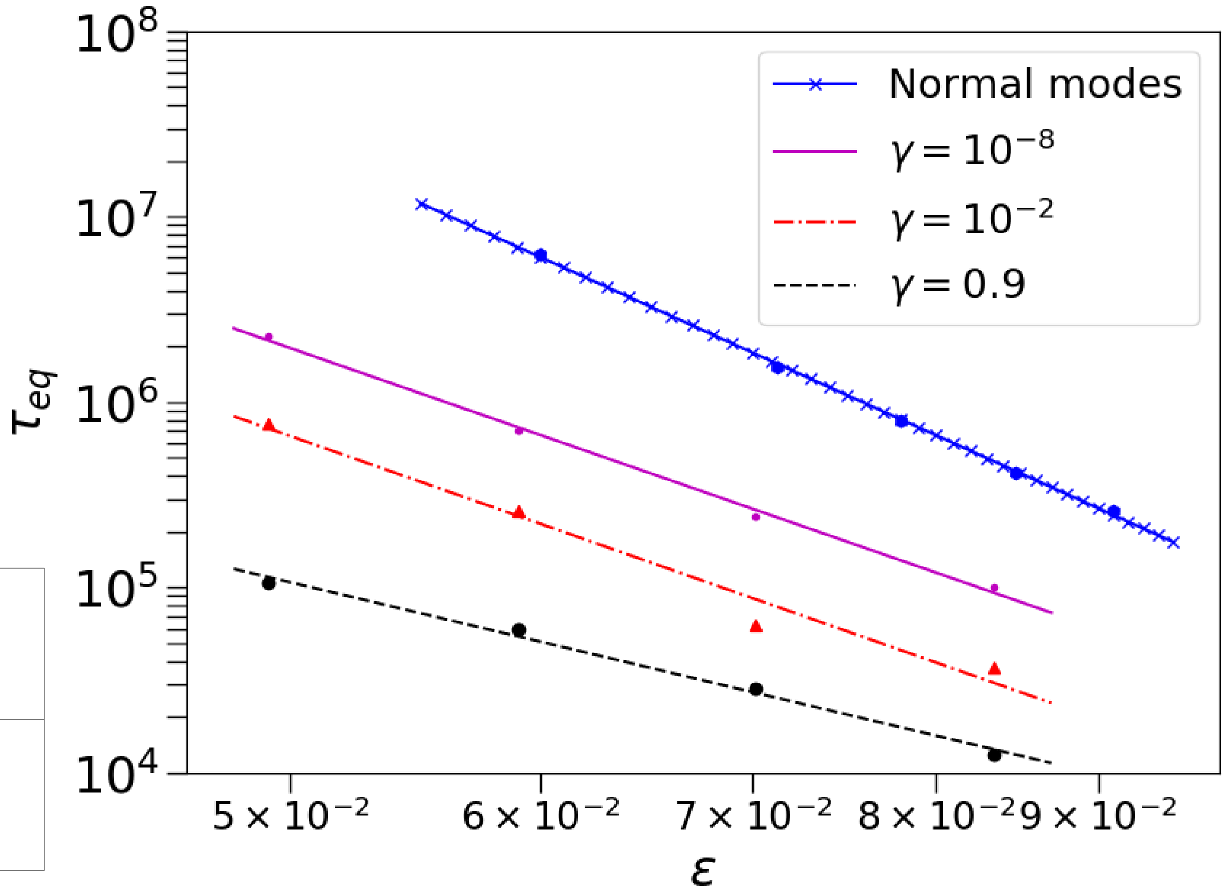


Dependence of τ on the nonlinearity parameter $\varepsilon=\alpha\sqrt{(E/N)}$

$\tau \sim 1/\varepsilon^a$ dependent on:

1. equipartition among normal mode energies – a = 8.
2. equipartition among local observables: γ dependent.

γ	0.9	0.01	10^{-8}
a	4	6	5.9



Relation to chaos

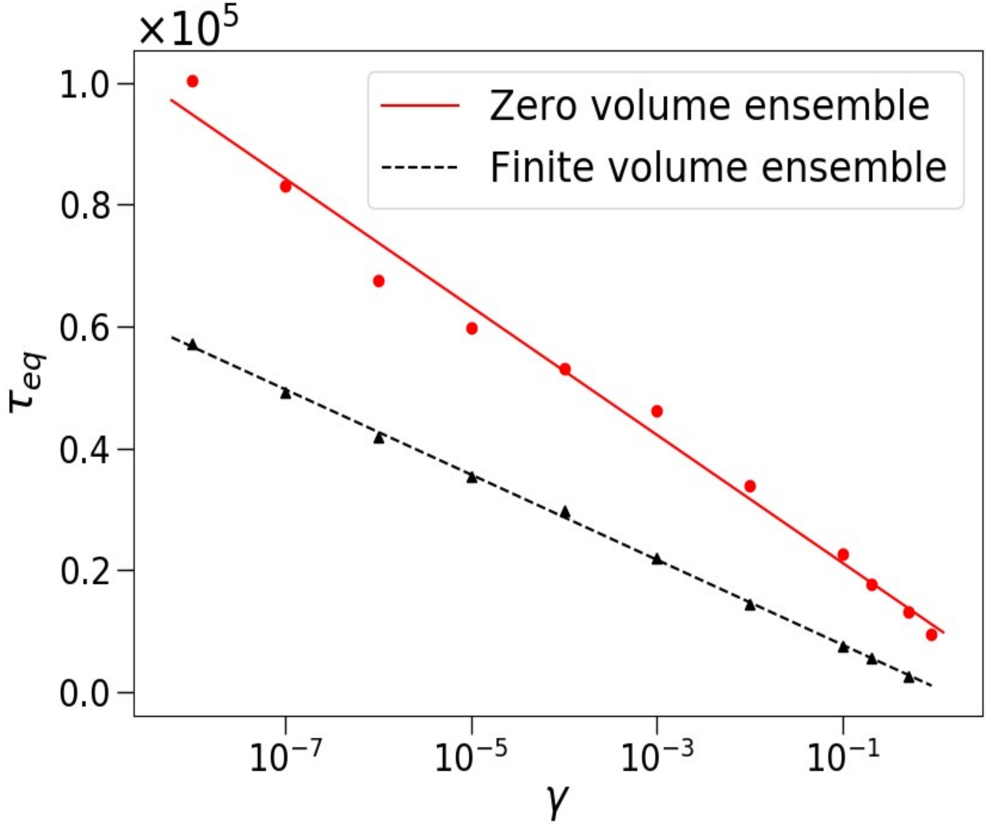
$$D(t) \sim \begin{cases} D(0)e^{\Lambda t} & \text{for FPUT} \\ D(0)t & \text{for Toda.} \end{cases}$$

$$\log(D(t)) \sim \begin{cases} \Lambda t + \log(\gamma) & \text{for FPUT,} \\ \log(t) + \log(\gamma) & \text{for Toda.} \end{cases}$$

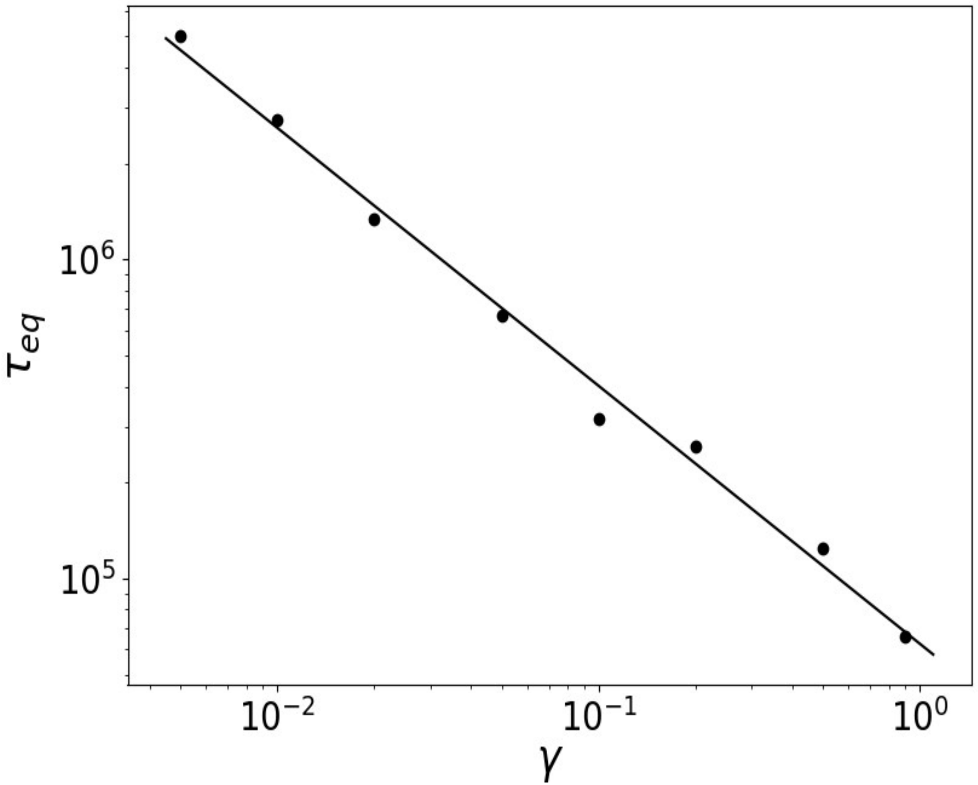
- Exponential separation of the nearby trajectories in the FPU problem would result in a faster thermalization.
- Linear separation of the nearby trajectories in the Toda chain leads to a slower thermalization.
- No separation of the nearby trajectories in the harmonic chain results in no thermalization.

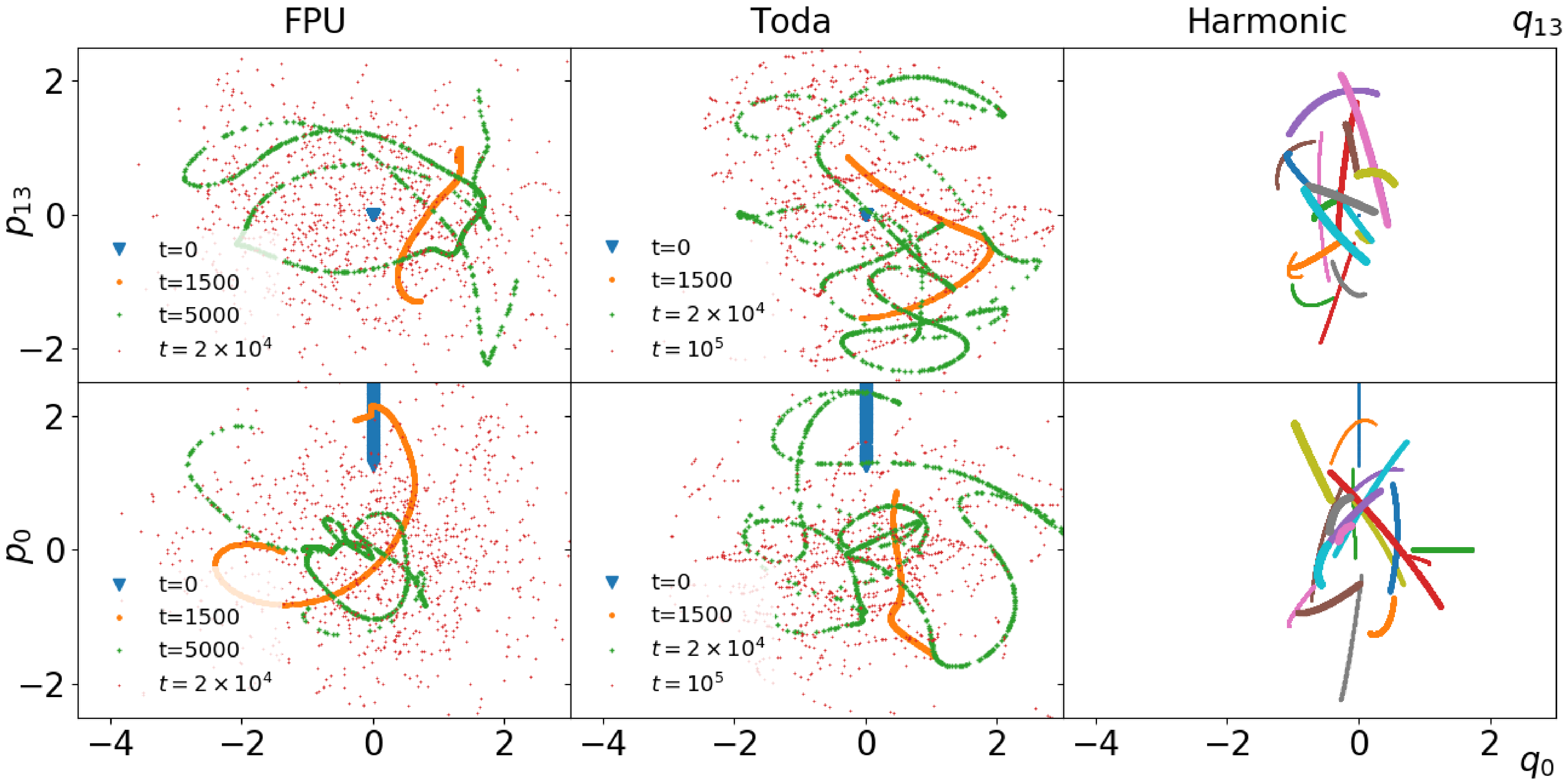
Dependence of τ on γ

α-FPUT



Toda





FPU
Toda
Harmonic
q_{13}
p_{13}
p_0
q_0
t=0
t=1500
t=5000
$t = 2 \times 10^4$
t=0
t=1500
$t = 2 \times 10^4$
$t = 10^5$

Conclusion

- $\tau \sim 1/\varepsilon^a$ dependent on:
1. equipartition among normal mode energies – a = 8.
2. equipartition among local observables: γ dependent.

a lies between 4 and 6.

- Local observables equilibrate faster than normal modes.
- Averaging is needed in order to observe thermalization.
- Relation between thermalization (equilibration of local observables) and chaos (sensitive dependence on initial conditions).