Equilibrium and thermalization in integrable systems: The case of Toda model and harmonic systems

GRAN SASSO SCIENCE INSTITUTE
CNRNANOTEC INSTITUTE OF NANOTECHNOLOGY

Angelo Vulpiani,
Marco Baldovin,
Niccolo' Cocciaglia,
Giacomo Gradenigo

MIUR-PRIN2017 CONEST

May 2023

Outline

Why should we trust equilibrium statistical mechanics?

Empirical fact: Equilibrium statistical mechanics correctly describes the behaviour of thermodynamic observables in physical systems with many degrees of freedom.

Consider a mechanical system $\{q_i, p_i\}$, $i = 1, ..., N \gg 1$, with Hamiltonian $\mathcal{H}(\mathbf{q}, \mathbf{p})$, whose evolution reads

$$\begin{cases} \dot{q}_i = \frac{\partial \mathcal{H}}{\partial p_i} \\ \dot{p}_i = -\frac{\partial \mathcal{H}}{\partial q_i} \end{cases},$$

and some observable $\mathcal{F}(\mathbf{q}, \mathbf{p})$.

Time average:

$$\overline{\mathcal{F}} = \lim_{T \to \infty} \frac{1}{T} \int_0^T \mathcal{F}(\mathbf{q}(t), \mathbf{p}(t))\, dt$$

(measured in experiments)

Phase average (microcanonical):

$$\langle \mathcal{F} \rangle_E = \frac{1}{\omega(E)} \int \mathcal{F}(\mathbf{q}, \mathbf{p}) \delta(\mathcal{H}(\mathbf{q}, \mathbf{p}) - E)\, \mathcal{D}\mathbf{q} \mathcal{D}\mathbf{p}$$

(equilibrium statistical mechanics)

- Phase averages can be computed (at least in principle) once $\mathcal{H}(\mathbf{q}, \mathbf{p})$ is known.
- $\overline{\mathcal{F}} = \langle \mathcal{F} \rangle_E \longrightarrow$ validity of statistical mechanics

Birkhoff theorem

- Ω: invariant part of the phase space with a finite volume
- $\mathcal{F} : \Omega \to \mathbb{R}$ phase function summable over Ω, determined at all points $\mathbf{X} \in \Omega$

Then Birckhoff theorem states that:

1. The limit
$$\overline{\mathcal{F}} = \lim_{T \to \infty} \frac{1}{T} \int_0^T \mathcal{F}(\mathbf{X}(t))dt \tag{1}$$
exists for almost all initial conditions $\in \Omega$.

2. If Ω cannot be divided into invariant subsets of positive measures (metrical indecomposability), then
$$\overline{\mathcal{F}} = \frac{1}{\mu(\Omega)} \int_\Omega \mathcal{F}(\mathbf{X}) \mathcal{D}\mathbf{X} \,. \tag{2}$$
where $\mu(\Omega)$ is the Lebesgue measure.

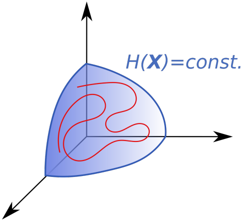
Ergodicity and chaos

As a consequence, time averages and microcanonical phase averages coincide if

- $\Omega = \Omega(E)$ is the phase-space hypersurface at constant energy E;
- $\Omega(E)$ is metrically indecomposable.

One may assume the metrical indecomposability of $\Omega(E)$.

- "Any" trajectory is allowed to explore the "whole" hypersurface $\mathcal{H}(\mathbf{q}, \mathbf{p}) = const.$ (excluding sets with vanishing measure);
- equivalent to the ergodic hypothesis.

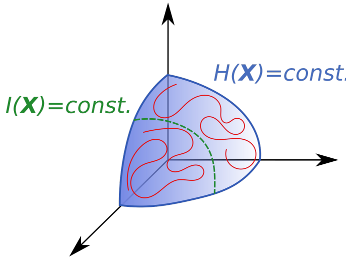


Arguments in favour of this point of view are usually based on chaos theory: validity of equilibrium statistical mechanics $\longleftrightarrow$ positive Lyapunov exponents.
P. Gaspard, *"Chaos, Scattering and Statistical Mechanics"*, Cambridge Univ. Press, (1998)

$\longrightarrow$ Validity of statistical mechanics crucially depends on the properties of the dynamics

Limits of ergodicity

Unfortunately, in many cases $\Omega(E)$ is not metrically indecomposable.



E.g., if the dynamics admits an integral of motion $I(\mathbf{X}) \neq \mathcal{H}(\mathbf{X})$, the condition $I(\mathbf{X}) = const.$ will in general cut $\Omega(E)$ into two invariant sets.

$\mathcal{H}(\mathbf{X}) = const.$ is, in principle, as significant as any other $I(\mathbf{X}) = const.$ hypersurface: we should take into account all constraints coming from independent integrals.

- If we knew the values of all first integrals $I_1, I_2, ..., I_n$, in principle we could compute phase averages over some phase-space set $\Omega'(E, I_1, ..., I_n)$, introducing some generalized microcanonical ensemble.
- The above strategy is for sure unfeasible in integrable systems, where N independent conserved quantities can be found.

Khinchin's approach: beyond ergodicity

Under rather general assumptions, Khinchin showed that if

- the system is composed by a large number of degree of freedom, i.e. $N \gg 1$;
- the particles interact weakly;
- we limit our attention to the sum functions usually encountered in statistical mechanics, of the form

$$\mathcal{F}(\mathbf{q},\mathbf{p}) = \sum_{i=1}^{N} f(q_i, p_i)$$

then:

the relative measure of the sets of points for which

$$\left| \frac{\overline{\mathcal{F}}}{\langle \mathcal{F} \rangle} - 1 \right| > K N^{-1/4} \qquad K = const.$$

is a small quantity $\leq O(N^{-1/4})$.

A.I.Khinchin, *"Mathematical Foundations of Statistical Mechanics"*, Dover, New York, (1949)

$\longrightarrow$ Validity of statistical mechanics due to the large number of degrees of freedom and the sensible choice of the observables.

Purpose

Two alternative interpretations:

- Equilibrium as a property of the model
- Equilibrium as a property of the chosen observable

A quite severe test to the latter is the study of integrable systems, where no chaotic behaviour is present.

We will focus on the Toda model (nonlinear integrable Hamiltonian) and harmonic systems (trivially integrable)

Idea: numerical study of canonical variables which do not diagonalize $\mathcal{H}(\mathbf{q}, \mathbf{p})$.

- Does this description reach thermalization in Khinchin's sense?
- Do time averages over long trajectories coincide with phase averages?

$\longrightarrow$ Possible analogy with thermalization in quantum mechanics:

- Is unitary dynamics an obstacle to thermalization?

Toda: an integrable model

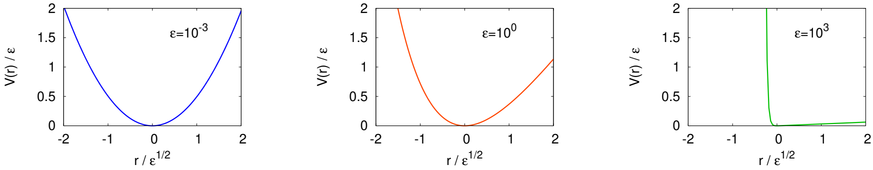
Toda model:

$$\mathcal{H}(\mathbf{q},\mathbf{p}) = \sum_{i=1}^{N} \frac{p_i^2}{2} + \sum_{i=0}^{N} V(q_{i+1} - q_i)\,, \quad \text{with} \quad V(x) = e^{-x} + x - 1\,.$$

M.Toda, *"Vibration of a Chain with Nonlinear Interaction"*, J. Phys. Soc. Jpn. **22**, 431-436 (1967)

- Completely integrable nonlinear Hamiltonian system;
- a set of N independent integrals of motion is known;
- solitonic solutions, close relation to the FPUT Hamiltonian and its phenomenology.

Small energy $\approx$ harmonic oscillators chain | Energy $\simeq O(1)$ | High energy $\approx$ hard spheres in 1D



Integrals of Toda model

Defining $X_i = e^{-(q_{i+1}-q_i)}$, Hénon showed that N integrals of the Toda model with periodic boundary conditions can be found as

$$I_m = \sum p_{i_1}...p_{i_k}(-X_{j_1})...(-X_{j_l})\,, \qquad \text{with} \quad k+2l=m\,,$$

where the sum is computed over all m-uples $(i_1, ..., i_k, j_1, j_1+1, ..., j_l, j_l+1)$, with no repetition of indexes, leading to different terms.
M.Hénon, *"Integrals of the Toda lattice"*, Phys. Rev. B **9**, 1921 (1974)

The complete integrability can be also proved by considering the Lax pair:

$$\begin{cases} \mathcal{L}\mathbf{e_i} = \frac{1}{2}\left[X_i^{1/2}\mathbf{e_{i+1}} + X_{i-1}^{1/2}\mathbf{e_{i-1}} - p_i\mathbf{e_i}\right] \\ \mathcal{P}\mathbf{e_i} = \frac{1}{2}\left[X_i^{1/2}\mathbf{e_{i+1}} - X_{i-1}^{1/2}\mathbf{e_{i-1}}\right]\,. \end{cases}$$

It can be easily verified that

$$\frac{d}{dt}\mathcal{L}(t) = [\mathcal{P}(t), \mathcal{L}(t)]$$

is equivalent to the original dynamics $\longrightarrow$ the eigenvalues of $\mathcal{L}$ are invariant in time.
H.Flaschka, *"The Toda lattice. II. Existence of integrals"*, Phys. Rev. B **9**, 1924–1925 (1974)

Relation with the FPUT problem

In the Fermi-Pasta-Ulam-Tsingou numerical experiment, the nonlinear Hamiltonian model

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

is prepared in a initial condition such that all energy is assigned to the first Fourier mode:

$$\omega_k^2 \mathcal{Q}_k^2 = \mathcal{P}_k^2 = \begin{cases} E_0 & k=1 \\ 0 & k \neq 1 \,. \end{cases}$$

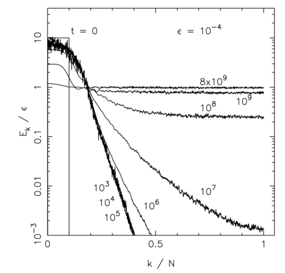
where

$$\begin{cases} \mathcal{Q}_k &= \sqrt{\frac{2}{N+1}} \sum_{i=1}^{N} q_i \, \sin\left(\frac{\pi i k}{N+1}\right) \\ \mathcal{P}_k &= \sqrt{\frac{2}{N+1}} \sum_{i=1}^{N} p_i \, \sin\left(\frac{\pi i k}{N+1}\right) \end{cases}, \qquad \omega_k = 2\sin\frac{\pi k}{2(N+1)}$$

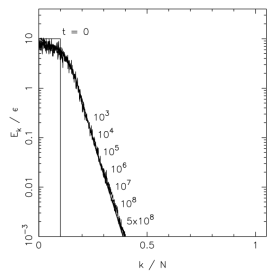
Despite the presence of nonlinearity, for small specific energies the normal modes take extremely long times to reach equipartition.

Relation with the FPUT problem

FPUT



Toda



G.Benettin, H.Chrisodoulidi, A.Ponno, *"The Fermi-Pasta-Ulam Problem and Its Underlying Integrable Dynamics"*,J Stat Phys (2013) 152:195–212

Energy distribution between normal modes identical to the Toda case for quite long times.

⟶ FPUT phenomenology seems to be due to its similarity with Toda model.

Thermalization to equilibrium

- Toda model is completely integrable, but in general I_m will depend on all Fourier modes.
- It is observed that, when energy is small, Fourier modes take extremely long times to equilibrate in the Toda model
- ... but is this also true for specific energy $\simeq O(1)$?

We know that there exist N conserved quantities that will never equilibrate.
But if we can observe equilibration for other sets of canonical variables, this means that equilibrium is an observable-dependent property $\longrightarrow$ Khinchin's perspective

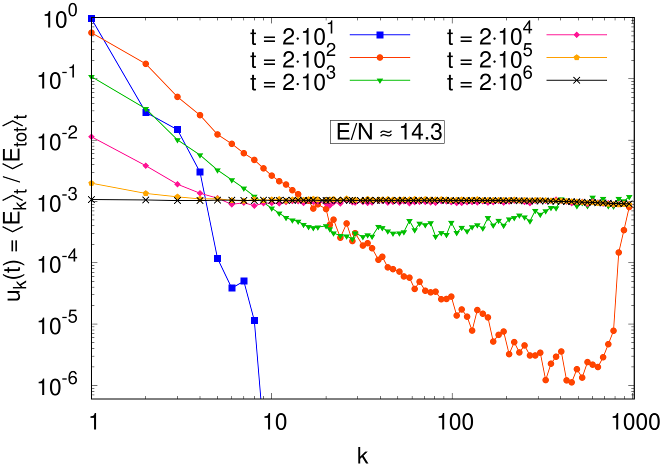
Numerical experiment "FPUT-like":

1. initialize the system in a state in which only the first Fourier mode is excited: atypical initial condition;
2. consider cumulative time averages for the harmonic energy of the k-th mode
3. verify equipartition.

M.Baldovin, A.Vulpiani, G.Gradenigo, *"Statistical mechanics of an integrable system"*, J Stat Phys (2021) 183, 41

"FPUT-like" numerical experiment

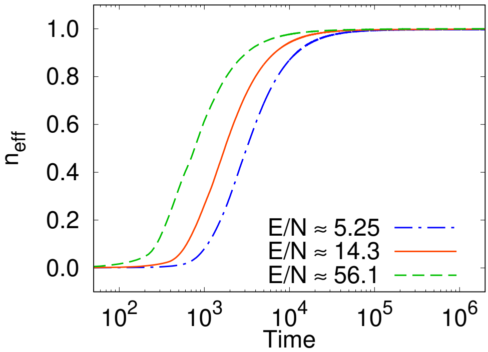
$$\langle E_k \rangle_t = \int_0^t ds\, E_k(s) \qquad \langle E_{tot} \rangle_t = \int_0^t ds \sum_k E_k(s) \qquad u_k(t) = \frac{\langle E_k \rangle_t}{\langle E_{tot} \rangle_t}$$



Spectral density

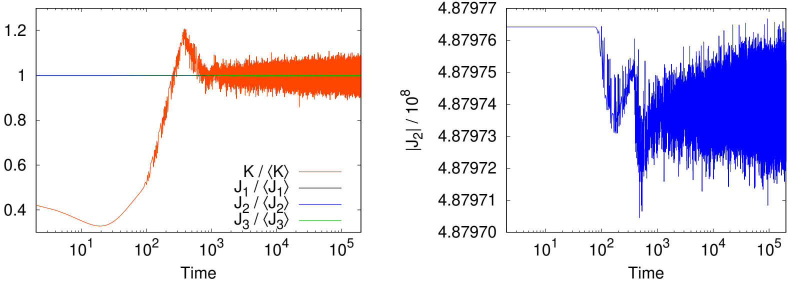
Spectral entropy: $$S_{\text{sp}}(t) = -\sum_{k=1}^{N} u_k(t)\log u_k(t)$$

Density of effective degrees of freedom: $$n_{\text{eff}}(t) = \frac{\exp\left(S_{\text{sp}}\right)}{N}$$



- Relaxation time increasing for decreasing energies
- Consistent with previous results about harmonic localization in low-energy FPUT and Toda

First integrals



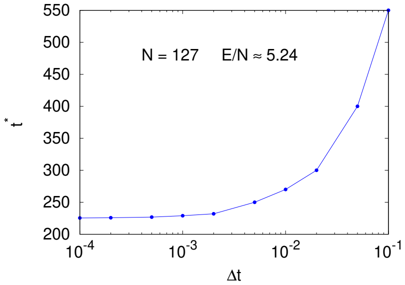
Technical note: we consider fixed boundary conditions:
the complete set of first integrals $\{J_n\}$ is obtained as the N first integrals with even index in a chain of $2N$ particles with periodic BC and antisymmetric initial conditions.

In order to be sure that our numerical approach is working correctly, we should check all first integrals...

Numerical stability

We are using a symplectic Velocity Verlet Update. It can be shown[1] that symplectic integrators preserve the Hamiltonian flux, but for a correction depending on Δt.

t^* $\longrightarrow$ Time at which $n_{eff} \geq 0.5$.



- The plateau at small Δt seems to exclude the possibility of artifact thermalization due to numerical effects.

[1] G.Benettin, A.Giorgilli, *"On the Hamiltonian interpolation of near-to-the-identity symplectic mappings with application to symplectic integration algorithms"*, J. Stat. Phys. **74**, 1117 (1994)

Equilibrium properties

Canonical partition function (potential part):

$$\mathcal{Z}_N^{(\mathrm{P})}(\beta) = e^{\beta N} \int_{-\infty}^{\infty} \prod_{i=1}^{N+1} dr_i \; e^{-\beta \sum_{i=1}^{N+1} \exp(-r_i)} \; \delta\left(\sum_{i=1}^{N+1} r_i\right) .$$

We can take the Lalpace transform and compute $\mathcal{Z}_N^{(\mathrm{P})}(\beta)$ as a Bromwich integral:

$$\begin{aligned}\mathcal{Z}_N^{(\mathrm{P})}(\beta) &= e^{\beta N} \int_{s_0 - i\infty}^{s_0 + i\infty} \frac{ds}{2\pi i} \int_{-\infty}^{\infty} \prod_{i=1}^{N+1} dr_i \;\; \exp\left(-\beta \sum_{i=1}^{N+1} \exp(-r_i) + s \sum_{i=1}^{N+1} r_i\right) \\ &= e^{\beta N} \int_{s_0 - i\infty}^{s_0 + i\infty} \frac{ds}{2\pi i} \;\; \exp\left\{N \log z_\beta(s)\right\}\end{aligned}$$

with

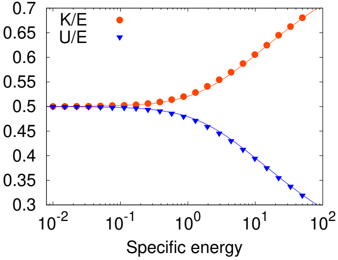
$$z_\beta(s) = \int_{-\infty}^{\infty} dr \;\; \exp\left(-\beta e^{-r} + sr\right) \quad \longrightarrow \quad \text{Saddle point:} \quad \psi(s) = \log(\beta)$$

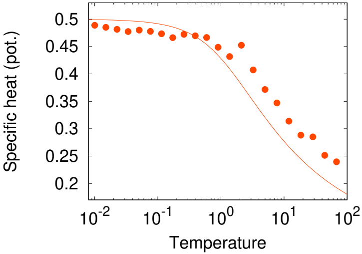
- Equilibrium averages can be derived in the canonical ensemble.

Thermodynamic observables

Average kinetic and potential energy can be studied as functions of the specific energy $\varepsilon = E/N$.

- "Equilibrium" initial conditions (equipartition between kinetic degrees of freedom)
- Agreement between time averages (simulations, points) and phase averages (theory, lines).

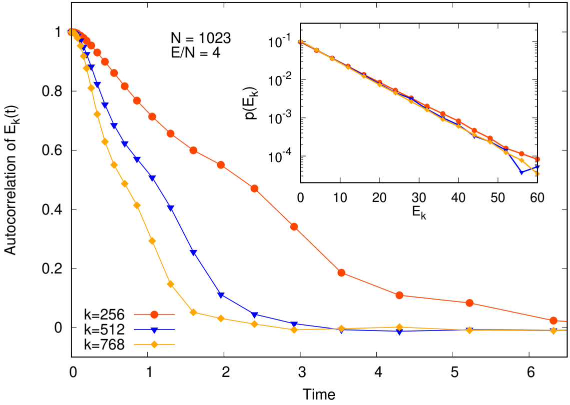




An exact relation can be also found for the specific heat. It can be numerically tested by measuring energy fluctuations in subsets of the chain.

- "Severe" test.
- Worse agreement at high energies due to hard spheres limit?

Fourier modes



- The energy of Fourier modes decorrelates in finite time;
- Energy distribution $\propto \exp(-\beta E_k)$

Thermalization of Harmonic Systems

Consider now the harmonic system

$$\mathcal{H}(\mathbf{q},\mathbf{p}) = \sum_{i=1}^{N} \frac{p_i^2}{2} + \sum_{i=0}^{N} \frac{1}{2}(q_{i+1} - q_i)^2$$

if the initial condition is such that if only one harmonic k is excited, for all $q \neq k$, energy is never shared among Fourier modes due to the lack of interaction.
Introduce the variables:

$$z_k = \frac{P_k + iQ_k}{\sqrt{2\omega_k}} \quad , \quad z_k^* = \frac{P_k - iQ_k}{\sqrt{2\omega_k}}$$

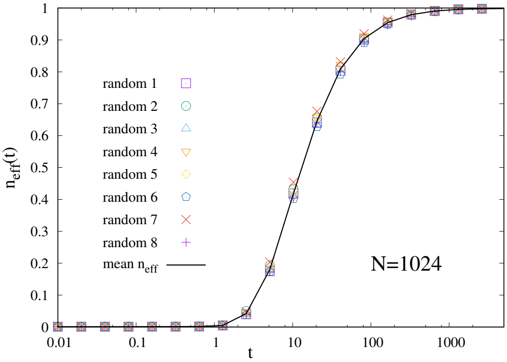
and a "random rotation" $M(\theta)$ i.e. a unitary matrix depending of N angles $\theta_1, \theta_2, ..., \theta_N$, and the new (random) Fourier modes

$$Z_k(\theta) = \sum_q M_{kq}(\theta) z_q$$

Let us wonder what happen if we look at the the variables $Z_k(\theta)$, in particular the relaxational dynamics when energy is initially fed to a single random mode.

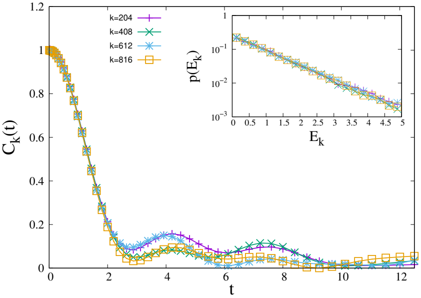
Numerical Results for the random Harmonic Systems

- The behavior of the density of effective degrees of freedom: $n_{\text{eff}}(t) = \frac{\exp(S_{\text{sp}})}{N}$ obtained by the spectral entropy: $S_{\text{sp}}(t) = -\sum_{k=1}^{N} u_k(t) \log u_k(t)$ is quite similar to that one observed for the Toda.



Effective number of degrees of freedom as a function of time, $n_{\text{eff}}(\theta, t)$ vs t : the continuous (black) line represents the average over 30 choices of the random modes basis, points represent the individual behaviour of 8 different instances.

Time correlation and energy distribution of the random modes



Time auto-correlation function $C_k(t)$ as a function of time for different choices of the random modes index k; in the inset: probability distribution of random-modes energy E_k for some values of k, system size $N = 1023$.

Considerations of the statistical features of the random Harmonic Systems

- In some sense, anyone of the N random modes plays a role akin to that of a particle in the harmonic chain; this is evident from the time autocorrelation function for the random Fourier modes for the harmonic system.
- Physically, the difference between random modes and particles is that the former are all in interaction while the latter have only first neighbour interactions. Despite integrability thermalization is observed even in the harmonic chain, provided the "right variables" are considered.
- What is most remarkable, thermalization looks as the typical phenomenon, while the lack of it is specific only to the representation of the chain configuration in Fourier space.
- The idea that in the large-N limit the relevant thermodynamic properties of a system cannot be tight to a particular choice of coordinates.

What about quantum mechanics?

A related problem about thermalization and equilibrium is found in quantum mechanics of many-body isolated systems:

- unitary evolution of the state ψ;
- large dimensionality D of the Hilbert space $\mathcal{H}$ corresponding to a certain energy shell;
- justification needed to thermalization and equilibrium.

Idea of Von Neumann's "Quantum Ergodic Theorem":
If the Hilbert space is divided into orthogonal subspaces $\mathcal{H}_\nu$ with $\dim \mathcal{H}_\nu = d_\nu$, and such d_νs are large enough, then

$$||P_\nu \psi_t||^2 \approx \frac{d_\nu}{D} \quad \text{for all } \nu\,,$$

for most choices of the decomposition, where P_ν is the projection operator for the subspace $\mathcal{H}_\nu$.

S.Goldstein, J.L.Lebowitz, R.Tumulka, N.Zanghi, *"Long-Time Behavior of Macroscopic Quantum Systems: Commentary Accompanying the English Translation of John von Neumann's 1929 Article on the Quantum Ergodic Theorem"*, European Phys. J. H 35: 173-200 (2010)

Some conclusions

1. Even starting from atypical initial conditions, as in the "FPUT-like" experiment, we observe thermalization in Toda model, as soon as "generic" canonical coordinates are chosen (i.e., not those diagonalizing the dynamics).

2. In typical conditions, fair agreement between phase averges and time averages is found.

3. Integrability does not seem to hinder thermalization and the applicability of statistical mechanics $\longrightarrow$ The possibility to reach equilibrium is linked to the choice of the observables, rather than to the features of the dynamics.

4. In this sense, statististical mechanics of integrable systems is the classical analogue of many-body quantum mechanics: also in the latter case , for most "descriptions" of the system, equilibrium is reached despite the unitary evolution (Von Neumann's "Quantum Ergodic Theorem").

References:

[1] P. Gaspard, *"Chaos, Scattering and Statistical Mechanics"*, Cambridge Univ. Press (1998)

[2] A.I.Khinchin, *"Mathematical Foundations of Statistical Mechanics"*, Dover, New York (1949)

[3] M.Toda, *"Vibration of a Chain with Nonlinear Interaction"*, J. Phys. Soc. Jpn. **22**, 431-436 (1967)

[4] M.Hénon, *"Integrals of the Toda lattice"*, Phys. Rev. B **9**, 1921 (1974)

[5] H.Flaschka, *"The Toda lattice. II. Existence of integrals"*, Phys. Rev. B **9**, 1924–1925 (1974)

[6] G.Benettin, H.Chrisodoulidi, A.Ponno, *"The Fermi-Pasta-Ulam Problem and Its Underlying Integrable Dynamics"*,J Stat Phys (2013) 152:195–212

[7] M.Baldovin , A.Vulpiani, G.Gradenigo, *"Statistical mechanics of an integrable system"*, J Stat Phys (2021) 183, 41

[8] G.Benettin, A.Giorgilli, *"On the Hamiltonian interpolation of near-to-the-identity symplectic mappings with application to symplectic integration algorithms"*, J. Stat. Phys. **74**, 1117 (1994)

[9] N.Cocciaglia, A.Vulpiani, G.Gradenigo, *"Thermalization without chaos in harmonic systems"*, Physica A 601, 127581 (2022)

[10] S.Goldstein, J.L.Lebowitz, R.Tumulka, N.Zanghi, *"Long-Time Behavior of Macroscopic Quantum Systems: Commentary Accompanying the English Translation of John von Neumann's 1929 Article on the Quantum Ergodic Theorem"*, European Phys. J. H 35: 173-200 (2010)

Thank you for your attention