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Thermalization without chaos in harmonic systems

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ABSTRACT

Recent numerical results showed that thermalization of Fourier modes is achieved in short time-scales in the Toda model, despite its integrability and the absence of chaos. Here we provide numerical evidence that the scenario according to which chaos is irrelevant for thermalization is realized even in the simplest of all classical integrable system: the harmonic chain. We study relaxation from an atypical condition given with respect to *random* modes, showing that a thermal state with equilibrium properties is attained in short times. Such a result is independent from the orthonormal basis used to represent the chain state, provided it is a random basis.

1. Introduction

Whether chaos is a necessary or just a sufficient condition in order for many-body Hamiltonian systems to exhibit thermalization is an old debate, to which a final assessment has not yet been given [1–3]. A possibility, outlined with an interesting mathematical argument first by Khinchin in 1949 [4] and then by Mazur and van der Linden [5], is that the applicability of the statistical mechanics description to a macroscopic object relies on the number of its microscopic constituents being very large, irrespective to details of their dynamics. There are in fact examples showing that chaos is not necessary to have good statistical features [6], sometimes being not even sufficient [7,8]. It is in this spirit that two of us recently investigated how an atypical initial condition relaxes to equipartition in an integrable Hamiltonian system, the Toda chain [9]. It turned out that in order to see fast relaxation to thermal equilibrium it is sufficient to consider appropriate observables, for instance observables almost independent from the conserved quantities of the integrable system [9]. For what concerns the Toda model at not too low energies this is for instance the case of the Fourier modes harmonic energies, which thermalize fast. On the other hand, one could say that thermalization of Fourier modes in the Toda chain is specific to the choice of variables and to its intricate relation with the Toda modes; in fact it is well known that, if one considers the Toda modes, the thermodynamic of the system is well described by the Generalized Gibbs Ensemble [10–13]. The goal of the present work is to give further and more stringent evidences in favour of the scenario tested numerically in [9] and at the basis of the Khinchin approach [4]: in the large-N limit details of the microscopic dynamics are not relevant for statistical mechanics.

In the present paper we discuss an alternative way to study the behaviour of a system which is a textbook example: the harmonic chain. Our goal is to show that the lack of thermalization is a property *specific* of the Fourier modes, in the sense that there are infinitely many other choices of canonical variables to represent the chain state and that using such variables one can see fast relaxation to a thermal state. In order to complement the results of [9] we will present here

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the numerical evidence of two important facts: (1) there are *many* (ideally, infinitely many) independent sets of canonical variables with respect to which the system shows thermalization and (2) the relaxation to a thermal state is a large-N effect. The fact that the validity of statistical mechanics can be generally claimed for any system *only* in the large-N limit is particularly relevant for integrable systems, for which at small sizes the regular behaviour of the dynamics is manifest. It is therefore definitely worth to recall the enunciate of the Khinchin result, in order to grasp the relevance of the bound imposed by the large-N limit. Given that $f(q,p) : \mathbb{R}^{2dN} \to \mathbb{R}$ is an observable of our many-body classical Hamiltonian system (with d the number of space dimensions and N the number of degrees of freedom), with $\langle f \rangle$ and $\bar{f}$ respectively its statistical and time averages, if f is a sum function, namely something of the kind $f(q,p) = \sum_{i=1}^{N} f_i(q_i, p_i)$ (in practice any sort of additive quantity which can be measured as a function of small portions of the system), then under quite general hypothesis [4] one has that the probability to have a difference between $\langle f \rangle$ and $\bar{f}$ small in N is itself small in N, namely it decreases when N increases, as well expressed by Eq. (1) below. By denoting as $\mathcal{P}$ this probability, in formulas we have:

$$\mathcal{P}\left(\left|\frac{\bar{f} - \langle f \rangle}{\langle f \rangle}\right| \geq \frac{C_1}{N^{1/4}}\right) \; < \; \frac{C_2}{N^{1/4}}, \tag{1}$$

where C_1 and C_2 are $\mathcal{O}(1)$ constants which do not depend on N. The necessity of having many degrees of freedom ($N \gg 1$) and that of avoiding "strange" initial conditions for the equilibrium statistical mechanics description to hold have been stressed in a clear way by a group of scientist around Lebowitz, see e.g. [14,15], in terms of typicality. It is not difficult to realize that there is a strong relationship between the typicality and the Khinchin approach. Without going in the mathematical details, we can notice that the key idea of typicality is in agreement with our results: irrespective to the nature of the microscopic dynamics, ensemble and dynamical averages are for practical purposes equivalent in the large-N limit. Let us note that often in non-equilibrium problems it is not possible to use in a simple way the Khinchin idea: for instance the study of transient properties necessarily requires initial conditions which are not typical, so that numerical simulations are unavoidable.

2. Model

Let us consider a harmonic chain with the following Hamiltonian

$$\mathcal{H}(q,p) = \sum_{j=1}^{N} \frac{p_j^2}{2m} + \frac{k}{2} \sum_{j=0}^{N} (q_{j+1} - q_j)^2, \tag{2}$$

where we can set masses and the elastic coefficient of the springs to $m = k = 1$. We consider fixed boundary conditions, $q_0 = q_{N+1} = 0$. The Hamiltonian in Eq. (2) can be easily put in a diagonal form with the following change of variables

$$\begin{aligned} Q_k &= \sqrt{\frac{2}{N+1}} \sum_{j=1}^{N} q_j \; \sin\left(\frac{\pi j k}{N+1}\right) \\ P_k &= \sqrt{\frac{2}{N+1}} \sum_{j=1}^{N} p_j \; \sin\left(\frac{\pi j k}{N+1}\right). \end{aligned} \tag{3}$$

By applying the above transformation, which is a canonical change of coordinates, one gets:

$$\mathcal{H}(Q,P) = \frac{1}{2} \sum_{k=1}^{N} (P_k^2 + \omega_k^2 Q_k^2) \tag{4}$$

where

$$\omega_k = 2 \sin\left(\frac{\pi k}{2N+2}\right), \tag{5}$$

is the angular frequency of the kth normal mode. It is then convenient for our purposes to introduce the semi-canonical complex variables:

$$\begin{aligned} z_k &= \frac{P_k + i\omega_k Q_k}{\sqrt{2\omega_k}} \\ z_k^* &= \frac{P_k - i\omega_k Q_k}{\sqrt{2\omega_k}}, \end{aligned} \tag{6}$$

such that

$$\begin{aligned} \mathcal{H}(z,z^*) &= \sum_{k=1}^{N} \omega_k \; |z_k|^2 \\ \{z_k^*, z_q\} &= i \; \delta_{k,q} \end{aligned} \tag{7}$$

3. Random modes thermalization

The considered system is such that if only one harmonic is excited at the beginning, i.e., one sets as initial condition $|z_k|^2 = E$, for a given k and $|z_q|^2 = 0$ for all $q \neq k$, energy is never shared among Fourier modes due to the lack of interaction. In other words, Fourier modes are integrability Liouville–Arnol'd theorem variables, so that no signature of thermalization can be found by definition looking at such variables. But let us consider a different point of view. The harmonic chain is a system characterized by a set of $2N$ real coordinate-momenta variables, or by a set of N complex coordinates, which can be chosen at will. The complex coordinates z_k represent just one of the infinitely many choices available. Any random rotation in the N-dimensional complex space leads to another possible system of coordinates. Let us denote with the symbol

$$\theta = \{\theta_1, \ldots, \theta_N\}, \tag{8}$$

the N random angles which define a random rotation in $\mathbb{C}^N$ and with $M(\theta)$ the unitary matrix, $M(\theta) \in U(N)$, which represent this rotation. In particular we have

$$M^\dagger M = M M^\dagger = \mathbf{1}, \tag{9}$$

where $M^\dagger$ means transpose and complex conjugate. We thus have infinitely many choices of *"random modes"*, which we define as random rotations of the Fourier modes and indicate as:

$$z_k(\theta) = \sum_{q=1}^{N} M_{kq}(\theta)\, z_q. \tag{10}$$

It is easy to check that the random rotation does not alter the Poisson parentheses structure between the variables:

$$\left\{z_p(\theta), z_q^*(\theta)\right\} = \sum_{ij} M_{pi}(\theta)\, M_{qj}^*(\theta)\, \left\{z_i, z_j^*\right\} = i \sum_{i=1}^{N} M_{pi}(\theta)\, M_{iq}^\dagger(\theta) = i\, \delta_{pq} \tag{11}$$

Clearly, in terms of these random modes the Hamiltonian is not anymore diagonal:

$$\mathcal{H}(z(\theta), z^*(\theta)) = \sum_{qp=1}^{N} c_{qp}(\theta)\, z_q^*(\theta)\, z_p(\theta), \tag{12}$$

where

$$c_{qp} = \sum_{k=1}^{N} \omega_k\, \mathcal{M}_{kq}^*(\theta)\, \mathcal{M}_{kp}(\theta), \tag{13}$$

with $\mathcal{M}(\theta) = [M^{-1}(\theta)]$, $\mathcal{M}(\theta) \in U(N)$.

We then define the energy of the random mode k as

$$\mathcal{E}_k(\theta) = c_{kk}(\theta)|z_k(\theta)|^2, \tag{14}$$

since $c_{kk}(\theta)$ is real then also $\mathcal{E}_k(\theta)$ is real. We have in fact by definition $c_{kk}(\theta) = c_{kk}^*(\theta)$, see Eq. (13). We can thus write the Hamiltonian by separating the diagonal from the non-diagonal contribution as

$$\mathcal{H}(z(\theta), z^*(\theta)) = \sum_{k=1}^{N} \mathcal{E}_k(\theta) + \sum_{q \neq p}^{N} c_{qp}(\theta)\, z_q^*(\theta)\, z_p(\theta), \tag{15}$$

and then perform the standard FPUT numerical experiment, which amounts to the numerical study of the relaxational dynamics when energy is initially fed to a single random mode:

$$\mathcal{E}_k = \begin{cases} E_0 & k = 1 \\ 0 & k \neq 1\,. \end{cases} \tag{16}$$

It is important to stress that, while it is true that at $t = 0$ the energy of the random mode with $k = 1$ is the total energy of the systems, since for all $k \neq 1$ we have $z_k(\theta, t = 0) = 0$ and hence all non-diagonal terms in Eq. (15) vanish, this is not true for any $t > 0$: due to the dynamics energy is shared among random modes and the off-diagonal terms of Eq. (15) also contribute at later times. We have checked that the amount of energy transferred to the off-diagonal terms in Eq. (15) amounts to less than the 1% of the total energy, on average in time, so that the random modes still represent physically meaningful variables, as long as they carry (on average) almost all the energy of the system. In the numerical simulations we used a symplectic algorithm to study the dynamics of a harmonic chain made of $N = 1023$ particles. The configuration of the system is evolved according to its Hamiltonian dynamics in the particles coordinate and momenta representation.

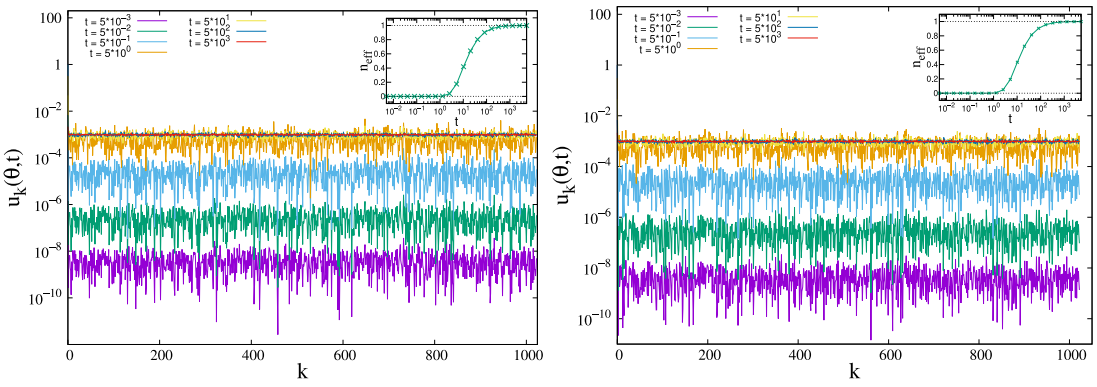

Fig. 1. Panels (a) and (b) show two different choices of *random modes*, i.e., two independent choices of the unitary random matrix $M(\theta)$. *Main*: Normalized random modes energy spectrum at different times, $u_k(\theta, t)$ vs k for increasing values of t; *Inset*: effective number of degrees of freedom as a function of time, $n_{eff}(\theta, t)$ vs t. The fact that at $t = 0$ energy is concentrated on the $k = 1$ mode, thus guaranteeing overall energy conservation, is emphasized in Fig. 2.

In agreement with the traditional approach to the Fermi–Pasta–Ulam–Tsingou problem [16–20] we have monitored along the dynamics the behaviour of the energy spectrum and of the *effective number* of degrees of freedom n_{eff}, an observable, defined below in Eq. (19), raising from $n_{\text{eff}} = 0$ when energy is concentrated on few modes to $n_{\text{eff}} = 1$ when energy is perfectly equipartited. The simplest way to study the degree of equipartition is obtained by considering the spectrum of $u_k(\theta, t)$:

$$u_k(\theta, t) = \frac{\langle \mathcal{E}_k(\theta) \rangle_t}{\langle \mathcal{E}_{tot}(\theta) \rangle_t}\,, \tag{17}$$

where $\langle \mathcal{E}_{tot}(\theta) \rangle_t = \sum_{k=1}^{N} \langle \mathcal{E}_k(\theta) \rangle_t$ and we consider cumulative time averages of the kind

$$\langle \mathcal{E}_k(\theta) \rangle_t = \frac{1}{t} \int_0^t ds\ \mathcal{E}_k(\theta, s)\,. \tag{18}$$

The strategy of considering time averages of single degree of freedom energies is quite common in the FPUT literature [18], although averages over initial conditions are considered as well [21]. While in non-pathological cases these two kind of averages are usually expected to yield the same kind of results, there are situations where the choice of initial conditions and the choice of the averaging procedure are of crucial importance, in particular for the behaviour of transients. This issue has been investigated in depth for the FPUT model [21–24], for which it has been shown explicitly how some particular choices of initial conditions, e.g., the choice of Fourier modes initial phases [22], strongly affect the duration of transients. Quite remarkably, in [24] it was then presented a first evidence that an appropriate choice of conditions (or, more generally, an appropriate choice of degrees of freedom as we will show in the following) allows to find thermalization even in the Toda model, a result in perfect agreement with the recent findings of two of us [9]. Coming back to the definition of $n_{\text{eff}}(\theta, t)$, which, physically, is analogous to an inverse participation ratio, we have that it reads as:

$$n_{\text{eff}}(\theta, t) = \frac{\exp\left(S_{\text{sp}}(\theta, t)\right)}{N}. \tag{19}$$

where $S_{\text{sp}}(\theta, t)$ is the so-called *spectral entropy*:

$$S_{\text{sp}}(\theta, t) = -\sum_{k=1}^{N} u_k(\theta, t) \log u_k(\theta, t), \tag{20}$$

a sort of entropy quite common in the FPUT literature [18], which is maximal when the degree of equipartition between the variables considered is maximal.

The parametric dependence of the spectrum $u_k(\theta, t)$ on the time variable t that we have found in numerical simulations is illustrated in Fig. 1 for two different choices of the random rotation θ. Two remarkable observations are in order: first, equipartition among random modes is fast; second, the phenomenon takes place on the same time-scale for different choices of the random rotation θ. We have therefore an indication that, apart the Fourier basis, fast relaxation to a thermal state seems to be the *typical* phenomenon for a random choice of the basis used to represent the chain configuration. The inset of each of the two panels of Fig. 1 represents the behaviour of the effective number of degrees of freedom $n_{\text{eff}}(t)$: the typical sigmoidal shape with a fast convergence to $n_{\text{eff}}(t) \approx 1$ signals the reaching of equipartition. Let us also point out a difference between Fig. 1 and similar ones which can be typically found in the literature on the Fermi–Pasta–Ulam–Tsingou problem, see for instance Fig. 1 in [20]. In the present case, when initially starting with energy only on the

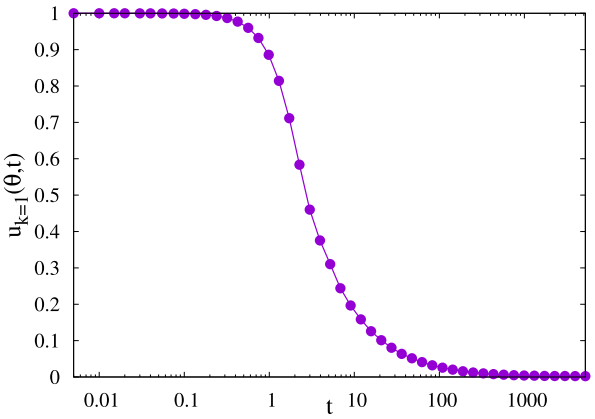

Fig. 2. Behaviour as a function of time of the normalized energy on the random mode with $k = 1$, $u_{k=1}(t)$ vs t.

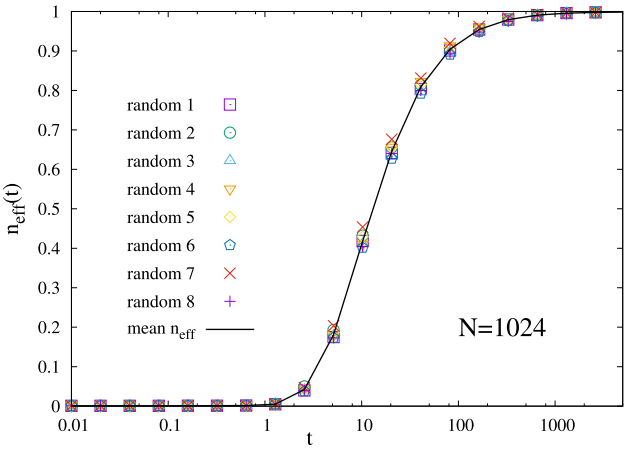

Fig. 3. Effective number of degrees of freedom as a function of time, $n_{eff}(\theta, t)$ vs t: the continuous (black) line represents the average $\overline{n_{eff}}(t)$ over 30 choices of the random modes basis, points represent the individual behaviour of 8 different instances.

$k = 1$ mode, there is no such thing as the two-stage relaxation process consisting first in the formation of a *packet* of excited modes with k close to $k = 1$ on a short time scale which is then followed by relaxation to equipartition at later times. This can be seen very clearly from Fig. 1 of the present paper: the energy stored initially on the $k = 1$ random mode is shared democratically at all times among all other modes. While from Fig. 1 it might be not clear that a decreasing amount of energy is left on $u_{k=1}$, this is clarified by Fig. 2, where it is represented the behaviour of $u_{k=1}(t)$ as a function of time. The overall trend of energy equipartition between random modes tells us that in this case the "wave-number" k does not represent indeed any length-scale, but is just a label for N independent random combinations of the Fourier modes. In some sense, anyone of the N random modes plays a role akin to that of a particle in the harmonic chain, as it is evident from the comparison of the time autocorrelation function shown in Fig. 3 of [6] and the autocorrelation function discussed later in this work (see Fig. 4). 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. And, what is most remarkable, *thermalization looks as the typical phenomenon* (see Fig. 3 below), 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 was at the basis of an averaging strategy proposed already in [25] to capture the essential thermodynamic features of the low temperature glassy phase of an optimization problem.

In Fig. 3 the behaviour of the effective number of degrees of freedom averaged over $M = 30$ instances of the random modes, where $\overline{n_{\text{eff}}}(\theta, t)$ (continuous line in Fig. 3) is defined as

$$\overline{n_{\text{eff}}}(t) = \frac{1}{M} \sum_{i=1}^{M} n_{\text{eff}}(\theta_i, t), \tag{21}$$

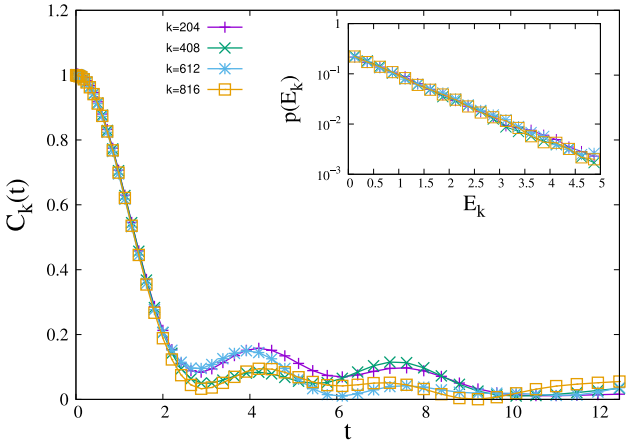

Fig. 4. *Main*: time auto-correlation function $C_k(t)$ as a function of time for different choices of the random modes index k, system size $N = 1023$; *Inset*: probability distribution of random-modes energy $\mathcal{E}_k$ for some values of k, system size $N = 1023$.

is compared with the behaviour for single instances of the random modes, $n_{\text{eff}}(\theta, t)$ (points): there is a clear evidence that for a chain of $N = 1023$ the behaviour of $n_{\text{eff}}(\theta, t)$ for each single instance is typical. Let us stress that the time average which is implicit in the definition of $n_{\text{eff}}(\theta, t)$ from the definition of $u_k(\theta, t)$ (see Eq. (17)), is not a necessity but is customarily used to smooth out the finite-N fluctuations. At large enough N the same behaviour is obtained from instantaneous configurations, as pointed out also in a recent paper on the thermodynamic behaviour of an ideal gas [26].

4. Equilibrium dynamics: importance of the large-*N* limit

Beside the "standard" FPUT-like numerical experiment discussed in the previous section, namely the study of relaxation from an atypical initial condition to a thermal state, it is important to investigate the equilibrium dynamics of the system. This will show that thermalization is achieved not only as equipartition among the chosen set of degrees of freedom, but also in the form of a Boltzmann-like equilibrium distribution of their energies. We present first the numerical results for the single-mode energy probability distributions, simply defined as the histogram of values taken by $\mathcal{E}_k$. In the inset of Fig. 4 it is shown that $p(\mathcal{E}_k)$, plotted for different values of k, has in all cases a nice exponential behaviour, as expected from a thermal ensemble:

$$p(\mathcal{E}_k) \sim \exp\left(-b\mathcal{E}_k\right), \tag{22}$$

where the value of b, proportional to the inverse of energy per degree of freedom, is identical for all random modes k. How to chose the degrees of freedom so that, even in an integrable systems, they thermalize? A conjecture about that, clearly inspired by the features of the random modes studied here, will be discussed in "Conclusions" paragraph. The second important test of thermalization is to check that the auto-correlation functions of the observables of interest decay in time fast enough. Clearly this is an heuristic approach: by definition, since our system is integrable it will always retain memory of the initial conditions. But one can adopt a pragmatic point of view: just look at the random modes energies and ignore that the system is integrable. How does look like an time auto-correlation function $C_k(t)$ of the energy on the random mode k? Let us define $C_k(t)$ as

$$C_k(t) = \frac{\langle \mathcal{E}_k(t)\mathcal{E}_k(0)\rangle - \langle \mathcal{E}_k\rangle^2}{\langle \mathcal{E}_k^2\rangle - \langle \mathcal{E}_k\rangle^2}\,. \tag{23}$$

In the main panel of Fig. 4 it is shown the behaviour of $C_k(t)$ for different values of k: the function rapidly decays and then oscillates in the vicinity of $C_k = 0$. How it is possible that an integrable system, moreover characterized by simple linear interactions, presents such good signatures of an equilibrium behaviour? Isn't it inconsistent with integrability? The way out to this apparent contradiction comes by taking into account the same two points which are the cornerstones of the Khinchin theorem: the consideration of the right observables and the large-N limit. The dynamics of Fourier modes amplitudes in the harmonic chain can be described analytically, as it is done, for instance, in a very insightful paper of Mazur and Montroll [6]. In fact, already in [6] it was shown that even in the harmonic chain, if one considers the energy of a single particle of the chain, the time-autocorrelation function decays fast to zero. In [6] the signature of integrability in the single particle dynamics was traced back to the quasi-periodic oscillations around zero of amplitude $N^{-1/2}$ in the time-autocorrelation function. The general picture emerging already from [6] and corroborated by the present results on random modes is therefore clear: if one considers as observables functions which are a (random) combinations of *all* the coordinates diagonalizing the Hamiltonian, integrability effects are small in N. For instance, if one considers the motion

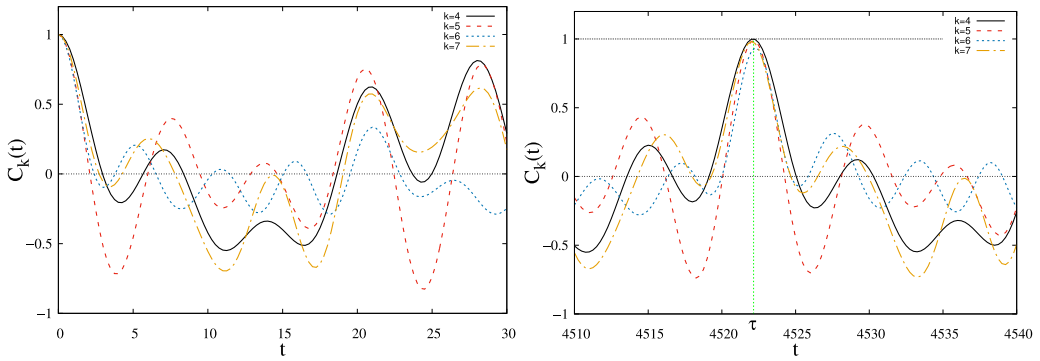

Fig. 5. Time autocorrelation function $C_k(t)$ as a function of time for different choices of the random-modes index k, system size $N = 7$.

of a single particle in a harmonic chain they are of order $\mathcal{O}(N^{-1/2})$ [6]. For what concerns the present work we have shown that the autocorrelation function of a random mode energy is for all practical purposes equivalent to that of single particle in the harmonic chain, since they both result from the combination of all Fourier modes. In agreement with the results of [6], it is worth showing that even in the present case the fast decay of $\langle \mathcal{E}_k(t)\mathcal{E}_k(0)\rangle$ is a large-N effect. Without going through a too much detailed finite-size analysis, we show here in Fig. 5 that for small system sizes (e.g., $N = 7$ particles) the recurrent nature of the integrable dynamics clearly emerges. In Fig. 5 it can be seen how the autocorrelation function defined in Eq. (23) depends on time for a harmonic chain of $N = 7$ particles and for some values of k: it is clear that at a characteristic time $\tau \approx 4520$ the system has gone back to the initial condition.

5. Overlaps distribution

Let us now represent in a quantitatively precise manner the statement, already stressed by some of us in [9], that the variables allowing to see thermalization in an integrable system must be *almost uncorrelated* to those diagonalizing the Hamiltonian. The purpose of the present section is therefore to stress, with the help of a quantitative evidence, that almost all the infinitely many possible choices of a random basis to represent the chain configuration, all corresponding to perfectly legitimate semi-canonical change of variables, correspond to variables statistically uncorrelated to Fourier modes. To this purpose let us introduce a more convenient bra–ket formalism. By considering a chain made of N particles we represent the harmonics of the chain as an orthonormal vector basis:

$$|z_k\rangle = \sqrt{\frac{2}{N+1}}\left\{\sin\left(\frac{\pi k}{N+1}\right), \ldots, \sin\left(\frac{\pi kN}{N+1}\right)\right\}, \tag{24}$$

with a scalar product defined as:

$$\langle z_q|z_k\rangle = \sum_{j=1}^{N}(z_q^j)^* z_k^j = \delta_{qk}, \tag{25}$$

where

$$z_k^j = \sqrt{\frac{2}{N+1}}\ \sin\left(\frac{\pi kj}{N+1}\right) \tag{26}$$

In this manner *any* state of the chain can be defined as

$$|\psi\rangle = \sum_{k=1}^{N} z_k|z_k\rangle, \tag{27}$$

where z_k is the quantity defined in Eq. (6). Using this formalism the energy of the system can be for instance represented as an operator such that

$$\hat{\mathcal{H}}|\psi\rangle = \sum_{k=1}^{N}\omega_k z_k|z_k\rangle, \tag{28}$$

so that the Hamiltonian of the systems simply reads as $\mathcal{H}(z^*, z) = \langle\psi|\hat{\mathcal{H}}|\psi\rangle$. Then, and here comes the usefulness of this formalism, it is straightforward to define a change of basis in the representation of the chain:

$$|z_k(\theta)\rangle = \sum_{q=1}^{N} M_{kq}(\theta)|z_q\rangle \tag{29}$$

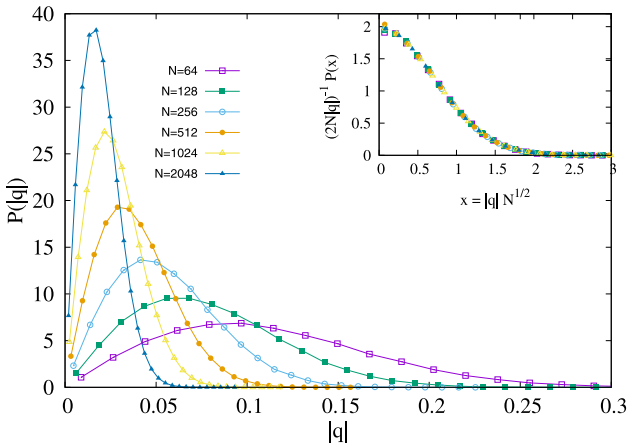

Fig. 6. *Main*: probability distribution $P(|q|)$ of the absolute value of the overlap between a Fourier mode and a random mode, for different sizes N of the system; *Inset*: collapsed data for different N.

It then comes natural the definition of the *overlap* between Fourier modes and random modes,

$$q_{kp} = \langle z_k(\theta)|z_q\rangle = \sum_{p=1}^{N} M^*_{kp}(\theta)\langle z_p|z_q\rangle = M^*_{kq}(\theta). \tag{30}$$

From the properties of random unitary matrices it is then possible to compute the probability distribution $\rho(|q|)$ of the overlap modulus. For the ease of the reader we report this elementary large deviation estimate in the Appendix, quoting here only the final result:

$$\rho(|q|) = 2N|q|\exp\left(-N|q|^2\right) \tag{31}$$

By recalling that we are dealing with a complex variable, $q \in \mathbb{C}$, the linear dependence on $|q|$ in front $\rho(|q|)$ is simply the Jacobian for the representation of a complex variable in polar coordinates, so that the probability distribution of the overlap, $\mathcal{P}(q) : \mathbb{C} \to \mathbb{R}$, is in fact simply a Gaussian with variance 1/N:

$$\mathcal{P}(q) \propto \exp\left(-Nq^2\right), \tag{32}$$

which completes our discussion about choosing a set of canonical coordinates which are *random combination* of the coordinates which make the integrable nature of the system manifest. In addition to what already observed in [9], in the present work we provided some further evidence in favour of the hypothesis that the set of (semi) canonical coordinates which behaves "thermally" are "many", most likely those corresponding to all the random unitary transformations $M(\theta) : \mathbb{C}^N \to \mathbb{C}^N$ not too close to the identity. It is remarkable how the large-N prediction of Eq. (31) is in good agreement with the numerical estimates of the probability distribution of overlaps at finite N, which is shown in Fig. 6. The numerical results of this paper cannot be clearly conclusive, but strongly suggest that a generic choice of a random modes basis allows to detect good thermalization properties. Once proved more rigorously, this result would be very close to a property outlined in [27] for random choices of eigenfunction basis in quantum systems.

6. Conclusions

The results presented in this work aim at clarifying a foundational problem in statistical mechanics: is dynamical chaos really a necessary condition to guarantee the thermalization of systems with many degrees of freedom? Our results generalize and strengthen the conclusions drawn for the Toda model in [9]: thermalization is achieved even in an integrable system, provided that an appropriate choice of the observables is made. The study of the harmonic chain added an insight: we have shown that in this system there are many (ideally, infinitely many) different choices of canonical coordinates which allow to detect thermalization. This evidence tells us that the lack of equilibrium is really a specific property of the coordinates which diagonalizes the Hamiltonian. Robust thermodynamic properties must be independent from the choice of the coordinates used to write the partition sum, an idea already exploited with success in replica calculations for *ordered* systems with a glassy phase [25]. This idea, which is substantiated mathematically by the Khinchin approach and of which we presented numerical evidence in this paper, tells us that even for integrable systems there are no *a priori* reasons to not expect the validity of equilibrium ensembles. This of course is not in contradiction with well established frameworks for integrable systems such as the Generalized Gibbs Ensemble [10–13,28–31], the latter being just specific of particular choice of the canonical coordinates. At the same time it is clear that the possibility

of unveiling specific properties of the dynamics crucially depends on the choice of variables, in particular for system where ergodicity is spontaneously broken as spin glasses [32–35] or systems highly structured and intrinsically characterized by multiple length/time scales like macro-molecules [36]. From the results of the present work and from that of [9], we are led to the conjecture that the observables following a Boltzmann–Gibbs statistics could be those defined in the following manner. Let $\mathcal{A}_i$ with $i = 1, \ldots, N$ be the N conserved quantities of our integrable system. An observable with good thermal properties should be each function B "independent enough" from any of the conserved quantities, that is, any function whose Poisson parenthesis with each conserved quantity is small in N, say $\{\mathcal{A}_i, B\} \sim 1/\sqrt{N}$ for each i. This condition is for instance the one fulfilled by what we have called "random modes".

As a final remark, let us notice that a generalization of the present results to quantum mechanics may provide further insights on the thermalization mechanism in quantum isolated systems [37], a theoretical issue which is the object of renewed interest thanks to the possibilities, offered by new technologies, to manipulate nanostructured materials suitable for quantum computing tasks. The point made by our findings on the *irrelevance of chaos* for the thermalization of harmonic systems are in fact quite similar to the Von Neumann quantum ergodic theorem approach [38,39]. According to the latter thermalization is in fact related to an appropriate choice of observables, rather than to the spectral properties of the Hamiltonian. The same scenario, where the choice of observables plays a central role, is the one underlying the Eigenstate Thermalization Hypothesis [40,41]. Numerical experiments to better explore the analogies between statistical mechanics foundations in classical and quantum systems, for instance simulations aimed at investigating thermal ensembles applicability in the presence of an external driving [42], in particular the study of fluctuation–dissipation relations, would be for instance very interesting.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix

In this Appendix we show how to compute the probability distribution of the generic matrix element M_{ki} (for simplicity of notation, let us omit the angle $\boldsymbol{\theta}$). To this aim it is possible to exploit the fact that each row/column of the matrix represents one (normalized) element of an eigenvector basis of $\mathbb{C}^N$, so that the following condition holds:

$$\sum_{i=1}^{N} |M_{ki}|^2 = A \qquad \forall k \,, \tag{33}$$

where A is the normalization that we will fix to 1 at the end of the calculation. Changing the notation so that: $\zeta_i = M_{ki}$, we have that the volume spanned by the elements of a row in M reads:

$$\Omega_N(A) = \int \prod_{i=1}^{N} d\,\mathrm{Re}(\zeta_i) d\,\mathrm{Im}(\zeta_i)\; \delta\left(A - \sum_{i=1}^{N} |\zeta_i|^2\right) \,, \tag{34}$$

so that the joint probability density is:

$$\rho(\zeta_1, \ldots, \zeta_N | A) = \frac{1}{\Omega_N(A)}\; \delta\left(A - \sum_{i=1}^{N} |\zeta_i|^2\right) \,. \tag{35}$$

Since we are looking for the distribution of a single matrix element, we are interested in the marginal:

$$\rho(\zeta_1 | A) = \int \prod_{i=2}^{N} d\,\mathrm{Re}(\zeta_i) d\,\mathrm{Im}(\zeta_i)\; \rho(\zeta_1, \ldots, \zeta_N | A) \,. \tag{36}$$

In order to compute $\Omega_N(A)$, let us switch to polar coordinates $\begin{cases} \mathrm{Re}(\zeta_i) = r_i \cos(\phi_i) \\ \mathrm{Im}(\zeta_i) = r_i \sin(\phi_i) \end{cases}$:

$$\Omega_N(A) = (2\pi)^N \int_0^{\infty} \left[\prod_{i=1}^{N} dr_i\; r_i\right]\; \delta\left(A - \sum_{i=1}^{N} r_i^2\right) \,. \tag{37}$$

In order to get to the result, we compute its Laplace transform:

$$\begin{aligned}\Omega_N(\mu) &= \int_0^\infty dA\ e^{-\mu A}\ \Omega_N(A)\\ &= (2\pi)^N \int_0^\infty \left[\prod_{i=1}^N dr_i\ r_i\right]\ \exp\left[-\mu \sum_i r_i^2\right] =\\ &= \left[2\pi \int_0^\infty dr\ r\ e^{-\mu r^2}\right]^N = \left(\frac{\pi}{\mu}\right)^N\\ &= \pi^N\ \exp\left[-N \log \mu\right]\end{aligned} \tag{38}$$

and then its inverse transform by applying the saddle point approximation, in the large-N limit:

$$\begin{aligned}\Omega_N(A) &= \frac{1}{2\pi i} \int_{\mu_0 - i\infty}^{\mu_0 + i\infty} d\mu\ e^{\mu A}\ \Omega_N(\mu)\\ &= \frac{\pi^N}{2\pi i} \int_{\mu_0 - i\infty}^{\mu_0 + i\infty} d\mu\ e^{N[\mu a - \log \mu]}\\ &= \frac{\pi^N}{2\pi i}\ \exp\left\{N[\mu^*(a)a - \log \mu^*(a)]\right\}\ ,\end{aligned} \tag{39}$$

having put $a = A/N$ and defined $\mu^*(a)$ as the saddle point value, which can be explicitly computed using the saddle point equation:

$$\frac{\partial}{\partial \mu}\left[\mu a - \log(\mu)\right] = 0 \quad \Longrightarrow \quad \mu^* = \frac{1}{a} = \frac{N}{A} = N\ , \tag{40}$$

having finally imposed the normalization condition: $A = 1 \longrightarrow a = 1/N$. Since we selected the value of μ which corresponds to the correct normalization of eigenvectors, we can simply compute the Laplace transform of the unnormalized marginal $\rho(\zeta|A)$ and plug in the correct value of μ^* in order to estimate its leading behaviour. Namely, we first consider:

$$\rho(r|A) \propto \int_0^\infty \left[\prod_{i=2}^N dr_i\ r_i\right]\ r\ \delta\left(A - r^2 - \sum_{i=2}^N r_i^2\right) \tag{41}$$

and then its Laplace transform, with the same procedure we already employed:

$$\rho(r|\mu) \propto \theta(r)\ re^{-\mu r^2} \qquad \overset{\mu^* = N}{\longrightarrow} \qquad \rho(r|N) = \mathcal{N}\ \theta(r)\ re^{-Nr^2}\ , \tag{42}$$

where $\theta(\cdot)$ is the Heaviside function and $\mathcal{N}$ the normalization factor. Therefore, considering that $r_i = |\zeta_i| = |M_{ki}|$, it is been shown that the probability distribution of the overlap between one of the normal modes and one of the random ones, in the large-N limit, is the product of a linear function and a Gaussian centred in $r = 0$ with standard deviation: $\sigma_g \sim 1/\sqrt{N}$. We can easily compute the normalization factor of the distribution, as well as the mean value and the variance, by solving Gaussian integrals; the results are:

$$\begin{aligned}A &= 2N\\ \langle r\rangle &= \sqrt{\frac{\pi}{4N}}\\ \sigma^2 &= \langle r^2\rangle - \langle r\rangle^2 = \left(1 - \frac{\pi}{4}\right)\frac{1}{N}\end{aligned} \tag{43}$$

In conclusion, the probability distribution for the overlaps $|q|$ (dropping the indices) reads:

$$\rho(|q|) = 2N|q|e^{-N|q|^2} \tag{44}$$

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