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Statistical Mechanics of an Integrable System

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Abstract
We provide here an explicit example of Khinchin's idea that the validity of equilibrium statistical mechanics in high dimensional systems does not depend on the details of the dynamics, as it is basically a matter of choosing the "proper" observables. This point of view is supported by extensive numerical simulation of the one-dimensional Toda chain, an integrable non-linear Hamiltonian system where all Lyapunov exponents are zero by definition. We study the relaxation to equilibrium starting from very atypical initial conditions and focusing on energy equipartion among Fourier modes, as done in the original Fermi-Pasta-Ulam-Tsingou numerical experiment. We consider other indicators of thermalization as well, e.g. Boltzmann-like probability distributions of energy and the behaviour of the specific heat as a function of temperature, which is compared to analytical predictions. We find evidence that in the general case, i.e., not in the perturbative regime where Toda and Fourier modes are close to each other, there is a fast reaching of thermal equilibrium in terms of a single temperature. We also find that equilibrium fluctuations, in particular the behaviour of specific heat as function of temperature, are in agreement with analytic predictions drawn from the ordinary Gibbs ensemble. The result has no conflict with the established validity of the Generalized Gibbs Ensemble for the Toda model, which is on the contrary characterized by an extensive number of different temperatures. Our results suggest thus that even an integrable Hamiltonian system reaches thermalization on the constant energy hypersurface, provided that the considered observables do not strongly depend on one or few of the conserved quantities. This suggests that dynamical chaos is irrelevant for thermalization in the large-N limit, where any macroscopic observable reads of as a collective variable with respect to the coordinate which diagonalize the Hamiltonian. The possibility for our results to be relevant for the problem of thermalization in generic quantum systems, i.e., non-integrable ones, is commented at the end.

Keywords Hamiltonian dynamics · Integrable systems · Thermal equilibrium · Gibbs ensemble

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1 Introduction

It is common wisdom that statistical mechanics works rather well at a practical level, meaning that its predictions about the relevant observables of a macroscopic system, based on equilibrium ensemble averages, correctly describe the actual behavior measured in experiments or numerical simulations [1,2]. For instance, statistical mechanics allows us to understand the features of macroscopic objects, including intriguing phenomena such as criticality and scale invariance. It is then quite natural to wonder about the origin of such a great success.

The problem of statistical mechanics foundations in weakly non-linear Hamiltonian systems has been widely investigated. A paradigmatic and historically crucial example is the Fermi-Pasta-Ulam-Tsingou (FPUT) problem [3–7]; many works originated by the study of this model showed that there are two main competing ingredients which allow for the emergence of a thermal phase in non-linear high-dimensional systems: *(i)* dynamical chaos, favouring thermalization, and *(ii)* the formation of stable or metastable recurrent excitations (breathers, solitons, etc.), which on the contrary slow down or completely arrest the relaxation to a thermal state [8–10].

This said, the true relevance of chaos to legitimate statistical mechanics is still an open issue. Roughly speaking the different points of view may be traced back to two opposite schools: *(i)* the "chaotic" one (based on the work of Prigogine and of his followers [11]), according to which a key role is played by the dynamics and, consistently, the presence of chaos is regarded as the basic ingredient for the validity of the statistical mechanics; *(ii)* the "traditional" one, following the original Boltzmann's ideas [12–16], which stresses the role of the large number of degrees of freedom. Important contributions to the latter point of view are due to Khinchin [12], as well as to Mazur and van der Linden [17]. Their results show that, although for most physical systems the ergodic hypothesis does not hold *mathematically*, it is *physically* valid in the following sense: if we limit our interest to collective variables, in systems with a large number of degrees of freedom N, the measure of the regions where ergodicity fails vanishes in the limit $N \to \infty$. In this respect the dynamics plays a marginal role, the key ingredient being only the assumption $N \gg 1$ and the use of collective observables, i.e., functions of *all* canonical coordinates (or, at least, of a finite fraction of them). Khinchin's approach has some practical limitations, in particular it is not constructive from the point of view of finding criteria to assess thermalization. For a given setup, i.e., a given choice of the observable and the initial conditions, it gives no hints about thermalization timescales. Despite these difficulties, Khinchin's point of view still seems to us the most promising way to gain some insight into the reason why macroscopic systems do actually thermalize.

To show this point, in this paper we consider a well known integrable Hamiltonian system, whose dynamics is, by definition, non chaotic. We will show that, even in this case, when thermalization indicators are measured with respect to canonical variables different from those which diagonalize the Hamiltonian, thermal equilibrium is reached within very reasonable times. Our numerical results strongly support the following agnostic scenario: *thermalization* is not an intrinsic property of the system but rather a property of the chosen description. It is from this point of view that our results are not in conflict with recent results on the Toda lattice [18], according to which the thermodynamics of this system is described by the Generalized Gibbs Ensemble (GGE). GGE is a Gibbs-like ensemble, initially introduced for isolated quantum systems [19,20], where to each conservation law of the Hamiltonian dynamics is associated a different temperature. In practice in the GGE the partition function reads as $\mathscr{Z} = \mathrm{Tr}[e^{-\sum_{i=1}^{N} \beta_i Q_i}]$, where the Q_i's represent the quantities conserved by the

dynamics, i.e., classically, $\{Q_i, \mathscr{H}\} = 0$, with $\{\cdot, \cdot\}$ being the Poisson parentheses. Although this ensemble provided consistent predictions for correlation functions in integrable models, initially with a big emphasis on quantum systems [19–24] and more recently also on classical ones [18,25–29], we believe that it is just a particular choice to describe the system. In fact, there are as many ways to write the partition function of a Hamiltonian system as are the possible choices for canonically conjugated variables. GGE represents a natural choice to emphasize the existence of many time scales and many energy scales in an integrable system. But is the knowledge of all these time and energy scales really necessary for the calculation of relevant macroscopic properties of the system? In particular is the GGE really necessary to estimate, just to make an example, the time average of global observables which depend, in general, on an extensive number of conserved quantities? These are in our opinion open questions which call for further investigations. In particular, the contribution of this paper is the presentation of neat numerical data which suggest that thermalization occurs at a single temperature for generic macroscopic observables, and their comparison with analytical calculations in the standard Gibbs ensemble. It is worth mentioning that in small systems even generic observables keep a strong correlation with conserved quantities, see for instance [30]: in this respect the large-N limit of the Khinchin approach seems to be crucial. Focusing on classical integrable systems is from this point of view particularly convenient since much larger sizes, compared to the quantum case, can be tested numerically.

The idea that the possibility to achieve thermalization depends on the choice of the observed degrees of freedom was proposed for instance in the domain of disordered systems with ergodicity breaking transitions: it is well known that in the replica-symmetry-broken phase of spin-glasses some degrees of freedom reach fast equilibration with the thermostat whereas others never equilibrate [31]. And this idea was proposed already before in [32,33]. Incidentally, from this point of view intriguing similarities between spin glasses and the GGE have been recently put in evidence in a series of papers focused on the idea of describing the broken-ergodicity phase of the spin glass as a multithermal system [34–36]. Given these premises, what we want to stress here is that for an appropriate choice of observables this multithermal description of integrable systems, or more in general systems with broken ergodicity, is not necessary. Here we want to stress much further this concept by showing that thermalization takes place also in integrable systems.

Let us notice that the Hamiltonian of an integrable system takes the form of a sum function, i.e., it can be written as $\mathscr{H} = \sum_{i=1}^{N} f_i(Q_i, P_i)$, where (Q_i, P_i) are the canonical variables which allow to diagonalize the Hamiltonian. This is exactly the original case discussed in Khinchin's book [12]; however it is worth reminding that Mazur and van der Linden [17] were able to prove an analogous result for Hamiltonians which are perturbations of an integrable system.

Bearing in mind the traditional approach of Ma's book [1], we adopt the following pragmatic definitions: (a) a system is at *equilibrium* if the time averages of relevant macroscopic observables, computed during suitably long time intervals, are in agreement with the corresponding ensemble averages; (b) *thermalization* occurs when, starting from an initial condition far from equilibrium, after a finite time the system reaches an equilibrium state, as defined above. To the best of our knowledge, the choice of the "relevant" observables, as already stressed by Ma [1], Onsager and Machlup [37], remains a subtle point, which cannot be easily bypassed.

The main message of the paper is that any generic Hamiltonian system in the large-N limit exhibits good thermalization and equilibrium properties irrespectively to whether or not ergodicity holds in the strict mathematical sense, provided that one considers "egalitarian" observables. By "egalitarian" we mean functions involving a finite fraction of the degrees of

freedom of the system, as suggested by Khinchin's approach. In practice, we are going to show that the the time averages are well approximated by analytic predictions drawn from equilibrium ensembles.

2 Model

We study numerically the Hamiltonian dynamics of the Toda model [38]. The system is constituted by N classical particles on a line connected by non-linear springs. We design with q_i the displacement from the equilibrium position of the i-th particle, $i = 1, ..., N$, and with p_i its conjugated momentum. The dynamics is defined by the following Hamiltonian:

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

where $V(x)$ is the Toda potential

$$V(x) = \exp(-x) + x - 1, \tag{2}$$

and we consider fixed boundary conditions, i.e. $q_0 = q_{N+1} = 0$. It has been shown by Hénon in [39] that in the Toda lattice there are N conserved quantities, i.e., N functions $\mathscr{I}_k$ such that $\{\mathscr{H}, \mathscr{I}_k\} = 0$, with $k = 1, \ldots, N$; as a consequence, model (1) is integrable. The explicit expression of the first few Hénon's integral of motion for a periodic system and how this definition can be adapted to a system with fixed boundary conditions can be found in Appendix 1.

The key idea of this paper is to study indicators of thermal equilibrium with respect to a set of canonical variables different from those which diagonalize the Hamiltonian, i.e. the Toda modes. In particular, we focus our attention on the Fourier modes, which do not diagonalize the Hamiltonian in Eq. (1) but nevertheless represent a complete basis for any configuration of the chain. These modes are defined from the set of canonical coordinates (q_i, p_i) by means of the following sine Fourier transform,

$$\begin{aligned} Q_k &= \sqrt{\frac{2}{N+1}} \sum_{i=1}^{N} q_i \ \sin\left(\frac{\pi i k}{N+1}\right) \\ P_k &= \sqrt{\frac{2}{N+1}} \sum_{i=1}^{N} p_i \ \sin\left(\frac{\pi i k}{N+1}\right), \end{aligned} \tag{3}$$

which represents a canonical change of coordinates. In terms of the Fourier modes the Hamiltonian in Eq. (1) is highly non-linear. In particular, it has nonlinearities at all orders, reading as

$$\mathscr{H}(Q, P) = \frac{1}{2} \sum_{k=1}^{N} (P_k^2 + \omega_k^2 Q_k^2) + \sum_{p=3}^{\infty} \sum_{k_1, \ldots, k_p} \alpha_{k_1 \ldots k_p} \ Q_{k_1} \cdots Q_{k_p} \,, \tag{4}$$

where

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

is the angular frequency of the k-th normal mode in the small-energy limit and $\{\alpha_{k_1 \ldots k_p}\}$ are suitable coefficients.

Let us ignore for a moment that Toda model is integrable: by just looking at Eq. (4), very naively we may conclude that energy exchanges between Fourier modes are very efficient and that the system, whatever the initial condition, relaxes to equilibrium quickly. This is exactly what we find, notwithstanding integrability. Very roughly, the behavior of the system meets the most naive expectation that the energy stored in the infinitely many non-linear terms on the right-hand side of Eq. (4) acts as a thermal bath for the harmonic terms. We present evidences of this behavior both studying the relaxation to equilibrium from a very atypical initial configuration and also studying how phase space is sampled by the "equilibrium" dynamics of the system, i.e., the Hamiltonian dynamics initialized with a *typical* initial condition. Clearly, we assume a definition of what is "typical" or "not typical" having in mind the presumed equilibrium measure, i.e., the uniform measure on constant energy hypersurfaces.

3 Relaxational Dynamics

First, we have repeated the celebrated FPUT experiment, i.e. we have studied how an atypical initial condition, obtained by assigning all harmonic energy to the lowest mode of the chain, relaxes to equilibrium, here identified by equipartition among all modes.

The initial conditions for this non-equilibrium relaxation dynamics are:

$$\omega_k^2 Q_k^2 = P_k^2 = \begin{cases} E_0 & k = 1 \\ 0 & k \neq 1 \,. \end{cases} \tag{6}$$

Therefore the value of E_0 set in the initial condition does not correspond to the total energy of the system, which comprises the non-linear terms of Eq. (4). Along the non-equilibrium dynamics we have monitored two indicators, one qualitative the other quantitative. The first is the power spectrum of the system,

$$u_k(t) = \frac{\langle E_k \rangle_t}{\langle E_{tot} \rangle_t} \,, \tag{7}$$

where E_k denotes the harmonic energy

$$E_k = \frac{1}{2} \left[P_k^2 + \omega_k^2 Q_k^2 \right] \,, \tag{8}$$

while $E_{tot} = \sum_{k=1}^{N} \langle E_k(t) \rangle$ and we consider cumulative time averages of the kind

$$\langle E_k \rangle_t = \frac{1}{t} \int_0^t ds \; E_k(s) \,. \tag{9}$$

From Fig. (1) it is clear that after a transient where the harmonic energy remains concentrated on the low-k modes it is then shared among all modes. Quantitatively this information is encoded in the behavior of the spectral entropy $S_{\rm sp}$ and of the effective number of degrees of freedom $n_{\rm eff}$, which are defined as follows:

$$\begin{aligned} S_{\rm sp}(t) &= -\sum_{k=1}^{N} u_k(t) \log u_k(t) \\ n_{\rm eff}(t) &= \frac{\exp\left(S_{\rm sp}\right)}{N} . \end{aligned} \tag{10}$$

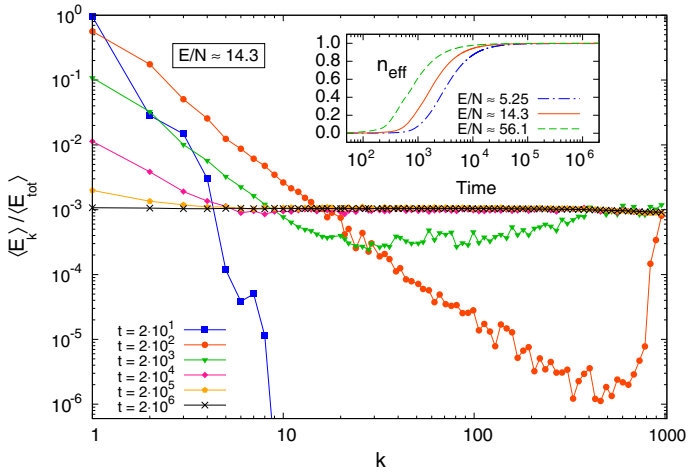

Fig. 1 *Main*: Energy spectrum of Fourier modes, $\langle E_k \rangle / \langle E_{tot} \rangle$ vs k, at different times (different symbols) for a Toda lattice with $N = 1023$ particles and total energy $E/N \simeq 14.3$ (here $E_0 = 4.0$). *Inset*: Effective number of degrees of freedom, n_{eff}, as function of time for different values of the energy. The value $n_{eff} = 1$ signals equipartition. Time-step for integration: $\Delta t = 0.02$

The behavior of $n_{\text{eff}}(t)$ is shown in the inset of Fig. 1: we find the typical sigmoidal shape starting from small values at the initial times, where energy is localized in the spectrum, and approaching $n_{\text{eff}} = 1$, the value typical of equipartition at later times. We thus see that, notwithstanding the fact that all Lyapunov exponents are zero, the system exhibits an *emerging* relaxational timescale. In the main panel of Fig. 1 we show results for a given value of the total energy E; from the behavior of $n_{\text{eff}}(t)$ for various choices of the total energy E in the inset it is clear that the qualitative feature does not change at varying E. Problems such as the dependence of the characteristic timescale on the initial energy and more in general the dependence on the initial condition and on the system size N are of course technically interesting, but are left for future investigations.

Before presenting other tests of thermalization let us comment on the reliability of numerics, usually characterized by unavoidable approximations such as the study of finite-size systems, finite lapses of time and discrete time dynamics. In fact, there are two sources of troubles which cannot be avoided in the numerical integration of differential equations: (a), the algorithm for the integration from time t to $t + \Delta t$ cannot be exact; (b), the computer necessarily works with integer numbers. Numerical simulations of dynamical systems cannot achieve arbitrary precision. Therefore, even if the system is strictly deterministic, as is the case of Hamiltonian systems, its numerical study is always affected by a small amount of "randomness" due to numerical roundings. Nevertheless, it has been shown that symplectic algorithms are rather efficient in limiting the spreading of numerical errors in the simulation of Hamiltonian systems; this is related to the (important) fact that, at variance with other popular algorithms (e.g. Runge-Kutta) they allow to preserve the Hamiltonian structure during the time evolution. For this reason in our numerical simulations we used the well-known leap-frog symplectic integrator [40].

To test the stability of numerical results is a compelling issue, in particular for the conclusions drawn in this paper. Fast equipartition between Fourier modes starting from very atypical initial configurations, although in agreement with the premises of Khinchin's approach, is a rather unexpected result for an integrable system. Usually non-linear Hamiltonian systems

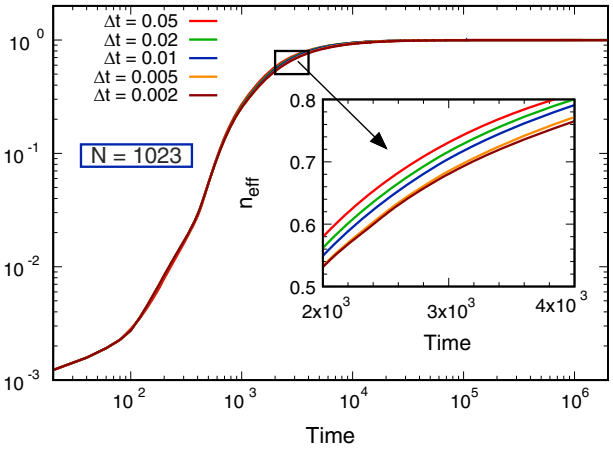

Fig. 2 *Main*: Effective number of degrees of freedom as a function of time, $n_{eff}(t)$ vs t, for different choices of timestep Δt in the numerical integration algorithm. All results are for the system size $N = 1023$. *Inset*: Zoom of the curves

are characterized by long time-scales emerging in the proximity of an integrable limit [5,7]. And in general, for classical integrable systems, one expects signatures of integrability to be manifest in every cirmustance [18,25] (not even to mention the case of integrable quantum systems [24,26,28]). A study of how equipartition times depend on the numerical protocol is therefore mandatory in the present situation. In order to check that equipartition between Fourier modes is not an artifact of the numerical protocol we have verified that our results do not depend on the time-step of the algorithm. This has been done for a chain of $N = 1023$ particles. In particular in Fig. 2 we show that varying Δt does not lead to any sensible increase of relaxation time. This result is not a proof, of course, but it gives us a very reasonable argument to expect that thermalization also occurs in the infinite precision limit, $\Delta t \to 0$.

Leaving apart the above practical test, in order to support the validity of our conclusions on thermalization it is worth to recall a result demonstrated mathematically only for Anosov system but accepted in more generic situations. What has been shown in [41,42] is that for a high precision integration algorithm, even in the case of arbitrary deviations of the numerical trajectories from the "true" ones (same initial conditions) due to rounding errors, the dynamical averages performed along the "original" trajectory and the one perturbed by rouding errors do coincide. This means that, assuming some weak form of ergodicity, the "statistical reproducibility" of the true dynamics by the numerical simulations is typical [41, 42].

4 Equilibrium Dynamics

Initial conditions which are both good to mimic thermal equilibrium and to set precisely the initial value of the energy are obtained by putting all initial amplitudes Q_k equal to zero and taking

$$\sum_{k=0} P_k^2 = 2E_0 \tag{11}$$

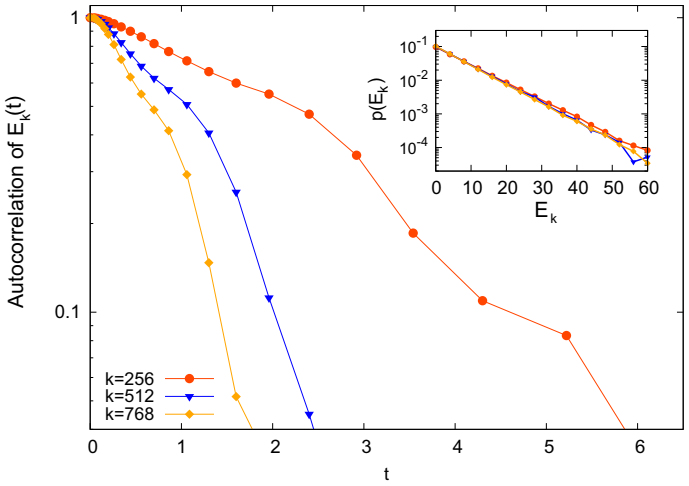

Fig. 3 *Main*: Time correlation function for the harmonic energy at different values of k: $k = 256, 512, 768$ for a Toda lattice with $N = 1023$ particles and energy $E/N = 4.0$. *Inset*: Probability distribution of the harmonic energy ε_k for different values of k

This condition can be obtained quite easily by sampling the initial velocity of each particle from a Gaussian distribution, which guarantees a good degree of randomization, and then rescaling all velocities according to the chosen value of E_0. One then considers equilibrium observables such as the time decay of the harmonic energies self-correlations:

$$C_k(t) = \frac{\langle E_k(t)E_k(0)\rangle - \langle E_k\rangle^2}{\langle E_k^2\rangle - \langle E_k\rangle^2}\,, \tag{12}$$

and the probability distribution of the harmonic energy of a given mode $p(E_k)$, which is simply defined as the histogram of values taken by E_k. In Fig. 3 it is shown that $C_k(t)$, for some given values of k, rapidly decays to zero. At the same time we find a nice exponential behavior for $p(E_k)$:

$$p(E_k) \sim \exp\left(-bE_k\right), \tag{13}$$

where the value of b is close to the inverse of the temperature in the simulation at small energies while it deviates at high energies. The description of the system in terms of normal modes is indeed appropriate for energy not too large while in the opposite limit of very high energy the system becomes similar to hard spheres.

Let us now compare the time average of some observables of obvious interest computed in simulations with initial conditions as in Eq. (11) with the prediction which can be worked out explicitly from the calculation of the partition function

$$\mathscr{Z}_N(\beta) = \mathscr{Z}_N^{(\mathrm{K})}(\beta)\cdot\mathscr{Z}_N^{(\mathrm{P})}(\beta), \tag{14}$$

where the kinetic and the potential contributions, respectively $\mathscr{Z}_N^{(\mathrm{K})}(\beta)$ and $\mathscr{Z}_N^{(\mathrm{P})}(\beta)$, are factorized and read respectively as

$$\mathscr{Z}_N^{(\mathrm{K})}(\beta) = \beta^{-N/2}$$

$$\mathscr{Z}_N^{(\mathrm{P})}(\beta) = \int_{-\infty}^{\infty} \prod_{i=1}^{N+1} dr_i \; e^{-\beta V(r_i)} \; \delta\left(\sum_{i=1}^{N+1} r_i\right)$$
$$= e^{\beta N} \int_{s_0-i\infty}^{s_0+i\infty} \frac{ds}{2\pi i} \; \exp\left\{N \log z_\beta(s)\right\}, \tag{15}$$

with

$$z_\beta(s) = \int_{-\infty}^{\infty} dr \; \exp\left(-\beta e^{-r} + sr\right). \tag{16}$$

The partition function $\mathscr{Z}_N^{(\mathrm{P})}$ can be computed exactly in the large-N limit (details can be found in App. 2), yielding:

$$\mathscr{Z}_N^{(\mathrm{P})} = e^{\beta N} \; \beta^{-\mu(\beta)} \; \Gamma[\mu(\beta)], \tag{17}$$

where the function $\mu(\beta)$ is determined implicitly by the condition:

$$\frac{\Gamma'(\mu)}{\Gamma(\mu)} = \log(\beta), \tag{18}$$

and does not have in general an explicit expression. For the comparison between simulation and theory let us now focus *only* on the potential energy partition function $\mathscr{Z}_N^{(\mathrm{P})}(\beta)$. By plugging the expression of $\mathscr{Z}_N^{(\mathrm{P})}(\beta)$ from Eq. (17) into the standard formulas

$$\langle u \rangle = -\frac{1}{N} \frac{\partial}{\partial \beta} \log \mathscr{Z}_N^{(\mathrm{P})}(\beta)$$
$$C_V = \frac{\beta^2}{N} \frac{\partial^2}{\partial \beta^2} \log \mathscr{Z}_N^{(\mathrm{P})}(\beta), \tag{19}$$

one obtains the analytical predictions for the average potential energy $\langle u \rangle$ and the specific heat C_V which are plotted in Fig. 4, where they are also compared with the numerical data. Apart from small discrepancies for C_V, probably due to the lack of large enough statistics, it is clear that the numerical behavior is well reproduced by the exact computation of C_V done assuming thermal equilibrium in the canonical ensemble. The formula of C_V cannot be given in the general case explicitly in terms of β, because one needs the knowledge of $\mu(\beta)$, which is determined only implicitly by Eq. (18). An expression of C_V in terms of $\mu(\beta)$ can be found in App. 2. What can be written explicitly are the asymptotic behaviors, which read:

$$T \to 0 \quad \Longrightarrow \quad \langle u \rangle = \frac{T}{2}; \qquad C_V = \frac{1}{2}$$
$$T \to \infty \quad \Longrightarrow \quad \langle u \rangle \sim \frac{T}{\log(T)}; \quad C_V \sim \frac{1}{\log(T)}. \tag{20}$$

Asymptotically, we have

$$C_V \approx \langle u \rangle / T, \tag{21}$$

which nicely compares with the results shown in Fig. 4. We have thus shown that, despite the Toda model being integrable, its behavior is strikingly well captured by equilibrium statistical mechanics formulas. In order to simulate a canonical ensemble avoiding any noise source modeling the heat bath, we have just studied the Hamiltonian dynamics of a systems with N particles and focused our attention on subsystems of N_* particles each, with $1 \ll N_* \ll N$. For instance we have considered the subsystems in the central part of the chain, in such a

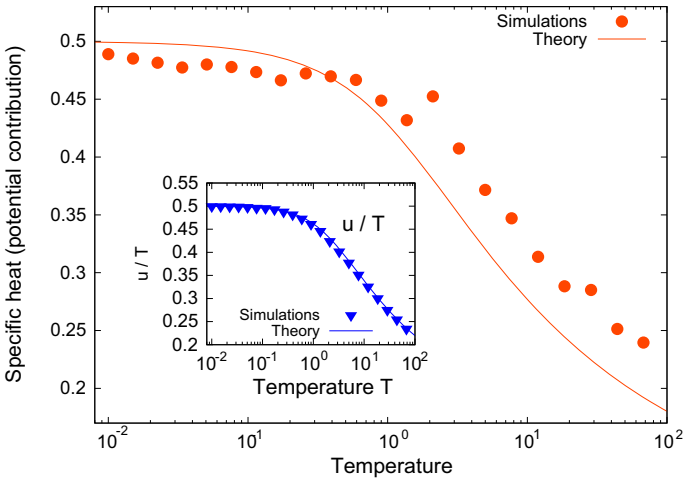

Fig. 4 *Main*: Potential contribution of the specific heat C_V as a function of temperature T. Points: numerical data obtained by using Eq. (22) with $N_* = 50$ and averaging over 10 different subsystems, for a total time $\mathscr{T} = 5 \cdot 10^6$; lines: analytical prediction. *Inset*: average *potential* energy as a function of temperature T; points, numerical data; lines, analytical prediction

way that the fixed boundary conditions are not very relevant. In the simulations the specific heat has been computed as

$$C_V = \frac{\langle E_*^2 \rangle - \langle E_* \rangle^2}{N_* T^2}, \tag{22}$$

where E_* is the energy in the subsystem with N_* particles and temperature is defined as $T = \langle p^2 \rangle$.

Let us stress that the good agreement between equilibrium calculations and numerical simulations is not particularly surprising for what concerns the behavior of the average energy $\langle u \rangle$: basically, it is a sort of virialization of the global kinetic energy starting from initial conditions which are not at equilibrium. On the contrary the test for the specific heat, which involves the behavior of the energy fluctuations of a subsystem, is rather severe. Let us note that this result for the specific heat is quite analogous to the one obtained in the FPUT system [43], where chaos is present.

5 Conclusions

We have shown, by comparing analytical results with numerical simulations, that even the dynamics of an integrable system such as the Toda chain has good "equilibrium" properties, provided one looks at "generic" observables. In the present context a good definition of "generic" looks as the one of *"collective with respect to the canonical coordinates which diagonalize the Hamiltonian"*. This observation suggests the possibility to generalize the implications of our results to generic quantum systems, i.e. to the *non-integrable* quantum unitary dynamics. The Schrödinger equation has in fact, by construction, properties very similar to integrable systems. In particular, the coherent motion of the eigenvectors phases is analogous, in the case of a N-dimensional system, to the one of the N angles of the Liouville-Arnold's theorem action-angle pairs. The analogy between *generic* quantum systems and

integrable classical ones stems from the conservation along quantum dynamics of the N projectors on energy eigenstates, $\hat{P}_\alpha = |\varepsilon_\alpha\rangle\langle\varepsilon_\alpha|$. We do not consider here the more subtle case of *integrable* quantum systems, where these N global conservation laws are also accompanied by the conservation of N local charges Q_i. Finding what is the "classical analog" of an integrable quantum system is therefore a subtler issue: one needs to find a system with $2N$ conservation laws, among which N are global and N are local. On the other hand, the problem of thermalization is interesting already in the case of non-integrable quantum systems. For instance in the case of small systems sizes, where the validity of "bona-fide" ergodicity assumptions as the Eigenstate Thermalization Hypothesis is not granted [44,45], one finds clear signatures of the built-in integrability due to quantum unitary dynamics [30].

If we thus try to extrapolate the implications of our results to quantum systems, we may say that the decoherence between the phases of different eigenvectors may be *not necessary* for the thermalization of the system: to detect thermalization one just needs to look at observables uniformly spread on *all* eigenvectors. This last conclusion seems quite in line with Von Neumann's "quantum ergodic theorem" [46,47]. According to the latter, relaxation to a thermal state is a property of the chosen observables rather than of the energy eigenmodes (absence of) structure. Structureless eigemodes are in fact the landmark of the so-called "quantum chaos" [48]. A similar thing happens also for the Eigenstate Thermalization Hypothesis, which is regarded by someone as the modern version of the Von Neumann theorem. Then, what is similar between the Von Neumann quantum ergodic theorem and the results due to Khinchin, Mazur and van der Linden is the lack of any explicit mention to quantum or dynamical chaos. Our numerical results on the Toda model seem to be quite in line with the idea of *"thermalization without chaos"*. Further investigations are for sure needed to clarify the problem of thermalization in the presence of conservation laws in high-dimensional Hamiltonian systems, the study of thermal properties in isolated quantum systems and classical integrable ones is a topic which keeps on attracting many scholars, see also [47,49,50].

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Appendix

Integrals of Motion

Just for the sake of self-consistency we briefly remind here the conservation laws of the Toda system. In the case of a periodic lattice with N particles where $q_0 = q_N$ the first four integrals of motion read as:

$$\mathscr{I}_1 = \sum_{i=1}^{N} p_i$$

$$\mathscr{I}_2 = \sum_{i=1}^{N} \frac{p_i^2}{2} + \mathscr{U}_i$$

$$\mathscr{I}_3 = \sum_{i=1}^{N} \frac{p_i^3}{3} + (p_i + p_{i+1})\mathscr{U}_i$$

$$\mathscr{I}_4 = \sum_{i=1}^{N} \frac{p_i^4}{4} + (p_i^2 + p_{i+1}^2 + p_i\, p_{i+1})\mathscr{U}_i + \frac{\mathscr{U}_i^2}{2} + \mathscr{U}_i \mathscr{U}_{i+1}, \tag{23}$$

where $\mathscr{U}_i = e^{-(q_{i+1}-q_i)}$. Note that $\mathscr{I}_2$ is nothing but the energy (apart for an irrelevant additive constant). The expressions in Eq. (23), see, e.g., [39], can be extended to the case of fixed boundary conditions by conventionally defining a periodic chain with $2N+2$ particles where the coordinates from q_0 to q_{N+1} are identical to the original one, while those such as q_{N+1+i} with $i = 1, \ldots, N$ are defined in order to have an odd function with respect to the center of the lattice:

$$\begin{aligned} q_{N+1+i} &= -q_{N+1-i} \\ p_{N+1+i} &= -p_{N+1-i} \end{aligned} \tag{24}$$

Specific Heats

The first step to compute the specific heat is the calculation of the partition function. For consistency with the numerical simulations, we compute it with fixed boundary conditions. That is, we have N variables q_i with $i = 1, \ldots, N$ to integrate over, while

$$q_0 = q_{N+1} = 0 \tag{25}$$

By identifying with the same variable the two fixed boundaries, i.e., $q_0 = q_{N+1}$, we can thus change variables to

$$r_i = q_{i+1} - q_i, \tag{26}$$

with, in particular

$$\begin{aligned} r_N &= q_{N+1} - q_N, \\ r_{N+1} &= q_1 - q_{N+1}. \end{aligned} \tag{27}$$

We can thus safely integrate over the $N+1$ variables r_i under the global constraint $\sum_{i=1}^{N+1} r_i = 0$:

$$\mathscr{Z}_N^{(\mathrm{P})}(\beta) = e^{\beta N} \int_{-\infty}^{\infty} \prod_{i=1}^{N+1} dr_i \; e^{-\beta \sum_{i=1}^{N+1} \exp(-r_i)} \; \delta\left(\sum_{i=1}^{N+1} r_i\right). \tag{28}$$

In order to *unfold* the global constraint it is useful to exploit the inverse Laplace rapresentation of the partition function:

$$\begin{aligned} \mathscr{Z}_N^{(\mathrm{P})}(\beta) &= e^{\beta N} \int_{s_0-i\infty}^{s_0+i\infty} \frac{ds}{2\pi i} \int_{-\infty}^{\infty} \prod_{i=1}^{N+1} dr_i \; \exp\left(-\beta \sum_{i=1}^{N+1} \exp(-r_i) + s \sum_{i=1}^{N+1} r_i\right) \\ &= e^{\beta N} \int_{s_0-i\infty}^{s_0+i\infty} \frac{ds}{2\pi i} \left[\int_{-\infty}^{\infty} dr \; \exp\left(-\beta e^{-r} + sr\right)\right]^{N+1} \\ &= e^{\beta N} \int_{s_0-i\infty}^{s_0+i\infty} \frac{ds}{2\pi i} \; \exp\left\{N \log z_\beta(s)\right\} \end{aligned} \tag{29}$$

where we have introduced the partition function per degree of freedom:

$$z_\beta(s) = \int_{-\infty}^{\infty} dr \; \exp\left(-\beta e^{-r} + sr\right). \tag{30}$$

It is convenient to regard β as a parameter in Eq. (30) and consider $z_\beta(s)$ as a function of s in the complex s plane. Clearly the integral expression in Eq. (30) is well defined only for $\mathrm{Re}(s) < 0$, so that it is convenient to change variable in the integral of Eq. (29) from s to $\mu = -s$:

$$\mathscr{Z}_N^{(\mathrm{P})}(\beta) = e^{\beta N} \int_{\mu_0 - i\infty}^{\mu_0 + i\infty} \frac{d\mu}{2\pi i} \, \exp\left\{ N \log \hat{z}_\beta(\mu) \right\}, \tag{31}$$

where now the contour in the complex plane passes through $\mathrm{Re}(\mu_0) > 0$ and we have the partition function per degree of freedom defined as:

$$\hat{z}_\beta(\mu) = \int_{-\infty}^{\infty} dr \, \exp\left(-\beta e^{-r} - \mu r \right). \tag{32}$$

The partition function of the whole system $Z_N(\beta)$ can be computed from Eq. (31) by means of a saddle-point approximation in the large-N limit. But first we need to compute explicitly $\hat{z}_\beta(\mu)$ in Eq. (32). By going through two changes of variables, i.e.,

$$\begin{aligned} x \to u &= e^{-x} \\ u \to t &= \beta u, \end{aligned} \tag{33}$$

we obtain

$$\begin{aligned} \hat{z}_\beta(\mu) &= \int_0^\infty du \, u^{\mu-1} e^{-\beta u} = \frac{1}{\beta^\mu} \int_0^\infty dt \, t^{\mu-1} \, e^{-t} \\ \hat{z}_\beta(\mu) &= \frac{\Gamma(\mu)}{\beta^\mu}. \end{aligned} \tag{34}$$

In order to compute the integral in Eq. (31) by means of the saddle-point approximation we just need to solve the saddle-point equation

$$\begin{aligned} &\frac{\partial}{\partial \mu} \left(\log \Gamma(\mu) - \mu \log(\beta) \right) = 0 \\ \Longrightarrow \quad &\frac{\Gamma'(\mu)}{\Gamma(\mu)} = \log(\beta) \end{aligned} \tag{35}$$

At this stage, without doing any approximation and indicating as $\hat{\mu}(\beta)$ the function implicitly determined by the condition in Eq. (35), one has that the partition function of the system reads:

$$\mathscr{Z}_N^{(\mathrm{P})}(\beta) = e^{\beta N} \frac{\Gamma(\hat{\mu}(\beta))}{\beta^{\hat{\mu}(\beta)}}. \tag{36}$$

For instance the specific heat C_V, which can be obtained from Eq. (36) using the standard formula in Eq. (18) of the main text, reads as

$$C_V = -\frac{1}{\psi'(\hat{\mu}(\beta))} - \left[\psi(\hat{\mu}(\beta)) - \log(\beta) \right] \left(\frac{\psi''(\hat{\mu}(\beta))}{[\psi'(\hat{\mu}(\beta))]^3} + \frac{1}{\psi'(\hat{\mu}(\beta))} \right) + \hat{\mu}(\beta), \tag{37}$$

being $\psi(x)$ the so-called *digamma* function $\psi(x) = \Gamma'(x)/\Gamma(x)$. The expression in Eq. (37) is not very insightful, but is necessary to plot the full analytic behavior of the function. Similarly one can write down the expression for the temperature, but we leave this exercise to the willing reader.

On the contrary, what can be obtained explicitly, are the asymptotic behaviors for both the average potential energy $\langle u \rangle$ and the specific heat C_V in the limit of small and large

temperatures T. This is obtained by the knowledge of the two asymptotic behaviors of the digamma function $\psi(\mu)$:

$$\begin{aligned} \mu \to \infty \quad &\Longrightarrow \quad \psi(\mu) \sim \log(\mu) \\ \mu \to 0 \quad &\Longrightarrow \quad \psi(\mu) \sim -\frac{1}{\mu}. \end{aligned} \tag{38}$$

We thus have two different approximations for our saddle-point equations in the *low-temperature*, $\beta \to \infty$, or the *high-temperature*, $\beta \to 0$, limit:

$$\begin{aligned} \text{Low T:} \quad &\Longrightarrow \quad \log(\mu) = \log(\beta) \quad \Longrightarrow \quad \mu = \beta \\ \text{High T:} \quad &\Longrightarrow \quad -\frac{1}{\mu} = \log(\beta) \quad \Longrightarrow \quad \mu = -\frac{1}{\log(\beta)} \end{aligned} \tag{39}$$

Let us first consider the low-temperature case, where Toda is well-approximated by a system of weakly coupled harmonic oscillators, for which the specific heat is constant. In this case we get:

$$Z_N(\beta) \approx \exp\left((N+1)\left[\beta + \log\Gamma(\beta) - \beta\log(\beta)\right]\right). \tag{40}$$

By using the Stirling's approximation

$$\log\Gamma(\beta) = \beta\log(\beta) - \beta - \frac{1}{2}\log(\beta), \tag{41}$$

we thus get

$$Z_N(\beta) \approx \exp\left[-\frac{N}{2}\log(\beta)\right]. \tag{42}$$

From Eq. (42) and from the definition of C_V in Eq. (18) in the main text we get

$$C_V = \beta^2 \frac{\partial^2}{\partial\beta^2}\left(\frac{N}{2}\log(\beta)\right) = \frac{1}{2}. \tag{43}$$

In the light of the high-temperature expansion, we get

$$\beta \to 0 \Longrightarrow \mathscr{Z}_N(\beta) \approx \left\{N\left[\beta + \log\Gamma\left(-\frac{1}{\log(\beta)}\right)\right]\right\}. \tag{44}$$

By exploiting the identity of the Euler gamma function $z\Gamma(z) = \Gamma(z+1)$ one has that

$$z \to 0 \quad \Longrightarrow \quad \Gamma(z) \sim \frac{1}{z}, \tag{45}$$

from which we have

$$\begin{aligned} &\log\mathscr{Z}_N(\beta) \approx \left\{N\left[\beta + \log\left(-\log(\beta)\right)\right]\right\} \\ &\Longrightarrow \quad C_V \sim \frac{1}{\log(T)} \end{aligned} \tag{46}$$

In a similar manner one obtains the behavior of the average energy $\langle u\rangle$, which is reported in the main text.

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