Breakdown of Thermalization in Finite One-Dimensional Systems

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We use quantum quenches to study the dynamics and thermalization of hard core bosons in finite one-dimensional lattices. We perform exact diagonalizations and find that, far away from integrability, few-body observables thermalize. We then study the breakdown of thermalization as one approaches an integrable point. This is found to be a smooth process in which the predictions of standard statistical mechanics continuously worsen as the system moves toward integrability. We establish a direct connection between the presence or absence of thermalization and the validity or failure of the eigenstate thermalization hypothesis, respectively.

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A little more than 50 years ago, Fermi, Pasta, and Ulam (FPU) [1] set up a numerical experiment to prove the ergodic hypothesis for a one-dimensional (1D) lattice of harmonic oscillators once nonlinear couplings were added. Much to their surprise, the system exhibited long-time periodic dynamics with no signals of ergodicity. This behavior could not be explained in terms of Poincaré recurrences and motivated intense research [2], which ultimately gave rise to the modern chaos theory. It led to the discovery of solitons (stable solitary waves) in nonlinear systems and to the understanding of thermalization in terms of dynamical chaos [2]. In the latter scenario, there is a threshold below which the interactions breaking integrability are ineffective in producing chaotic behavior and the system cannot be described by standard statistical mechanics [3]. The FPU numerical calculations happened to be below that threshold [4].

More recently, experiments with ultracold gases in 1D geometries have challenged our understanding of the quantum domain [5]. After bringing a nearly isolated system out of equilibrium, no signals of relaxation to a thermal equilibrium distribution were observed. Some insight can be gained in the framework of integrable quantum systems [6], but then it remains the question of why thermalization did not occur even when the system was supposed to be away from integrability. In the latter regime, thermalization is expected to occur [7,8]. This new experimental result [5] has opened many questions such as: Will thermalization occur if one waits longer? Is there a threshold after which thermalization will occur? In this work we address some of these questions using numerical experiments.

In the limit in which the quantum system is integrable, it has been shown numerically [6] that observables such as the ones measured experimentally relax to an equilibrium distribution different from the thermal one. That a novel distribution is generated is the result of the conserved quantities that render the system integrable, and can be characterized by a generalization of the Gibbs ensemble (GGE) [6]. Several works since then have addressed the relevance and limitations of the GGE to various integrable systems and classes of observables [9]. Much less is known away from integrability where fewer analytical tools are available and numerical computations become more demanding. Early works in one dimension have provided mixed results; thermalization was observed in some regimes and not in others [10]. In two dimensions, thermalization was unambiguously shown to occur [8] and could be understood on the basis of the eigenstate thermalization hypothesis [7]. Recent works have also pointed out a possible intermediate quasisteady regime that could occur before thermalization in a class of fermionic systems [11]. Here we study how breaking integrability affects the thermalization of correlated bosons in a 1D lattice after a quantum quench.

We consider impenetrable bosons in a periodic 1D lattice with nearest-neighbor hopping t and repulsive interaction V, and next-nearest-neighbor hopping t' and repulsive interaction V' [12].

When $t' = V' = 0$ this model is integrable. In order to understand how the proximity to the integrable point affects equilibration, we prepare an initial state that is an eigenstate of a system with $t = t_{\rm ini}$, $V = V_{\rm ini}$, t', V' and then quench the nearest-neighbor parameters to $t = t_{\rm fin}$, $V = V_{\rm fin}$ without changing t', V'; i.e., we only change $t_{\rm ini}$, $V_{\rm ini} \to t_{\rm fin}$, $V_{\rm fin}$. The same quench is then repeated for different values of t', V' as one approaches $t' = V' = 0$. We have performed the exact time evolution of up to eight impenetrable bosons in lattices with up to 24 sites. Taking advantage of translational invariance, this required the full diagonalization of blocks in the Hamiltonian that contained up to 30 667 states.

Does integrability, or its absence, affect the relaxation dynamics of experimentally relevant observables? To answer that question, we examine two of those observables: the momentum distribution function $n(k)$ and the structure factor for the density-density correlations $N(k)$ [12]. Since the initial state wave function can be expanded in the eigenstate basis of the final Hamiltonian $\hat{H}$ as $|\psi_{\rm ini}\rangle = \sum_\alpha C_\alpha |\Psi_\alpha\rangle$, one finds that, if the spectrum is nondegenerate and incommensurate, the infinite time average of an observable $\hat{O}$ can be written as

$$\overline{\langle\hat{O}\rangle} \equiv O_{\rm diag} = \sum_{\alpha} |C_{\alpha}|^2 O_{\alpha\alpha}, \tag{1}$$

where $O_{\alpha\alpha}$ are the matrix elements of $\hat{O}$ in the basis of the final Hamiltonian. This exact result can be thought as the prediction of a "diagonal ensemble", where $|C_{\alpha}|^2$ is the weight of each state of this ensemble [8]. We then study the normalized area between our observables, during the time evolution, and their infinite time average; i.e., at each time we compute

$$\delta n_k = \frac{\sum_k |n(k) - n_{\rm diag}(k)|}{\sum_k n_{\rm diag}(k)} \tag{2}$$

and similarly for δN_k. If, up to small fluctuations, $n(k)$ and $N(k)$ relax to a constant distribution, it must be the one predicted by the infinite time average in Eq. (1), i.e., $\delta n(k)$, $\delta N(k) \to 0$.

In Fig. 1, we show results for δn_k and δN_k as a function of time τ for four different quenches as one approaches the integrable point. In Figs. 1(a) and 1(f), we compare the initial $n(k)$ and $N(k)$ with the predictions of Eq. (1) away from integrability. Interestingly, the time evolution of δn_k and δN_k in Figs. 1(b)–1(e) and 1(g)–1(j), respectively, can be seen to be very similar for all values of t' and V'. Hence, the dynamics are barely affected by the closeness to the integrable point [12]. In all cases, we find that there is a fast relaxation of $n(k)$ and $N(k)$ towards the diagonal ensemble prediction (in a time scale $\tau \sim 1/t_{\rm fin}$ [12]) and that later they fluctuate within 1% to 2% of that prediction. The latter differences decrease as one increases the system size and the energy, or the effective temperature [13] of the system [12]. From these results, we infer that, for very large system sizes and finite effective temperatures, $n(k)$ and $N(k)$ should in general relax to exactly the predictions of Eq. (1) even if the system is very close or at integrability.

Once it is known that the diagonal ensemble provides a very good description of observables after their relaxation dynamics, a question that remains to be answered is how good are standard statistical ensembles in reproducing the $n(k)$ and $N(k)$ distributions predicted by the diagonal ensemble as one approaches the integrable point? Based on the experimental results [5] one would expect conventional statistical mechanics to fail everywhere in one dimension or at least over a finite window in the vicinity of the integrable point. We find the latter scenario to be the one realized in our finite 1D lattices.

In the main panel of Fig. 2(a), we compare the diagonal ensemble results with the predictions of the microcanoni-

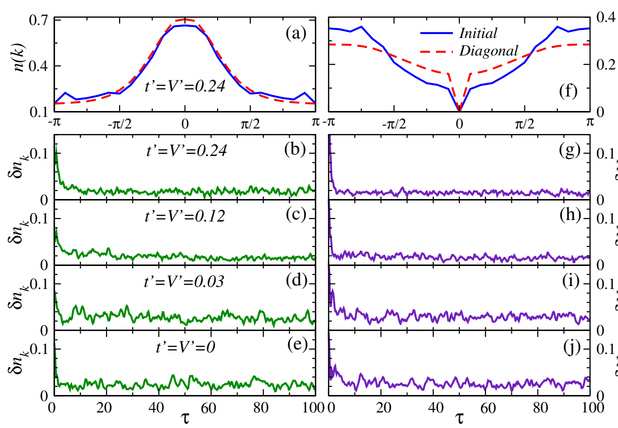

FIG. 1 (color online). Quantum quench from $t_{\rm ini} = 0.5$, $V_{\rm ini} = 2.0$ to $t_{\rm fin} = 1.0$, $V_{\rm fin} = 1.0$, with $t'_{\rm ini} = t'_{\rm fin} = t'$ and $V'_{\rm ini} = V'_{\rm fin} = V'$ in a system with eight hardcore bosons ($N_b = 8$) in 24 lattice sites ($L = 24$). The initial state was chosen within the eigenstates of the initial Hamiltonian with total momentum $k = 0$ in such a way that after the quench the system has an effective temperature $T = 2.0$ in all cases. Given the energy of the initial state in the final Hamiltonian $E = \langle\psi_{\rm ini}|\hat{H}_{\rm fin}|\psi_{\rm ini}\rangle$ the effective temperature is computed as described in Ref. [13]. (a) Initial and diagonal ensemble results for $n(k)$ when $t' = V' = 0.24$. (b)–(e) Time evolution of δn_k for $t' = V' = 0.24$, 0.12, 0.03, and 0.0, respectively. (f) Initial and diagonal ensemble results for $N(k)$ when $t' = V' = 0.24$. (g)–(j) Time evolution of δN_k for $t' = V' = 0.24$, 0.12, 0.03, and 0.0, respectively.

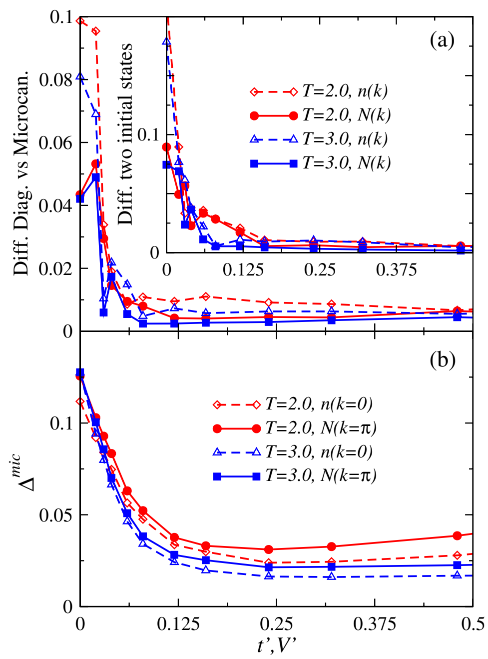

FIG. 2 (color online). Comparison between the predictions of different statistical ensembles for $n(k)$ and $N(k)$ after relaxation in a system with $L = 24$ and $N_b = 8$. Results are shown for $T = 2.0$ and $T = 3.0$. (a) (main panel) Relative difference between the predictions of the diagonal ensemble and the microcanonical ensemble. (a) (inset) Relative difference between the predictions of two diagonal ensembles generated by different initial states selected from the eigenstates of a Hamiltonian with $t_{\rm ini} = 0.5$, $V_{\rm ini} = 2.0$ and a Hamiltonian with $t_{\rm ini} = 2.0$, $V_{\rm ini} = 0.5$, and $L = 24$, $N_b = 8$. The final Hamiltonian ($t_{\rm fin} = 1.0$, $V_{\rm fin} = 1.0$) and the effective temperature are identical for both initial states. Relative differences are computed following Eq. (2). (b) Average relative deviation of eigenstate expectation values with respect to the microcanonical prediction (see text) as a function of t', V', for the same effective temperatures as in (a).

cal ensemble for our two observables of interest. We find the differences between them to be below 1% and decreasing with system size [12] when the system is far from integrability ($t' = V' > 0.1$). Thus, one can say that thermalization takes place in this case. As one approaches the integrable point, on the other hand, the differences between the diagonal and microcanonical ensembles increase, signaling a breakdown of thermalization in one dimension. This breakdown is accompanied by a dependence of the properties of the system after relaxation on the initial state, as can be seen in the inset in Fig. 2(a). There, we compare the predictions of the diagonal ensemble for two different initial states that have the same effective temperature. Those predictions are almost independent of the initial state for $t' = V' > 0.1$, but strongly dependent on it closer to integrability. In Fig. 2(a), it is remarkable to find that both $n(k)$ and $N(k)$ exhibit very similar quantitative behavior away from integrability, which is an indication of the generality of our results for few-body observables.

A clarification is in order at this point. It is usually assumed that, for extensive quantities, the predictions of conventional statistical mechanics ensembles such as the microcanonical and canonical ones are identical, provided the systems are large enough. We should stress that this is not the case in our small systems, and may not be the case for many experiments that are performed in similar setups. In Fig. 3 one can see that depending on the physical observable under consideration the differences between the predictions of those ensembles can be quite large [in particular for $n(k)$]. Interestingly, they are almost not affected by the proximity to integrability, and, as expected, can be seen to reduce with increasing system size.

One may wonder why conventional statistical mechanics ensembles can predict the exact values of few-body observables after relaxation at all, since these seem to be *a priori* fully dependent on the initial conditions through the values of $|C_\alpha|^2$ [see Eq. (1)]. In the main panel in Fig. 4(b), we show the distribution of $|C_\alpha|^2$ for one of the quenches that exhibited thermalization in Fig. 2(a). Figure 4(b) shows that the $|C_\alpha|^2$ distribution is clearly

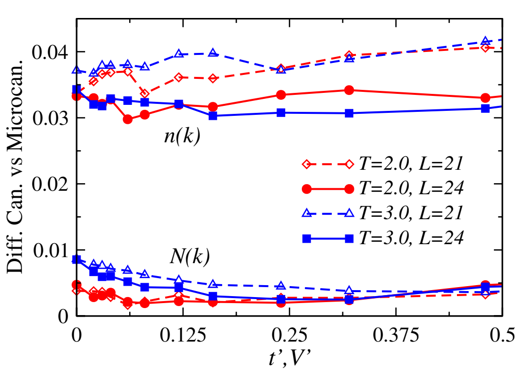

FIG. 3 (color online). Relative difference between the predictions of the microcanonical and canonical ensembles for our two observables of interest in systems with $L = 21$, $N_b = 7$ and $L = 24$, $N_b = 8$. Relative differences are computed following Eq. (2).

different from the microcanonical one, in which all states within an energy window are taken with the same weight. One can conclude then that something else is at play here.

A resolution to this puzzle was advanced by Deutsch and Srednicki in terms of the eigenstate thermalization hypothesis (ETH) [7]. ETH states that the fluctuation of eigenstate expectation values of generic few-body observables [$O_{\alpha\alpha}$ in Eq. (1)] is small between eigenstates that are close in energy, which means that the microcanonical average is identical to the prediction of each eigenstate, or what is the same that the eigenstates already exhibit a thermal value of the observable. If this holds, thermalization in an isolated quantum system will follow for any distribution of $|C_\alpha|^2$, as long as it is narrow enough in energy. This scenario was shown to be valid in isolated two-dimensional systems in Ref. [8].

In 1D systems, we find the onset of thermalization to be directly related to the validity of the eigenstate thermalization hypothesis. In the main panel in Fig. 4(a), we depict $n(k = 0)$ [similar results were obtained for $n(k \neq 0)$ and $N(k)$] in each eigenstate of the Hamiltonian as a function of the energy of the eigenstate, when the system is far from integrability. Figure 4(a) shows that after a region of low energies where the eigenstate expectation values exhibit large fluctuations follows another region where fluctuations are small and ETH holds. The inset in Fig. 4(a) shows that for a system close to the integrable point, in which thermalization is absent [Fig. 2(a)], the eigenstate to eigenstate fluctuations of $n(k = 0)$ are very large over the entire spectrum and ETH does not hold.

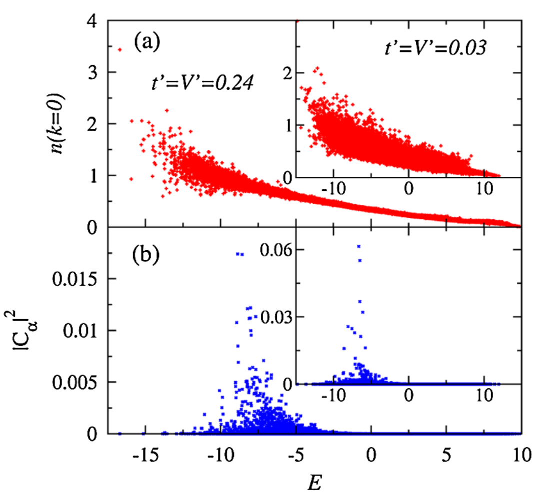

FIG. 4 (color online). (a) $n(k = 0)$ as a function of the energy for all the eigenstates of the Hamiltonian (including all momentum sectors). (main panel) $t = V = 1$ and $t' = V' = 0.24$. (inset) $t = V = 1$ and $t' = V' = 0.03$. The system has 24 lattice sites and 8 bosons for which the total Hilbert space consists of 735 471 states. (b) Distribution of $|C_\alpha|^2$ for the quench from $t_{\rm ini} = 0.5$, $V_{\rm ini} = 2.0$ to $t_{\rm fin} = 1.0$, $V_{\rm fin} = 1.0$ for an effective temperature $T = 2.0$. (main panel) $t = V = 1$ and $t' = V' = 0.24$, where $E = \langle\psi_{\rm ini}|\hat{H}_{\rm fin}|\psi_{\rm ini}\rangle = -6.85$. (inset) $t = V = 1$ and $t' = V' = 0.03$, where $E = -5.95$.

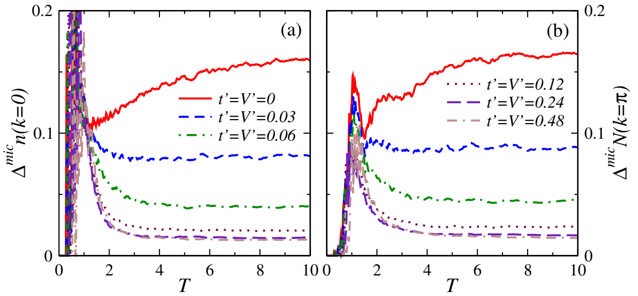

FIG. 5 (color online). Average relative deviation of eigenstate expectation values with respect to the microcanonical prediction as a function of the effective temperature of the microcanonical ensemble. Results are presented for: (a) $n(k=0)$ and (b) $N(k=\pi)$. These systems have 24 lattice sites, 8 bosons, and $t = V = 1.0$. An effective temperature $T = 2$ in these plots corresponds to an energy $E_{\rm mic} = -5.95$ for $t' = V' = 0.03$ and $E_{\rm mic} = -6.85$ for $t' = V' = 0.24$ and, $T = 10$ corresponds to an energy $E_{\rm mic} = -0.81$ for $t' = V' = 0.03$ and $E_{\rm mic} = -0.82$ for $t' = V' = 0.24$ (see the corresponding parts of the spectrum in Fig. 4).

In order to be more quantitative, and to understand how ETH breaks down as one approaches the integrable point, we have computed the average relative deviation of the eigenstate expectation values with respect to the microcanonical prediction ($\Delta^{\rm mic}$) for $n(k=0)$ and for $N(k=\pi)$ [12]. They are shown in Fig. 5(a) and 5(b), respectively, as a function of the effective temperature T corresponding to an energy E of the microcanonical ensemble [13]. Temperature in this plot is only used as an auxiliary tool for assessing how far from the ground state these systems are.

In Fig. 5 one can see that $\Delta^{\rm mic} n(k=0)$ and $\Delta^{\rm mic} N(k=\pi)$ exhibit very similar behavior. Below $T \simeq 1.5$ fluctuations are large and due to the relatively small number of states in some energy windows the use of the microcanonical ensemble may not be well justified. For $T \gtrsim 1.5$, the fluctuations saturate with increasing temperature, and $\Delta^{\rm mic} n(k=0)$ and $\Delta^{\rm mic} N(k=\pi)$ continuously increase, at any given temperature, as one approaches the integrable point. The latter is better seen in Fig. 2(b) for the two specific effective temperatures studied in Fig. 2(a). A comparison between Figs. 2(a) and 2(b), allows us to establish a direct connection between the breakdown of thermalization in one dimension and the increase of the eigenstate to eigenstate fluctuations in the Hamiltonian, or what is the same, the failure of ETH. We have also studied how these results are modified when changing the system size. We find that for our lattice sizes $\Delta^{\rm mic}$ still reduces as one increases the system size [12]. The relative reduction is more pronounced away from integrability.

Overall, our study shows that in finite 1D systems there is a regime close to integrability where thermalization fails to occur, and that this failure originates in the breakdown of ETH. We also find that ETH holds further departing from integrability explaining why thermalization can occur in one dimension. Since both experiments [5] and computations have been performed with relatively small systems, an important question that remains open is whether for sufficiently large system sizes thermalization will occur arbitrarily close to the integrable point or whether there will be a finite critical value starting from which integrability breaking terms will produce thermalization. For our finite systems all we see is a smooth breakdown of thermalization as one approaches integrability [14]. The answer to this question may be well suited for experimental analysis as it may be easier to study the scaling with system size in experiments than within our numerical computations, which scale exponentially with the system size. The addition of a lattice along the 1D tubes in the experiments [16] may help in addressing these issues.

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[1] E. Fermi *et al.*, Los Alamos Report No. LA-1940, 1955.
[2] See, e.g., Special issue on The "Fermi-Pasta-Ulam" Problem-The First 50 Years, edited by D. K. Campbell, P. Rosenau, and G. M. Zaslavsky [Chaos **15**, 015101 (2005)].
[3] B. V. Chirikov, J. Nucl. Energy, Part C **1**, 253 (1960).
[4] F. M. Izrailev *et al.*, Los Alamos Report No. LA-4440-TR, 1970.
[5] T. Kinoshita *et al.*, Nature (London) **440**, 900 (2006).
[6] M. Rigol *et al.*, Phys. Rev. Lett. **98**, 050405 (2007); Phys. Rev. A **74**, 053616 (2006).
[7] J. M. Deutsch, Phys. Rev. A **43**, 2046 (1991); M. Srednicki, Phys. Rev. E **50**, 888 (1994).
[8] M. Rigol *et al.*, Nature (London) **452**, 854 (2008).
[9] M. A. Cazalilla, Phys. Rev. Lett. **97**, 156403 (2006); P. Calabrese and J. Cardy, J. Stat. Mech. (2007) P06008; M. Cramer *et al.*, Phys. Rev. Lett. **100**, 030602 (2008); T. Barthel and U. Schollwöck, Phys. Rev. Lett. **100**, 100601 (2008); M. Eckstein and M. Kollar, Phys. Rev. Lett. **100**, 120404 (2008); M. Kollar and M. Eckstein, Phys. Rev. A **78**, 013626 (2008); M. Cramer *et al.*, Phys. Rev. Lett. **101**, 063001 (2008); D. Rossini *et al.*, Phys. Rev. Lett. **102**, 127204 (2009); A. Iucci and M. A. Cazalilla, arXiv:0903.1205.
[10] C. Kollath *et al.*, Phys. Rev. Lett. **98**, 180601 (2007); S. R. Manmana *et al.*, Phys. Rev. Lett. **98**, 210405 (2007).
[11] M. Moeckel and S. Kehrein, Phys. Rev. Lett. **100**, 175702 (2008); arXiv:0903.1561; M. Eckstein *et al.*, Phys. Rev. Lett. **103**, 056403 (2009).
[12] See EPAPS Document No. E-PRLTAO-103-021938 for supplementary material. For more information on EPAPS, see http://www.aip.org/pubservs/epaps.html.
[13] Given an energy E, the effective temperature T is defined by the expression $E = Z^{-1}\,{\rm Tr}\{\hat{H}\exp(-\hat{H}/k_B T)\}$, where $\hat{H}$ is the Hamiltonian for which E is measured, $Z = {\rm Tr}\{\exp(-\hat{H}/k_B T)\}$, and k_B is the Boltzmann constant.
[14] Its relation with the crossover between Poissonian and Wigner-Dyson level statistics is discussed in Ref. [15].
[15] L. F. Santos and M. Rigol (to be published).
[16] B. Paredes *et al.*, Nature (London) **429**, 277 (2004).