Generalized Thermalization in an Integrable Lattice System

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After a quench, observables in an integrable system may not relax to the standard thermal values, but can relax to the ones predicted by the generalized Gibbs ensemble (GGE) [M. Rigol *et al.*, Phys. Rev. Lett. **98**, 050405 (2007)]. The GGE has been shown to accurately describe observables in various one-dimensional integrable systems, but the origin of its success is not fully understood. Here we introduce a microcanonical version of the GGE and provide a justification of the GGE based on a generalized interpretation of the eigenstate thermalization hypothesis, which was previously introduced to explain thermalization of nonintegrable systems. We study relaxation after a quench of one-dimensional hard-core bosons in an optical lattice. Exact numerical calculations for up to 10 particles on 50 lattice sites ($\approx 10^{10}$ eigenstates) validate our approach.

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Once only of theoretical interest, integrable models of one-dimensional (1D) quantum many-body systems can now be realized with ultracold atoms [1]. The possibility of controlling the effective dimensionality and the degree of isolation have allowed access to the quasi-1D regime and to the long coherence times necessary to realize integrable models. Additionally, advances in the cooling and trapping of atoms have led to increased interest in dynamics following quantum quenches, where a many-body system in equilibrium is exposed to rapid changes in the confining potential or interparticle interactions.

In general, in integrable quantum systems that are far from equilibrium, observables cannot relax to the usual thermal state predictions because they are constrained by the nontrivial set of conserved quantities that make the system integrable [2]. Relaxation to nonthermal values were recently observed in a cold-atom system close to integrability [3]. At integrability, it is natural to describe the observables after relaxation by an updated statistical mechanical ensemble: the generalized Gibbs ensemble (GGE) [4], which is constructed by maximizing the entropy subject to the integrability constraints [5]. In recent studies of integrable systems [4,6,7], the GGE has been found to accurately describe various observables after relaxation, but a microscopic understanding of its origin and applicability remains elusive. In particular, an important question remains: how is it that expectation values after relaxation can be described by an ensemble with exponentially fewer parameters than the size of the Hilbert space? The full dynamics are determined by as many parameters as the size of the latter. At a microscopic level, thermalization for nonintegrable systems can be understood in terms of the eigenstate thermalization hypothesis (ETH) [8,9], which, however, breaks down as one approaches integrability [10].

This Letter is devoted to the study of how generalized thermalization, in the sense of relaxation to the predictions of the GGE, takes place in integrable systems. Answering this question is important not merely because of its relevance to the foundations of statistical mechanics in integrable systems, but also because it has become necessary to understand recent experiments with ultracold gases in quasi-1D geometries. For integrable systems, we compare the predictions of quantum mechanics with those of various statistical ensembles. In particular, we introduce a microcanonical version of the GGE, which we use to show that relaxation to the GGE can be understood in terms of a generalized view of the ETH.

We study the dynamics following an instantaneous quench of 1D hard-core bosons on a lattice, which is fully integrable. The Hamiltonian is given by

$$\hat{H} = -J\sum_{i=1}^{L-1}(\hat{b}_i^\dagger \hat{b}_{i+1} + \text{H.c.}) + V(\tau)\sum_{i=1}^{L}(i - L/2)^2 \hat{n}_i, \quad (1)$$

where J is the hopping parameter; $V(\tau)$ gives the curvature of an additional parabolic trapping potential for atoms on a lattice with lattice constant a; $\hat{b}_i^\dagger(\hat{b}_i)$ is the hard-core bosonic creation (annihilation) operator; and $\hat{n}_i = \hat{b}_i^\dagger \hat{b}_i$ is the number operator. In addition to the standard commutation relations for bosons, hard-core bosons satisfy the constraint $\hat{b}_i^{\dagger 2} = \hat{b}_i^2 = 0$, which forbids multiple occupancy of the lattice sites. This Hamiltonian can be mapped onto noninteracting fermions through the Jordan-Wigner transformation [11], and the many-body eigenstates can be constructed as Slater determinants of the single-particle fermionic eigenstates [12].

We will focus on the behavior of the momentum distribution function, $\langle \hat{n}_k \rangle = \sum_{l,m} e^{-ik(l-m)} \langle \psi | \hat{b}_m^\dagger \hat{b}_l | \psi \rangle / L$, for system sizes ranging from $N = 5$ bosons on $L = 25$ lattice sites to $N = 10$ bosons on $L = 50$ lattice sites ($\approx 10^{10}$ eigenstates). Initially, we prepare the system in the ground state $|\psi_0\rangle$ of a 1D lattice with hard-wall boundary conditions and an additional harmonic potential, with trapping strength $V = V_0$. At time $\tau = 0$, the harmonic trap is turned off, $V(\tau \geq 0) = 0$, and the state $|\psi(\tau)\rangle$ evolves under the influence of the final Hamiltonian. Hereafter, we refer to this state as it is immediately after the quench as the "quenched state." Its time evolution is given by $|\psi(\tau)\rangle = \sum_\alpha c_\alpha e^{-iE_\alpha \tau/\hbar}|\alpha\rangle$, where $|\alpha\rangle$ are the energy eigenstates of the final Hamiltonian with energies E_α, and $c_\alpha = \langle\alpha|\psi_0\rangle$ are the overlaps between the eigenstates of the final Hamiltonian and the quenched state. After relaxation, assuming the degeneracies in energy levels are irrelevant, the expectation value of an observable is expected to be given by the so called diagonal ensemble (DE) [7,9,10]

$$\langle\hat{A}\rangle_{\mathrm{DE}} = \lim_{\tau\to\infty}\frac{1}{\tau}\int_0^\tau d\tau'\langle\psi(\tau')|\hat{A}|\psi(\tau')\rangle = \sum_\alpha |c_\alpha|^2\langle\alpha|\hat{A}|\alpha\rangle.$$

We have checked numerically that, despite the integrability of our model, n_k relaxes to the DE prediction, with small fluctuations around this result [13].

Figure 1 shows the momentum distributions, n_k, before and after the quench, for two different initial trap strengths, which correspond to different energies per particle, ε, after the quench. These results are compared with those of various ensembles of statistical mechanics. The microcanonical ensemble (ME) is one in which all eigenstates in

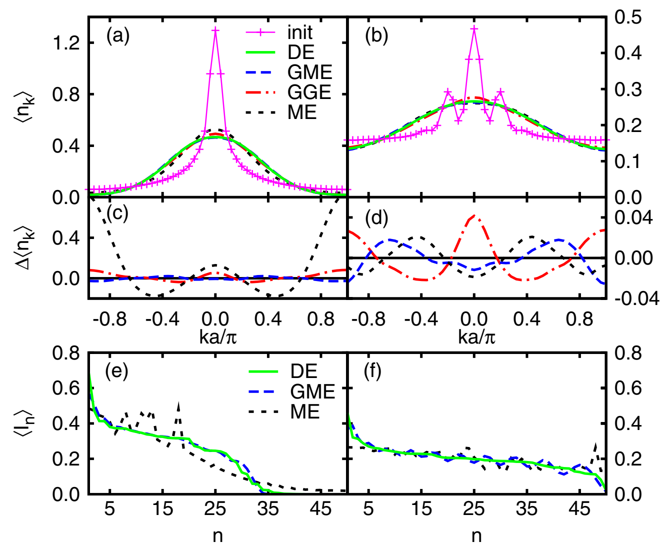

FIG. 1 (color online). (a),(b) Momentum distribution of the initial state (init), diagonal (DE), generalized microcanonical (GME), generalized Gibbs (GGE), and the microcanonical (ME) ensembles. (c),(d) Relative difference of the GME, GGE and ME from the DE. (e),(f) Conserved quantities, $\langle\hat{I}_n\rangle$, in the quenched state (identical to the DE), GME and ME. $\langle I_n\rangle$ are ordered in descending occupations in the quenched state. $L = 50$, $N = 10$, $\delta_{\mathrm{ME}} = 0.05J$, $\delta_{\mathrm{GME}} = 0.8$. (a),(c),(e) $\varepsilon = 0.72J$, $V_0 = 0.029J$. (b),(d),(f) $\varepsilon = 1.52J$, $V_0 = 0.125J$.

the relevant energy window have identical weights. Within the microcanonical ensemble, the expectation value of a generic observable A is $\langle\hat{A}\rangle_{\mathrm{ME}} = N^{-1}_{\varepsilon,\delta_{\mathrm{ME}}} \sum_{\alpha,|\varepsilon-\varepsilon_\alpha|<\delta_{\mathrm{ME}}}\langle\alpha|\hat{A}|\alpha\rangle$, where δ_{ME} is small, but still much greater than the mean many-body level spacing. $N_{\varepsilon,\delta_{\mathrm{ME}}}$ is the number of eigenstates in the energy window $|\varepsilon - \varepsilon_\alpha| < \delta_{\mathrm{ME}}$. We have checked that the results reported here are nearly independent of the specific value of δ_{ME}. The GGE is a grand-canonical ensemble that maximizes the entropy subject to the constraints associated with nontrivial conserved quantities of the quenched state. The density matrix takes the form [4]

$$\hat{\rho}_{\mathrm{GGE}} = Z_G^{-1}e^{-\sum\lambda_n\hat{I}_n}, \qquad Z_G = \mathrm{Tr}[e^{-\sum\lambda_n\hat{I}_n}], \tag{2}$$

where $\{\hat{I}_n\}$, $n = 1, \ldots, L$, are the conserved quantities. In our systems, these correspond to the occupation of the single-particle eigenstates of the underlying noninteracting fermions to which hard-core bosons are mapped, and $\{\lambda_n\}$ are Lagrange multipliers fixed by the initial conditions, $\lambda_n = \ln[(1 - \langle\psi_0|\hat{I}_n|\psi_0\rangle)/\langle\psi_0|\hat{I}_n|\psi_0\rangle]$ [4]. Observables within this ensemble are then computed as $\langle\hat{A}\rangle_{\mathrm{GGE}} = \mathrm{Tr}[\hat{A}\hat{\rho}_{\mathrm{GGE}}]$ following Ref. [12].

As a step towards understanding the GGE as well as developing a more accurate description of isolated integrable systems after relaxation, we introduce a microcanonical version of the GGE, which we call the generalized microcanonical ensemble (GME). Like the ME, where states within a small energy window contribute with equal weight, within the GME we assign equal weight to all eigenstates whose values of the conserved quantities are close to the desired values. The expectation value of a generic observable within the generalized microcanonical ensemble is given by $\langle\hat{A}\rangle_{\mathrm{GME}} = \mathcal{N}^{-1}_{\{I_n\},\delta_{\mathrm{GME}}} \sum_{\alpha,\delta_\alpha<\delta_{\mathrm{GME}}}\langle\alpha|\hat{A}|\alpha\rangle$, where $\sum_{\alpha,\delta_\alpha<\delta_{\mathrm{GME}}}$ is a sum over eigenstates that are within the GME window and $\mathcal{N}_{\{I_n\},\delta_{\mathrm{GME}}}$ is the number of states within that window and δ_α is a measure of the distance of eigenstate α from the target distribution.

In order to construct the GME, we include eigenstates of the Hamiltonian with a similar distribution of conserved quantities which once averaged reproduce the values of the conserved quantities in the quenched state. This approach is characterized by three ingredients [14]: (i) The ordered distribution (from largest to smallest) of the conserved quantities in the DE, $\langle I_n\rangle_{\mathrm{DE}} \equiv \sum_\alpha |c_\alpha|^2 I_{n,\alpha}$ [as in Figs. 1(e) and 1(f)], (ii) a target distribution of the nonzero expectation values of the conserved quantities $\{I^*_{n^*_i} = 1\}$, where the values of n^*_i ($i = 1, \ldots, N$) are chose to describe the distribution I_n in a coarse-grained sense [15], and (iii) for each individual many-body eigenstate, the distance from the target state, δ_α, which we define as $\delta_\alpha = [\frac{1}{N} \times \sum_{i=1}^N I_{n^*_i}(n_{i,\alpha} - n^*_i)^2]^{1/2}$. Here $n_{i,\alpha}$ ($i = 1, \ldots, N$) are the single-particle states occupied in eigenstate α, and $I_{n^*_i}$ are the interpolated values of $\langle I_n\rangle_{\mathrm{DE}}$, evaluated at n^*_i.

The definition of δ_α is not unique and several variants that do not change our conclusions were also considered [13].

To better visualize the differences between the results of the various ensembles in Figs. 1(a) and 1(b), we have plotted $\Delta\langle n_k\rangle_{\rm stat} = (\langle\hat{n}_k\rangle_{\rm DE} - \langle\hat{n}_k\rangle_{\rm stat})/\langle\hat{n}_k\rangle_{\rm DE}$, where "stat" stands for ME, GGE, or GME in Figs. 1(c) and 1(d). For weaker initial confinements [smaller ε—Fig. 1(c)], the GME is practically indistinguishable from the diagonal distribution. Both the GME and the GGE accurately capture the tails of n_k, while the thermal ensemble does not. For tighter initial traps [greater ε—Fig. 1(d)] all four ensembles are very similar (note the scale), suggesting that n_k in the final steady state is indistinguishable from that of the thermal state.

The close agreement between DE and ME results in Fig. 1(b) raises the question: how can an integrable system thermalize, given the constraints imposed by the complete set of conserved quantities? We conjecture that if the values of the conserved quantities in the quenched state are similar to those of the ME, then the latter will accurately describe observables after relaxation. This may occur for a variety of quenches.

In Figs. 1(e) and 1(f), we plot the values of the conserved quantities in the quenched state and compare them with the expectation values of those quantities in different statistical ensembles. (By definition, the distribution of conserved quantities in the DE and GGE are identical to that of the quenched state.) Figure 1(e) shows that the microcanonical values of the conserved quantities are clearly different from the values in the quenched state, while in Fig. 1(f) they are very similar. This supports our conjecture above, and demonstrates that thermalization can occur in integrable systems for special initial conditions. Additionally, the GME reproduces the correct distribution of the conserved quantities supporting the validity of our method for generating it.

To quantify the above observations, and to understand what happens in the thermodynamic limit, we have studied the difference between the predictions of the DE and the statistical ensembles for different system sizes. We compute the integrated relative differences, $(\Delta n_k)_{\rm stat} = \sum_k|\langle\hat{n}_k\rangle_{\rm DE} - \langle\hat{n}_k\rangle_{\rm stat}|/\sum_k\langle\hat{n}_k\rangle_{\rm DE}$, where again stat stands for ME, GGE, or GME.

In Fig. 2(a), we plot $(\Delta n_k)_{\rm ME}$ as a function of the final energy per particle, ε, for different lattice sizes, L. To perform finite-size scaling, ε and the filling factor ($\nu = N/L = 0.2$) are held constant as L changes. Figure 2(a) shows that for $\varepsilon \lesssim 1.3J$ the difference between the n_k in the DE and the ME increases with increasing L, indicating that the difference persists in the thermodynamic limit. For $\varepsilon \gtrsim 1.3J$, the opposite behavior is observed. From our previous discussion, one expects that $(\Delta n_k)_{\rm ME}$ should closely follow the behavior of the integrated differences between the conserved quantities in the quenched state and the ME, $(\Delta I_n)_{\rm ME} = \sum_n|\langle I_n\rangle_{\rm DE} - \langle I_n\rangle_{\rm ME}|/\sum_n\langle I_n\rangle_{\rm DE}$. This is seen by comparing Figs. 2(a) and 2(c), which leads us to conclude that n_k need not relax to the standard thermal prediction, except when $(\Delta I_n)_{\rm ME}$ becomes negligible. Qualitatively similar results were obtained in the canonical ensemble [13].

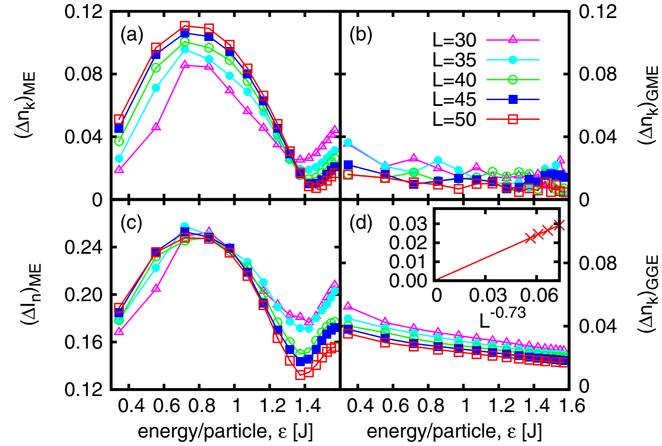

FIG. 2 (color online). (a) $(\Delta n_k)_{\rm ME}$ versus energy per particle of the quenched state. $\delta_{\rm ME} = 0.05J$. (b) $(\Delta n_k)_{\rm GME}$ vs ε, $\delta_{\rm GME} = 0.8$. (c) Integrated difference between the conserved quantities in the quenched state and the ME, $(\Delta I_n)_{\rm ME}$. (d) $(\Delta n_k)_{\rm GGE}$ vs ε. Inset: $(\Delta n_k)_{\rm GGE}$ vs $L^{-0.73}$ for $\varepsilon = 1.07J$, where a fit to $(\Delta n_k)_{\rm GGE} = zL^{-\gamma}$ gives $\gamma = 0.73 \pm 0.02$.

On the other hand, in Fig. 2(b) one can see that the differences between n_k in the diagonal and generalized microcanonical ensembles are very small and decrease with increasing system size, so that the former successfully describes this observable after relaxation. In the case of the GGE [Fig. 2(d)], $(\Delta n_k)_{\rm GGE}$ is in general larger than $(\Delta n_k)_{\rm GME}$, which is to be expected since the GGE is a grand-canonical ensemble. As the system size increases $(\Delta n_k)_{\rm GGE} \to 0$ as $L^{-\gamma}$, where $\gamma \approx 0.73$ [inset of Fig. 2(d)] and slightly depends on the energy [13].

The question that remains to be answered is why the generalized Gibbs and the generalized microcanonical ensemble are able to describe the n_k after relaxation, i.e., why $\langle\hat{n}_k\rangle_{\rm GGE} = \langle\hat{n}_k\rangle_{\rm GME} = \langle\hat{n}_k\rangle_{\rm DE} \equiv \sum_\alpha|c_\alpha|^2\langle\alpha|\hat{n}_k|\alpha\rangle$. Note that whereas $\langle\hat{n}_k\rangle_{\rm GGE}$ and $\langle\hat{n}_k\rangle_{\rm GME}$ are entirely determined by the L independent values of the conserved quantities in the quenched state, $\langle\hat{n}_k\rangle_{\rm DE}$ is determined by the exponentially larger $\binom{L}{N}$ values of the coefficients c_α.

To address this question, we perform a spectral decomposition of $\langle\hat{n}_k\rangle_{\rm DE}$ and $\langle\hat{n}_k\rangle_{\rm GME}$. Figure 3 displays a coarse-grained view of the weight which eigenstates with a given zero momentum occupancy $\langle\hat{n}_{k=0}\rangle_\alpha = \langle\alpha|\hat{n}_{k=0}|\alpha\rangle$ contribute to the DE [Fig. 3(a)] and the GME [Fig. 3(b)]. The correlation between the results in both figures is apparent. However, it is not clear why the details contained in the overlaps c_α are completely washed out so that the DE and the GME results coincide, while they are different from those in the ME. In the inset of Fig. 3(a), we plot a histogram of the values of $n_{k=0}$ for the DE, GME and the ME. Clearly the histograms for the DE and GME have a similar mean but different widths, while the ME has a different mean and width [13].

Ultimately, one is interested in what happens in the thermodynamic limit. For each k, we define the width of the distribution of $\langle\hat{n}_k\rangle_\alpha$ for each ensemble as

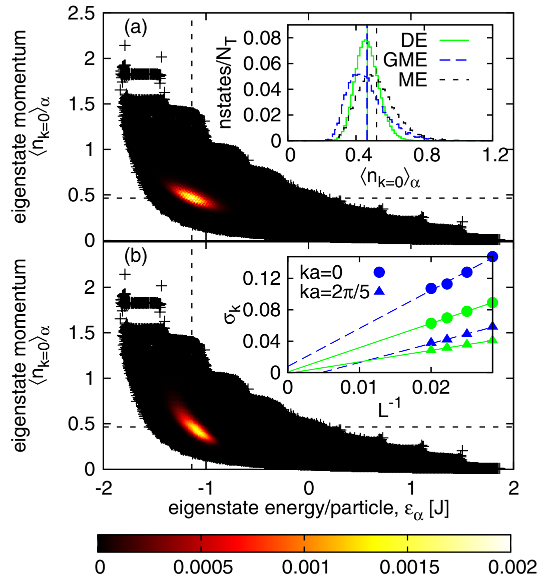

FIG. 3 (color online). Density plot of the coarse-grained weights with which eigenstates contribute to (a) the DE (sum over diagonal weights, $|c_\alpha|^2$) and (b) the GME (fractional number of states = number of states/total number of states) as a function of eigenstate energy and $\langle \hat{n}_{k=0}\rangle_\alpha$. The sums are performed over window of width $\delta n_k = 0.0067$, and $\delta\varepsilon = 0.035J$. The horizontal and vertical dotted lines are the expectation values of $\hat{n}_{k=0}$ and ε in each ensemble. $L = 45$, $N = 9$, $V_0 = 0.036J$, $\varepsilon = 0.72J$, $\delta_{\rm GME} = 0.85$. Inset in (a) Histogram of DE weights (green), fractional number of GME states (blue) and fractional number of ME states (black) summed over all energies. Bin width, $\delta n_k = 0.0067$. Vertical lines give the mean, $\langle \hat{n}_{k=0}\rangle$ within each ensemble. Inset in (b) Fluctuations of $\langle \hat{n}_{ka=0}\rangle$ (●) and $\langle \hat{n}_{ka=2\pi/5}\rangle$ (▲) within the DE (green) and GME (blue) as a function of inverse system size. $\varepsilon = 0.72J$.

$\sigma_k = \sqrt{\langle \hat{n}_k^2\rangle - \langle \hat{n}_k\rangle^2}$. The inset of Fig. 3(b), shows σ_k within the DE and the GME versus L^{-1}. The scaling is depicted for two k values and clearly shows that the widths of both distributions vanish in the thermodynamic limit. This demonstrates that the overwhelming majority of the states selected by the DE as well as by the GME, which have similar values of the conserved quantities, have identical expectation values of n_k. This is why details of the distribution of c_α no longer matter as L increases. We note that with increasing L, the number of eigenstates contained in the generalized microcanonical window increases exponentially; however, the ratio of the number of states in the GME and the ME vanishes [13].

The findings above provide a generalization of the ETH introduced previously to understand thermalization in nonintegrable systems [8,9]. The ETH states that the expectation values of few-body observables in generic systems do not fluctuate between eigenstates that are close in energy. Thus all eigenstates within a microcanonical window have essentially the same expectation values of the observables, and one can say that thermalization occurs at the level of eigenstates. As seen in Fig. 3, $\langle \hat{n}_k\rangle_\alpha$ exhibits large eigenstate-to-eigenstate fluctuations in our integrable system, showing that ETH is invalid. However, by selecting eigenstates with similar conserved quantities, ETH is restored, although in a weaker sense: the overwhelming majority of eigenstates with similar conserved quantities have similar values of n_k. These results pave the way to a unified understanding of thermalization in generic (nonintegrable systems) and its generalization in integrable systems. This opens many new questions, such as whether the concepts of typicality [16] and thermodynamics [17] can be generalized to isolated integrable systems.

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[13] See supplemental material at http://link.aps.org/supplemental/10.1103/PhysRevLett.106.140405.
[14] In each many-body eigenstate of the Hamiltonian, $|\alpha\rangle$, $I_{n,\alpha} = \langle\alpha|\hat{I}_n|\alpha\rangle$ can only be zero or one, because they are constructed by occupying single-particle fermionic states.
[15] We compute the n_i^*, which are not restricted to integers, as follows. The first one (n_1^*) is computed so that $\int_{0.5}^{n_1^*} I(x)dx = 0.5$, where $I(x) = I_n$, $x \in (n - 0.5, n + 0.5]$. For all other values of n_i^*, $\int_{n_{i-1}^*}^{n_i^*} I(x)dx = 1$.
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