

Relaxation in a Completely Integrable Many-Body Quantum System: An *Ab Initio* Study of the Dynamics of the Highly Excited States of 1D Lattice Hard-Core Bosons

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In this Letter we pose the question of whether a many-body quantum system with a *full set of conserved quantities* can relax to an equilibrium state, and, if it can, what the properties of such a state are. We confirm the relaxation hypothesis through an *ab initio* numerical investigation of the dynamics of hard-core bosons on a one-dimensional lattice. Further, a natural extension of the Gibbs ensemble to integrable systems results in a theory that is able to predict the mean values of physical observables after relaxation. Finally, we show that our generalized equilibrium carries more memory of the initial conditions than the usual thermodynamic one. This effect may have many experimental consequences, some of which have already been observed in the recent experiment on the nonequilibrium dynamics of one-dimensional hard-core bosons in a harmonic potential [T. Kinoshita *et al.*, *Nature (London)* **440**, 900 (2006)].

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Introduction.—Integrable quantum gases traditionally belong to the domain of mathematical physics, with little or no connection to experiments. However, the experimental work on confined quantum-degenerate gases has recently yielded faithful realizations of a number of integrable one-dimensional many-body systems, thus making them phenomenologically relevant. Examples include the gas of hard-core bosons (Girardeau) [1–3], realized in [4]; its lattice version [5] studied in our Letter, realized in [6]; finite-strength *s*-wave-interacting spin-0 bosons (Lieb, Liniger, and McGuire) [7,8], realized in [9–11] in the mean-field regime and in [12,13] in the regime of interactions of intermediate strength; and spin- $\frac{1}{2}$ fermions (Yang-Gaudin) [14], realized in [15]. The list has a potential to grow to include also the fermionic *p*-wave version of hard-core particles [16,17]; the gas of $1/r^2$ interacting atoms (Calogero and Sutherland) [18,19]; and the gas of fermions on a lattice (Fermi and Hubbard) [20]. The experiment [6]—which is a realization of the system whose time dynamics we study in the present Letter—used an optical lattice in the tight-binding regime [21,22]. The technique was originally developed to reach the superfluid–Mott-insulator transition [23] as achieved in [24]. We should also mention the experimental studies [25] of a related nonintegrable system, the one-dimensional lattice bosons with finite coupling.

An integrable model possesses many nontrivial integrals of motion, and it is natural to wonder what consequences this fact may have for time dynamics and kinetics. Perhaps the best known theoretical efforts in this vein are the attempts to explain the suppression of equilibration in the Fermi-Pasta-Ulam chains by the closeness to various integrable models (see [26] for a review). Another research direction concerns the effects of integrals of motion on the

autocorrelation properties of large systems, first studied in [27,28] and later specialized to spin systems [29,30]. More recent are the studies of the onset of thermalization in a large quantum system [31,32], and, in particular, in a mesoscopic-size Lieb-Liniger gas [33].

The major inspiration for our work—underlying especially Fig. 2 below—is the recent experiment on the nonequilibrium dynamics of one-dimensional hard-core bosons in a harmonic potential performed at Penn State University [34]. There it was found that hard-core bosons do not relax to the usual state of thermodynamic equilibrium. The question that intrigued us is whether nevertheless there exists *some* kind of equilibrium state to which a many-body integrable system relaxes in the course of time evolution from even a highly nonequilibrium initial state—and, if so, how to predict mean values of physical observables in such a state.

Generalized Gibbs ensemble.—We start with the latter question, for now simply assuming that an equilibrium state exists. We conjecture that then the standard prescription of statistical mechanics applies: one should maximize the many-body entropy $S = k_B \text{Tr}[\rho \ln(1/\rho)]$, subject to the constraints imposed by all the integrals of motion. This results in the following many-body density matrix:

$$\hat{\rho} = Z^{-1} \exp\left[-\sum_m \lambda_m \hat{I}_m\right], \quad (1)$$

where $\{\hat{I}_m\}$ is the *full* set of the integrals of motion, $Z = \text{Tr}[\exp(-\sum_m \lambda_m \hat{I}_m)]$ is the partition function, and $\{\lambda_m\}$ are the Lagrange multipliers, fixed by the initial conditions via

$$\text{Tr}[\hat{I}_m \hat{\rho}] = \langle \hat{I}_m \rangle(t=0). \quad (2)$$

The generalized Gibbs ensemble (1) reduces to the usual

grand-canonical ensemble in the case of a generic system, where the only integrals of motion are the total energy, the number of particles, and, for periodic systems, the total momentum. Conceptually, the ensemble (1) is close to the one E. T. Jaynes introduced in 1957 in the context of the so-called “subjective statistical mechanics” [35]. Girardeau used Jaynes’s concept to study the relaxation of magnetization in the XY model [36]. Below we test the predictive power of (1) and (2) on the example of hard-core bosons on a one-dimensional lattice, a system integrable via Jordan-Wigner mapping to free fermions.

The Hamiltonian and the (quasi-)momentum distribution of hard-core bosons on a lattice.—The Hamiltonian for hard-core bosons (HCB) on a one-dimensional lattice with L sites reads

$$\hat{H} = -J \sum_{i=1}^L (\hat{b}_i^\dagger \hat{b}_{i+1} + \text{H.c.}), \quad (3)$$

where

$$\begin{aligned} [\hat{b}_i, \hat{b}_j^\dagger] &= 0, & [\hat{b}_i, \hat{b}_j] &= [\hat{b}_i^\dagger, \hat{b}_j^\dagger] = 0 \\ & \text{for all } i \text{ and } j \neq i; \\ \{\hat{b}_i, \hat{b}_i^\dagger\} &= 1, & (\hat{b}_i)^2 &= (\hat{b}_i^\dagger)^2 = 0 \text{ for all } i. \end{aligned}$$

Here \hat{b}_i (\hat{b}_i^\dagger) is the annihilation (creation) operator for hard-core bosons, and J is the hopping constant. For our theoretical predictions we use a periodic lattice ($\hat{b}_{L+1} = \hat{b}_1$). However, the subsequent numerical studies are performed for the more experimentally relevant hard-wall boundary conditions. For sufficiently large lattice sizes L , the difference between real physical quantities calculated using these two settings is negligible [37].

Our primary observable of interest is the HCB (quasi-)momentum distribution $f(k) = \langle \hat{f}(k) \rangle$, normalized to the total number of particles N , where

$$\hat{f}(k) = \frac{1}{L} \sum_{i=1}^L \sum_{i'=1}^L e^{-i2\pi k(i-i')/L} \hat{b}_i^\dagger \hat{b}_{i'} \quad (4)$$

is the HCB (quasi-)momentum distribution operator.

Fermi-Bose correspondence.—Our bosonic system can be mapped to a free fermionic one via the Jordan-Wigner transformation $\hat{b}_i^\dagger = \hat{c}_i^\dagger \prod_{i'=1}^{i-1} e^{-i\pi \hat{c}_i^\dagger \hat{c}_{i'}}$, $\hat{b}_i = \prod_{i'=1}^{i-1} e^{i\pi \hat{c}_i^\dagger \hat{c}_{i'}} \hat{c}_i$, where \hat{c}_i (\hat{c}_i^\dagger) is the fermionic annihilation (creation) operator. (Note that since the spatial density operators for fermions and bosons are equal to each other, $\hat{c}_i^\dagger \hat{c}_i = \hat{b}_i^\dagger \hat{b}_i$, the inverse mapping is straightforward.) Under this transformation our Hamiltonian (3) becomes just the Hamiltonian for noninteracting fermions on a lattice:

$$\hat{H} = -J \sum_{i=1}^L (\hat{c}_i^\dagger \hat{c}_{i+1} + \text{H.c.}), \quad (5)$$

$$\{\hat{c}_i, \hat{c}_j^\dagger\} = 1, \{\hat{c}_i, \hat{c}_j\} = \{\hat{c}_i^\dagger, \hat{c}_j^\dagger\} = 0 \text{ for all } i \text{ and } j.$$

The corresponding fermions obey periodic (antiperiodic) boundary conditions for odd (even) numbers of particles: $\hat{c}_{L+1} = (-1)^{\hat{N}+1} \hat{c}_1$. Here and below $\hat{N} = \sum_{i=1}^L \hat{c}_i^\dagger \hat{c}_i = \sum_{i=1}^L \hat{b}_i^\dagger \hat{b}_i$ is the particle number operator, the same for both fermions and bosons.

Integrals of motion.—It is clear from the fermionic form (5) of the Hamiltonian that our system possesses as many conserved quantities as there are lattice sites: they are simply the fermionic (quasi-)momentum distribution operators

$$\hat{I}_k = \hat{f}^F(k) = \frac{1}{L} \sum_{i=1}^L \sum_{i'=1}^L \sigma_{i-i'}(\hat{N}) e^{-i2\pi k(i-i')/L} \hat{c}_{i'}^\dagger \hat{c}_i, \quad (6)$$

where $\sigma_{\Delta_i}(N) = 1$ for odd N , and $\sigma_{\Delta_i}(N) = e^{-i\pi \Delta_i/L}$ for even N .

Note that if expressed through the bosonic fields, the above integrals of motion become complicated many-body operators. Consider, for example, the lattice analog of the fourth moment of the fermionic (quasi-)momentum distribution \hat{I}_4 , defined as

$$\begin{aligned} \frac{1}{4} \left(\frac{2\pi}{L} \right)^4 \hat{I}_4 &= \sum_k \left(1 - \cos \frac{2\pi n}{L} \right)^2 \hat{f}^F(k) \\ &= \frac{3}{2} \hat{N} + \frac{1}{J} \hat{H} \\ &+ \frac{1}{4} \sum_{i=1}^L [\hat{b}_i^\dagger (1 - 2\hat{b}_{i+1}^\dagger \hat{b}_{i+1}) \hat{b}_{i+2} + \text{H.c.}]. \quad (7) \end{aligned}$$

It is one of the simplest linear combinations of the integrals of motion (6), but it becomes a two-body operator in the bosonic representation.

Fully constrained thermodynamic ensemble.—The density matrix for the fully constrained thermodynamic ensemble described above reads

$$\hat{\rho}_{\text{FC}} = Z_{\text{FC}}^{-1} \exp \left[- \sum_k \lambda_k \hat{f}^F(k) \right], \quad (8)$$

where $Z_{\text{FC}} = \text{Tr}[\exp(-\sum_k \lambda_k \hat{f}^F(k))] = \prod_k (1 + e^{-\lambda_k})$. The values of the Lagrange multipliers λ_k must be fixed by the requirement that the fermionic (quasi-)momentum distribution predicted by (8) be the same as the (quasi-)momentum distribution of fermions in the actual initial—or, for that matter, time-evolved—state of the system. This constraint leads to $\lambda_k = \ln \left(\frac{1-f^F(k)}{f^F(k)} \right)$. As we stated above, the density matrix given by (8) is assumed to predict correctly the values of the system’s observables after a complete relaxation from an initial state with the fermionic (quasi-)momentum distribution given by $f^F(k)$. Below, we test this conjecture numerically, using the bosonic (quasi-)momentum distribution as the figure of merit.

Numerical tests.—In order to verify our predictions we perform two series of textbooklike numerical experiments on the relaxation of an ensemble of hard-core bosons on a lattice from a highly nonequilibrium state. We have chosen

to study lattices in which the final size $L \gg N$, i.e., the average interparticle distance is much larger than the lattice spacing, so that our results are also of relevance to continuous systems [5]. The numerical technique has been described elsewhere [38].

In the first series we prepare our gas in the ground state of a hard-wall box, then let the gas expand to a larger box. For all sizes of the initial box, we find that the (quasi-)momentum distribution indeed converges to an almost time independent distribution (see Fig. 1). Next, we compare the result after relaxation with the predictions of standard statistical mechanics and of the fully constrained ensemble (1) and (8). We find that the fully constrained thermodynamics stands in an exceptional agreement with the results of the dynamical propagation. (See [39] for further details of the thermal algorithm.) The accuracy of the above predictions has been successfully verified for the whole range of available values of the size of the initial box, from $L_{\text{in}} = N = 30$ through $L_{\text{in}} = L = 600$.

In the second series (Fig. 2) we study the effects of the memory of the initial conditions that is stored in the fully constrained ensemble (1) and (8). Our setting is very similar to an actual experiment on relaxation of an ensemble of hard-core bosons in a harmonic potential [34]. There the momentum distribution was initially split into two peaks. After many periods of oscillation, no appreciable relaxation to a single-bell distribution was observed. In our case the system is initially in the ground state of a superlattice (spatially periodic background potential, see [40] for details) with period 4,

$$\hat{V}_{\text{ext}} = A \sum_i \cos \frac{2\pi i}{T} \hat{b}_i^\dagger \hat{b}_i, \quad T = 4, \quad (9)$$

and is subsequently released to a flat-bottom hard-wall box $\hat{V}_{\text{ext}} = 0$. Our results show that even after a very long propagation time, the four characteristic peaks in the (quasi-)momentum distribution remain well resolved, although their shape is modified in the course of the propagation. Our interpretation of both experimental and numerical results is as follows: if the initial (quasi-)momentum distribution consists of several well-separated peaks, the memory of the initial distribution that is stored in the ensemble (1) prevents the peaks from overlapping, no matter how long the propagation time. Note also that the residual broadening of the peaks seen in Fig. 2 is beyond the experimental accuracy in [34].

Summary.—We have demonstrated that an integrable many-body quantum system—one-dimensional hard-core bosons on a lattice—can undergo relaxation to an equilibrium state. The properties of this state are governed by the usual laws of statistical physics, properly updated to accommodate all the integrals of motion. We further show that our generalized equilibrium state carries more memory of the initial conditions than the usual thermodynamic one. It is in the light of that observation that we interpret the results of the recent experiment on the nonequilibrium

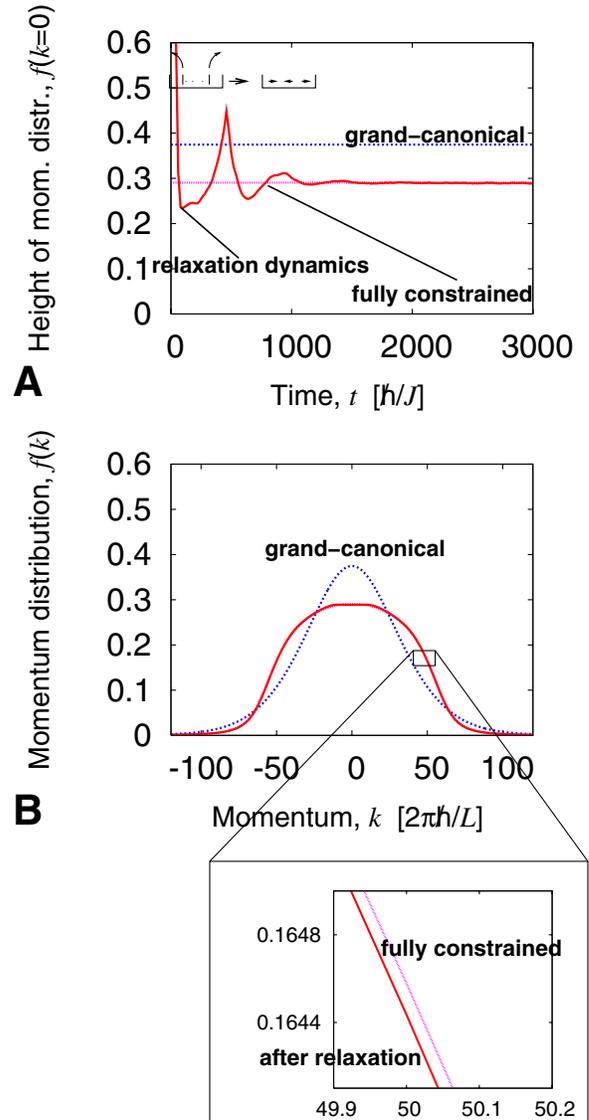


FIG. 1 (color online). Momentum distribution of $N = 30$ hard-core bosons undergoing a free expansion from an initial zero-temperature hard-wall box of size $L_{\text{in}} = 150$ to the final hard-wall box of size $L = 600$. The initial box is situated in the middle of the final one. (a) Approach to equilibrium. (b) Equilibrium (quasi-)momentum distribution after relaxation in comparison with the predictions of the grand-canonical and of the fully constrained (8) thermodynamical ensembles. The prediction of the fully constrained ensemble is virtually indistinct from the results of the dynamical simulation; see the inset for a measure of the accuracy. (An animation of the time evolution is posted online [41].)

dynamics of one-dimensional hard-core bosons performed at Penn State University [34], where an initial two-peaked (quasi-)momentum distribution failed to relax to a single-bell distribution.

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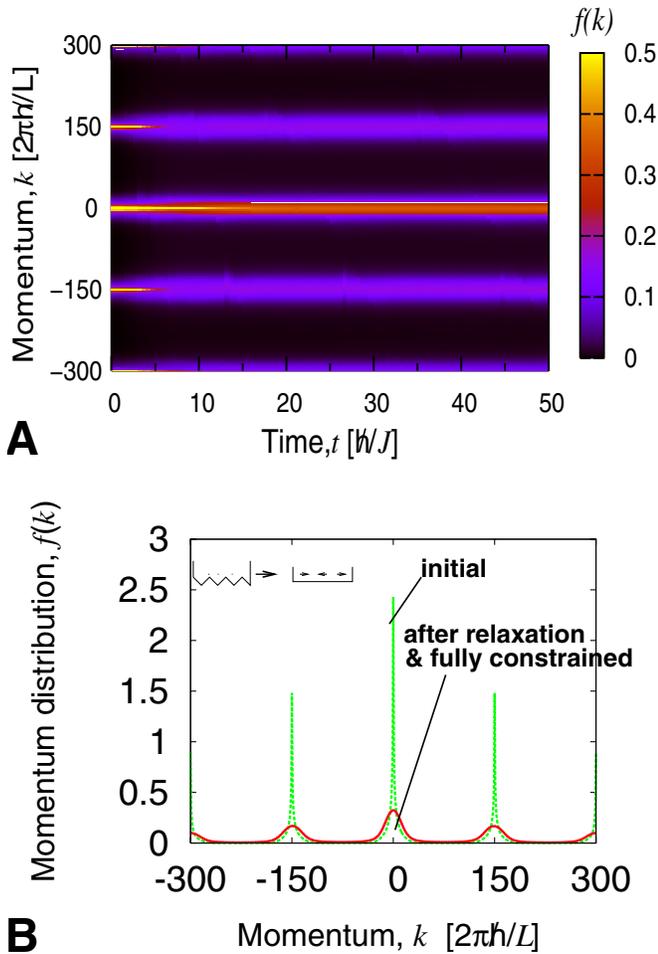


FIG. 2 (color online). Time evolution of the (quasi-)momentum distribution (a) and the (quasi-)momentum distribution after relaxation (b) of $N = 30$ hard-core bosons undergoing a free expansion from an initial zero-temperature superlattice with period four of half-depth $A = 8J$ and bound by a hard-wall box of size $L = 600$, to the final flat-bottom box ($A = 0$) of the same size. The discrepancy between the result of time propagation and the prediction of the fully constrained ensemble (8) [also shown in (b)] is less than the width of the line. Momentum peaks remain well-resolved during the whole duration of propagation; $t_{\text{fin}} = 3000\hbar/J$ for the subfigure (b). (An animation for the time evolution can also be found in [41].)

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