Irregular Dynamics in a One-Dimensional Bose System

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We study many-body quantum dynamics of δ-interacting bosons confined in a one-dimensional ring. Main attention is paid to the transition from the mean-field to the Tonks-Girardeau regime using an approach developed in the theory of interacting particles. We analyze, both analytically and numerically, how the Shannon entropy of the wave function and the momentum distribution depend on time for weak and strong interactions. We show that the transition from regular (quasiperiodic) to irregular ("chaotic") dynamics coincides with the onset of the Tonks-Girardeau regime. In the latter regime, the momentum distribution of the system reveals a statistical relaxation to a steady state distribution. The transition can be observed experimentally by studying the interference fringes obtained after releasing the trap and letting the boson system expand ballistically.

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The study of the quantum many-body dynamics of a Bose-Einstein condensate (BEC) is a major challenge in the physics of trapped gases. The mean-field Gross-Pitaevskii framework has successfully described an impressive set of experimental data [1], but it fails when genuine quantum many-body (QMB) correlations are important (e.g., in quantum phase transitions [2,3], in the design of quantum information devices [4] and interferometers [5], and near dynamically unstable regions where quantum corrections appear on a logarithmically short time scale [6]).

QMB effects also become particularly striking in low-dimensional systems, where the competition between quantum fluctuations and statistical properties is particularly enhanced. Recent experimental achievements in effective one-dimensional (1D) harmonically confined quantum degenerate systems [7] have stimulated several efforts to understand their main properties [8]. The 1D regime can be achieved in optical or magnetic traps when the radial degrees of freedom are frozen by tight transverse confinement. The Hamiltonian of the boson gas is given by the Lieb-Liniger model [9], where the two-body interaction is assumed to be pointlike. The thermodynamical properties of this Hamiltonian and its excitation spectra have been calculated analytically in [9]. An unexpected feature, predicted by Girardeau [10], is the onset of fermionization when $n/g \to 0$ (here n is the particle density, and g is the interatomic coupling constant which is inversely proportional to the 1D interatomic scattering length [11]). In this Tonks-Girardeau (TG) regime, the density of the interacting bosons becomes identical to that of noninteracting fermions (while, of course, the wave function keeps the bosonic symmetry). On the other hand, in the opposite limit, $n/g \to \infty$, the system is described in the mean-field (MF) approximation as a weakly interacting boson gas. The crossover between these two regimes occurs near $n/g \sim 1$. In this region the MF approach breaks down and more complicated two-body correlations become crucial.

While the thermodynamics of a 1D boson gas is fairly well understood, systematic studies of many-body dynamical properties of this system have been started only recently (see [12] and references therein). In this context, one should mention investigation of general quantum (beyond MF) properties of the dynamics of trapped bosons, which can be considered as the next frontier in BEC studies. In pursuit of this goal, in this Letter we study numerically the quantum dynamics of N interacting Bose particles on a one-dimensional ring of length L. Our main result is the discovery of a dynamical transition from regular to (quantum) irregular dynamics when $n/g \to 1$. This transition is accompanied by a linear increase of the Shannon entropy of the wave packets, which is directly related to the vanishing of the interference fringes which occurs after releasing the confinement and letting the bosons expand in a ballistic way.

Our model is specified by the Hamiltonian

$$\hat{H} = \sum_k \epsilon_k \hat{n}_k + \frac{g}{2L} \sum_{k,q,p,r} \hat{a}_k^\dagger \hat{a}_q^\dagger \hat{a}_p \hat{a}_r \delta(k + q - p - r). \tag{1}$$

Here $\hat{n}_k = \hat{a}_k^\dagger \hat{a}_k$ is the occupation number operator; $\hat{a}_s^\dagger$ and $\hat{a}_s$ are the creation-annihilation operators, and $\epsilon_k = 4\pi^2 k^2/L^2$. The classical analog of this model, which is originated from the nonlinear Shrödinger equation, has been analyzed in other papers. In the context of our study, the most interesting results have been obtained in [12], where the interchange between regular and irregular dynamics has been explored (without the connection with the Tonks-Girardeau regime). Note also that our model (1) is purely quantum, and the Hamiltonian is written in the operator form (see also [13]). Specifically, the occupation numbers for single-particle levels are not assumed *a priori* to be very large. To analyze this model, below we use the methods developed for quantum systems of interacting particles with complex behavior (see, e.g., [14] and references therein).

In what follows, we explore the situation when all bosons initially occupy the single-particle level with the angular momentum $k = 0$ or, equivalently, at $t = 0$ the system is in the unperturbed ($g = 0$) ground state $|\Psi_g\rangle$. Note that the total momentum is conserved in time. Our main interest is the evolution of the system for different values of the control parameter n/g. This type of experiment can be realized since the ratio n/g can be manipulated by tuning the interatomic scattering length.

It is convenient to label *single-particle states* $|k\rangle$ according to their momentum $k = 0, \pm 1, \pm 2, \ldots, \pm m, \ldots$. Then, any *many-body* state $|j\rangle$ can be represented as $|\ldots, n^j_{-m}, \ldots, n^j_0, \ldots, n^j_m, \ldots\rangle$, where n^j_k represents the number of particles in the single-particle level characterized by the momentum k of the jth state. In our numerical studies, we consider a finite number of particles N occupying $\ell = 2m + 1$ of single-particle states. Clearly, the number N of atoms and ℓ of levels should be chosen in a consistent way in order to extrapolate results to an arbitrary number of atoms. In a 1D geometry on a ring, N particles define the smallest spacing, which corresponds to the largest value of the momentum $m \approx N$. We satisfy the latter relation when changing values of N and m.

The transition from the MF to the TG regime can be understood using the following hand waving argument. Having all particles initially in the lowest state with $k = 0$, let us estimate the strength of the interaction necessary to move two particles from the unperturbed ground state to the upper (and lower) single-particle levels $k = \pm m$. One can expect that this interaction will result in an ergodic filling (in time) of all single-particle states. The energy required for the shift is approximately $m^2/L^2 \approx N^2/L^2$, and the matrix element of the interaction between the corresponding states is $\langle j|\hat{V}|j'\rangle \sim g\sqrt{N(N-1)}/L$. Equating these values, one can obtain $n = N/L \sim g$ which is associated with the crossover from the bosonic to fermionic regime. Dynamically this crossover is reflected by a rapid depletion of the fraction of particles in the lowest single-particle state with $k = 0$. Note that, at $n/g \sim 1$, the ratio $N_0/N \sim 1/2$, with $N_0 = \langle \hat{a}_0{}^\dagger \hat{a}_0\rangle$.

One of the most appropriate quantities to characterize the dynamical properties of this system is the Shannon entropy $S(t) = -\sum_j |\Psi_j(t)|^2 \ln|\Psi_j(t)|^2$ of the wave packet. Here $\Psi_j(t) = \langle j|\Psi(t)\rangle$ is the projection of the wave function onto the noninteracting many-body basis. After switching on the interaction, the wave function evolves according to the Hamiltonian, $\Psi(t) = e^{-iHt}\Psi_g(0)$, and spreads over the unperturbed basis.

The Shannon entropy $S(t)$ allows one to estimate the effective number of unperturbed many-body states that are involved in the dynamics due to the interparticle interaction, $N_{\mathrm{eff}}(t) \approx \exp\{S(t)\}$. A few examples of the time dependence of the entropy are reported in Fig. 1. One can see that for $n/g \gg 1$ the entropy oscillates in time, while for $n/g \ll 1$ there is a generic linear increase of $S(t)$ followed by a saturation.

While saturation is due to the finiteness of our Hilbert space, the linear growth in time of the entropy was shown [14] to be associated with the onset of chaos and thermalization in close systems of randomly interacting particles (see details in [15,16]). Specifically, for a strong enough interaction between particles the linear increase of $S(t)$ is due to an exponential increase in time of the number of many-body basis states involved in the dynamics. Although our model is not random, off-diagonal matrix elements determined by the particle interaction strongly fluctuate in time due to the different number of particles occupying single-particle levels. This fact allows us to apply the results obtained in [14] for our model.

When the probability of remaining in the originally excited state decreases exponentially, $W_0(t) = \exp(-\Gamma t)$, the entropy was found to increase linearly [14],

$$S(t) = \Gamma t \ln M, \tag{2}$$

apart from a generic quadratic increase that occurs at small times. Here the value of Γ is determined by the decay of the probability to stay in the unperturbed ground state, and $M = m$ is the number of many-body unperturbed states directly coupled to the initial state. As was shown in [14], the linear growth of entropy appears in the regime for which Γ is proportional to perturbation g.

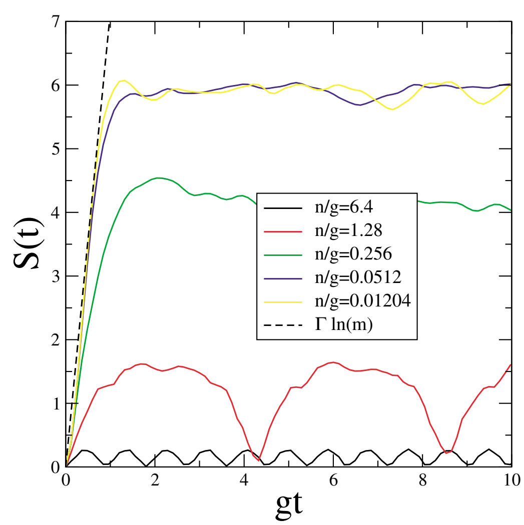

FIG. 1 (color online). Entropy as a function of the rescaled time gt for fixed $m = 6$ and different values of n/g. Data are given for $N = 6$. The saturation of $S(t)$ for small values of n/g manifests the onset of the Tonks-Girardeau regime. The dashed line corresponds to the theoretical prediction (2).

We have carefully checked the predictions (2) for $S(t)$. In particular, we have confirmed that the number of excited basis states grows in time exponentially fast before saturation. The saturation occurs because the total number of many-body states in our numerical simulation is finite. We also have found that the probability $W_0(t)$ decays exponentially in time. As a result, we were able to verify the increase of entropy given by Eq. (2) and indicated as a dashed line in Fig. 1.

We summarize our main results in Fig. 2. Here $S_{\rm ave}$ is the mean value of the entropy averaged over time after the saturation, and $N_{\rm H}$ is the dimension of the Hilbert space (the total number of many-body states defined by m and N). Entropy rescaling has been done in order to avoid its trivial dependence on the size of the Hilbert space. In this case, the plateau for $n/g \ll 1$ is independent of the choice of the number of particles and the number of levels. One can see that the renormalized entropy is a quantity that is very sensitive to the transition MF-TG regime. Also, as one can see, slight variations in the $m \approx N$ value does not change the results. This indicates the universal character of the entropy in the transition region. Note that the limiting value of the renormalized entropy is not 1, which would correspond to the prediction of random matrix theory. This deviation clearly indicates the influence of the dynamical nature of the Hamiltonian.

We now discuss how our predictions can be tested experimentally. Since the entropy of wave functions is not an easy quantity to measure experimentally, we need to relate it to an observable which can be measured directly. In cylindrical coordinates the boson field operator (defined on a ring of radius R in the plane $z = 0$) has the form $\hat{\psi}(\rho, \theta, z) = \hat{\delta}(z)\hat{\delta}(\rho - R)\hat{\psi}(\theta)$. Here the angle-dependent part can be expressed in terms of plane waves, $\hat{\psi}(\theta) = \sum_k \hat{a}_k e^{ik\rho\theta}$. Fourier transforming, $\hat{\chi}(\vec{p}) = \int d_3\vec{r}\, \hat{\psi}(\rho, \theta, z)e^{-i\vec{p}\cdot\vec{r}}$, and taking into account that $\vec{p} = p\hat{e}_y$ and $\vec{p} \cdot \vec{r} = p\rho \sin\theta$, we have,

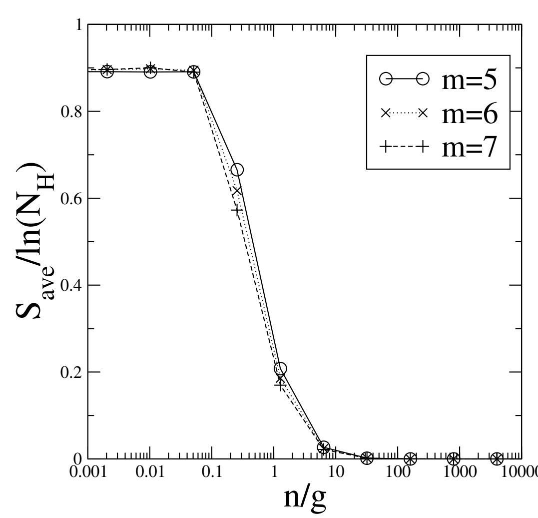

FIG. 2. Rescaled entropy as a function of n/g for $N = 6$ particles and different m as indicated in the inset.

$$\hat{\chi}(p) = C\sum_k \hat{a}_k \int_{\pi}^{\pi} d\theta\, e^{ikR\theta} e^{-ipR\sin(\theta)}, \tag{3}$$

where C is a normalization constant. Using periodic boundary conditions, $k = \frac{2\pi}{L} n = \frac{n}{R}$ with $n = 0, \pm 1 \pm 2 \ldots$, one obtains

$$\hat{\chi}(p) = C \sum_{n=-\infty}^{+\infty} J_n(pR)\hat{a}_n, \tag{4}$$

where $J_n(x)$ is the Bessel function of order n.

Expressing the wave function at time t in terms of the basis states $|j\rangle \equiv |n^j_{-\infty}, \ldots, n^j_0, \ldots, n^j_{+\infty}\rangle$, we obtain the occupation number distribution $n(p, t) = \langle\psi(t)|\hat{\chi}^\dagger(p)\hat{\chi}(p)|\psi(t)\rangle$. This quantity gives the probability density for finding a boson with momentum p along the y axis at time t. Using Eq. (4), we get

$$n(p, t) = \sum_{j,j'} \bar{\psi}_j(t)\psi_{j'}(t) \sum_{l,s=-\infty}^{+\infty} J_l(pR)J_s(pR)\langle j|\hat{a}_l^\dagger \hat{a}_s|j'\rangle. \tag{5}$$

Since the total momentum is zero, the selection rules $\langle j|\hat{a}_l^\dagger \hat{a}_s|j'\rangle = n^j_l \delta_{j,j'}\delta_{l,s}$ hold, where n^j_l is the number of particles occupying the single-particle level with momentum l in the jth basis state. Finally, we obtain

$$n(p, t) = C\sum_j |\psi_j(t)|^2 \sum_{l=-\infty}^{+\infty} J_l^2(pR)n^j_l, \tag{6}$$

where $C^{-1} = N^{-1} \int dp\, n(p, t)$.

Results are reported in Fig. 3. When $n/g \gg 1$, the momentum distribution does not practically change in time. All particles remain mainly in the condensate during the evolution. Close to the transition point $n/g \le 1$, the distribution begins to be flat, without relaxing to an asymptotic distribution. In this intermediate region, the

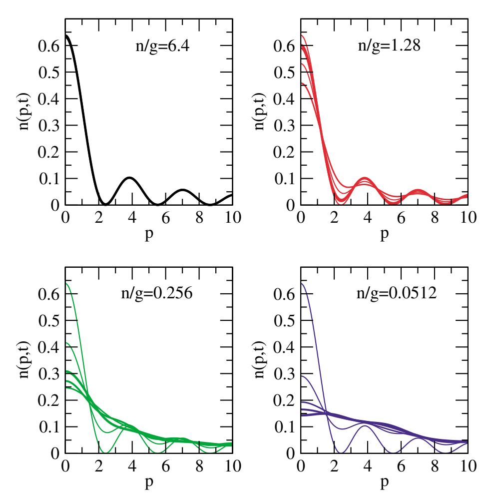

FIG. 3 (color online). Particle density in the momentum representation for four values of n/g, and for different rescaled times $gt = 0$, 0.2, 0.4, 0.6, and 0.8 (lines are thicker for later times).

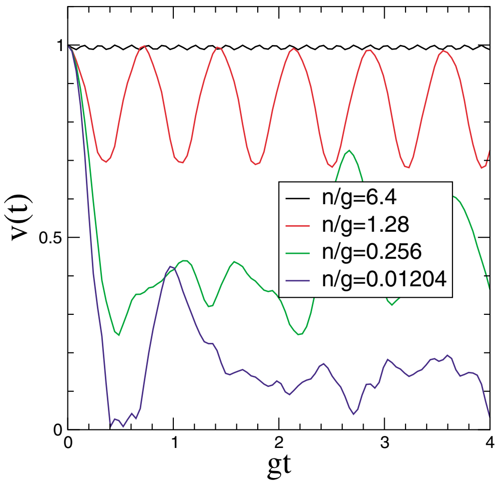

FIG. 4 (color online). Visibility as a function of time, for four values of rescaled interaction n/g. Here is $N = 6$ and $m = 6$.

occupation number distributions reveal a mixture of very slow relaxations and strong oscillations in time that was first observed [13] in a similar model and termed as "nonergodic behavior of interacting bosons."

Contrary to this, for $n/g \ll 1$, one can see a clear relaxation of the occupation number distribution to a steady state distribution. In fact, the onset of relaxation to the steady distribution means that the behavior of the model can be well described by statistical methods [17].

In order to characterize qualitatively the onset of relaxation in the TG regime, we propose to observe experimentally the *fringe visibility* defined as

$$v(t) = |I_{\max} - I_{\min}|/(I_{\max} + I_{\min}). \tag{7}$$

Here we chose $I_{\max} = n(p = 0, t)$, $I_{\min} = n(p_0, t)$ where $p_0 \simeq 2.41$ is the first zero of J_0. This quantity allows one to distinguish between periodic and aperiodic behavior of the occupation number distribution (see Fig. 4).

As one can see, the TG regime is characterized by a fast decay of the visibility with subsequent fluctuations that persist in time. These fluctuations are additional evidence of the statistical nature of the dynamics when the interparticle interaction is strong. When $n/g \gg 1$ (MF regime), the visibility oscillates, revealing collapses and revivals of the condensate fraction population, as the entropy does in the same regime (see Fig. 1). Therefore, there is a strict correspondence between the dynamical evolution of the entropy and the visibility of the momentum distribution. The interference properties of a thermal Tonks gas localized on one side of a ring have been studied in [18].

In conclusion, we have studied the dynamics of a Bose-Einstein condensate model on a torus by paying attention to the role of the interparticle interaction. Specifically, we considered the situation in which initially only the ground state, defined in the absence of the interaction, is populated. By switching on the interaction, we have found different regimes depending on the strength of interaction. The first regime (MF regime, $n/g \gg 1$) is characterized by regular dynamics associated with periodic oscillations in time of the Shannon entropy $S(t)$ and of the fringe visibility Eq. (7) of particle density. In the Tonks-Girardeau regime, $n/g \ll 1$, the Shannon entropy grows linearly in time in accordance with our analytical estimates. Even if these estimates are obtained for completely random models, they give a remarkable agreement with our data. Moreover, this approach allows one to understand the mechanism of the transition from the mean-field to Tonks gas regime.

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