Chaotic Properties of Quantum Many-Body Systems in the Thermodynamic Limit

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By using numerical simulations, we investigate the dynamics of a quantum system of interacting bosons. We find an increase of properly defined mixing properties when the number of particles increases at constant density or the interaction strength drives the system away from integrability. A correspondence with the dynamical chaoticity of an associated c-number system is then used to infer properties of the quantum system in the thermodynamic limit. [S0031-9007(96)01693-6]

Classical Hamiltonian systems are usually termed chaotic if their trajectories show local exponential instability, i.e., a positive Lyapunov exponent [1]. This definition reflects the generally nonlinear character of the differential equations of the classical motion. Here we will refer to this situation as *dynamical chaos.*

At quantum level, every system is described by a linear Schrödinger equation and dynamical chaos is not possible. One can resort to a definition of quantum chaos based on the correspondence principle. It is often assumed, but not rigorously proved, that classically chaotic systems give rise to quantum mechanical spectra whose statistical properties are well described by random matrix theory [2]. Indeed, a large class of numerical examples [3] and recent theoretical work [4] indicate that the nearest neighbor level spacing (NNLS) distribution of systems which are classically chaotic is well approximated by a Wigner distribution [1].

The above statements refer to confined systems with a finite number of degrees of freedom. Quantum mechanically these systems are characterized by a discrete spectrum. The situation is different if we consider a many-body system in the thermodynamic limit, i.e., when the number N of particles tends to infinity at constant density. In this limit the spectrum is, in general, continuous, and true chaotic phenomena are not excluded [5,6].

One should state clearly from the outset that in the thermodynamic limit chaotic behavior, in the sense that the system is mixing, can appear through a mechanism which has nothing to do with the nonlinearity of the interaction but is connected with the possibility of transforming space chaos into time chaos. This is true both at classical and quantum levels as it is illustrated in the case of an infinite system of linearly interacting oscillators classical [7], or quantum [8], and in the case of a gas of noninteracting particles classical [9], or quantum [10]. To clarify the point in question let us consider the case of a one-dimensional lattice of classical harmonic oscillators coupled in such a way that it may be considered as the discretization of the wave equation in one space dimension. As it is well known the solutions of this equation depend on the combination $x \pm t$, where x and t are the space and time coordinates, respectively. As a consequence, if the initial condition is a realization of a mixing stochastic process in space this is transformed by the dynamics into a mixing stochastic process in time at any point in space. If the system is in equilibrium at some temperature T, the initial conditions to be considered are typical realizations of the stochastic process corresponding to the equilibrium Gibbs measure. We shall call the chaotic behavior of noninteracting or linearly interacting many-body systems *kinematical chaos.* Clearly, in the cases considered in [8,10] Lyapunov exponents are zero because the dynamics in the thermodynamic limit is the limit of the finite-dimensional dynamics.

In this paper we want to investigate what happens when a nonlinear interaction is switched on, i.e., the Hamiltonian describing the system is not quadratic. We begin by recalling the general definition of mixing given in [8,10]. Let us consider N interacting particles in a volume $V \subset \mathbf{R}^d$ described by the Hamiltonian $\hat{H}$ and let $\hat{A}$ and $\hat{B}$ be two local observables. We shall say that the system has the property of quantum mixing in the thermodynamic limit if the following holds:

$$\lim_{t \to \infty} \lim_{\substack{N,V \to \infty \\ N/V \to \rho}} \langle \hat{A}(t)\hat{B} \rangle = \lim_{\substack{N,V \to \infty \\ N/V \to \rho}} \langle \hat{A} \rangle \lim_{\substack{N,V \to \infty \\ N/V \to \rho}} \langle \hat{B} \rangle, \qquad (1)$$

where

$$\langle \cdots \rangle = \frac{\mathrm{Tr} \ \ldots e^{-\hat{H}/k_B T}}{\mathrm{Tr} \ e^{-\hat{H}/k_B T}}, \qquad \hat{A}(t) = e^{(i/\hbar)\hat{H}t}\hat{A}e^{-(i/\hbar)\hat{H}t}.$$

As a rule, the limits on the left-hand side of (1) must be taken in the order indicated. However, for the systems discussed in [8,10] the limits can actually be inverted, and we shall assume that this applies also to the interacting systems considered in this paper.

Since, even if the interaction is nonlinear, the finite-dimensional dynamics is quasiperiodic, Lyapunov exponents are zero for any finite N and, therefore, also in the thermodynamic limit [11]. We expect, however, an influence of the nonlinearity on the mixing properties of the system. In particular, we expect that the strength of the nonlinearity will affect the rate of convergence of the t limit in (1) once the thermodynamic limit has been taken.

If N is finite, as will be the case in computer simulations, we expect the difference

$$\langle \hat{A}(t)\hat{B} \rangle - \langle \hat{A} \rangle \langle \hat{B} \rangle \tag{2}$$

to oscillate in time with an averaged amplitude [see Eq. (5)] which decreases when the interaction drives the system away from integrability. This amplitude should decrease also when the interaction strength is kept fixed and N increases with N/V constant.

We consider a system of N spinless bosons of charge q moving in a one-dimensional lattice with L sites and described by the Hamiltonian

$$\hat{H} = \sum_{j=1}^{L} [\alpha_j \hat{a}_j^\dagger \hat{a}_j - \beta_j (e^{i\theta} \hat{a}_{j+1}^\dagger \hat{a}_j + e^{-i\theta} \hat{a}_j^\dagger \hat{a}_{j+1})]$$
$$+ \sum_{j=1}^{L} \gamma_j \hat{a}_j^\dagger \hat{a}_j^\dagger \hat{a}_j \hat{a}_j, \tag{3}$$

where index correspondence $j \pm L = j$ is assumed. The operator $\hat{a}_j^\dagger$ creates a boson in the site j, and α_j, β_j, and γ_j are the site, hopping, and interaction energies, respectively. Dirichlet or periodic boundary conditions can be chosen. In the first case the sites lie on a segment and we put $\beta_L = 0$ and $\theta = 0$. In the second case the system represents a ring threaded by a line of magnetic flux ϕ. The phase factors are $\theta = 2\pi\phi/\phi_0 L$, where $\phi_0 = hc/q$ is the flux quantum. The system (3) has wide interest. Its time-dependent mean-field approximations have applications to molecular dynamics and nonlinear optics [12] and to electron transport in heterostructures [13].

For finite L and N the dimension of the Fock space spanned by the system (3) is finite and given by

$$D = \frac{(N + L - 1)!}{N!(L - 1)!}. \tag{4}$$

The D-dimensional matrix representing the Hamiltonian (3) in the base of the Fock states $|n_1^i \cdots n_L^i\rangle$, $i = 1, \ldots, D$, where n_j^i is the occupation number of the jth site in the ith Fock state and $\sum_{j=1}^{L} n_j^i = N$, can be diagonalized by standard numerical methods with negligible errors.

We have calculated the quantity (2) for different local operators $\hat{A}$ and $\hat{B}$ and for $N \leq 7$ with $N/L = 1$. Figure 1 shows typical results obtained at zero temperature for $\hat{A} = \hat{B} = \hat{a}_{k+1}^\dagger \hat{a}_k + \hat{a}_k^\dagger \hat{a}_{k+1}$ with $k = 3$. For simplicity, in the numerical simulation we put α, β, and γ independent of the site j. The number of particles and sites considered, $N = L = 5$ and $N = L = 7$, may look very small, but one has to remember that the complexity of the system is given by the Fock dimension D which is 126 and 1716, respectively. Up to such values of D we observe that the amplitude of the oscillations of (2) decreases in the presence of nonlinear interaction. By comparing Figs. 1(a) and 1(b), we have also evidence of a decrease of these oscillations with increasing N at constant density.

To make the above discussion quantitative we measure the oscillating behavior of (2) by introducing the follow-
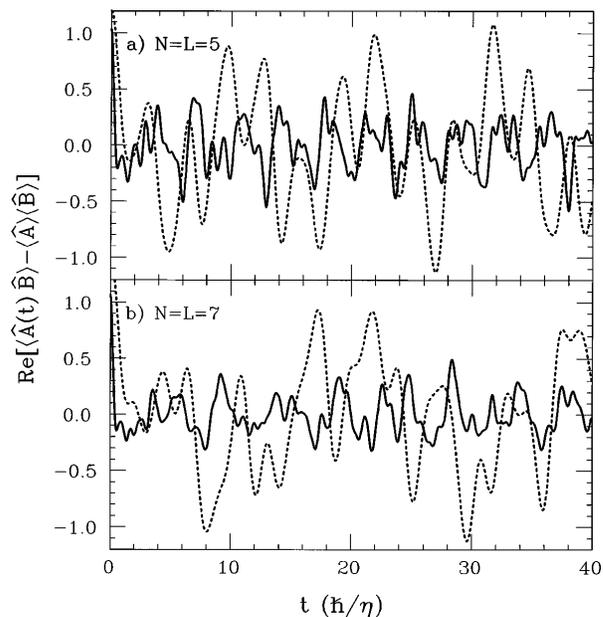
FIG. 1. Real part of (2) as a function of time for $N = L = 5$ (a) and $N = L = 7$ (b) at zero temperature. The system has periodic boundary conditions with $\phi/\phi_0 = 0.3$, $\alpha = 0$, $\beta = \eta$, and $\gamma = \eta$ (solid line) or $\gamma = 0$ (dashed line). The local operators considered are $\hat{A} = \hat{B} = \hat{a}_{k+1}^\dagger \hat{a}_k + \hat{a}_k^\dagger \hat{a}_{k+1}$ with $k = 3$.

ing indicator

$$\kappa_{\hat{A}\hat{B}} = \lim_{t \to \infty} \sqrt{\frac{1}{t} \int_0^t dt' \, |\langle \hat{A}(t')\hat{B} \rangle - \langle \hat{A} \rangle \langle \hat{B} \rangle|^2}. \tag{5}$$

Mixing implies that $\kappa_{\hat{A}\hat{B}} = 0$. If $\hat{A}$ or $\hat{B}$ commutes with the Hamiltonian $\hat{H}$, $\langle \hat{A}(t)\hat{B} \rangle - \langle \hat{A} \rangle \langle \hat{B} \rangle$ is identically zero at zero temperature. The limit (5) can be evaluated exactly and in Fig. 2 we show its value for the same observables of Fig. 1 as a function of the ratio γ/β at zero temperature. For fixed α, $\kappa_{\hat{A}\hat{B}}$ depends only on this ratio. Since the system considered is integrable for $\gamma = 0$ and $\beta = 0$ we expect a minimum of $\kappa_{\hat{A}\hat{B}}$, that is, a maximal chaoticity, between these two limits. For $\alpha = 0$ and $N/L = 1$, this minimum should take place at $\gamma/\beta \sim 1$. The results shown in Fig. 2 confirm this expectation as well the decrease of $\kappa_{\hat{A}\hat{B}}$ when N increases at constant density. Similar results are obtained at finite temperature.

There is a natural c-number system associated with a system of bosons like the one we consider. This is obtained by constructing a mean-field approximation which, when quantized, reproduces the exact quantum equation in the second quantization formalism [14]. We now provide evidence that there exists a strict correspondence between the dynamics of this c-number system and that of the quantum system by evaluating the maximal Lyapunov exponent of the mean-field dynamics as a function of the
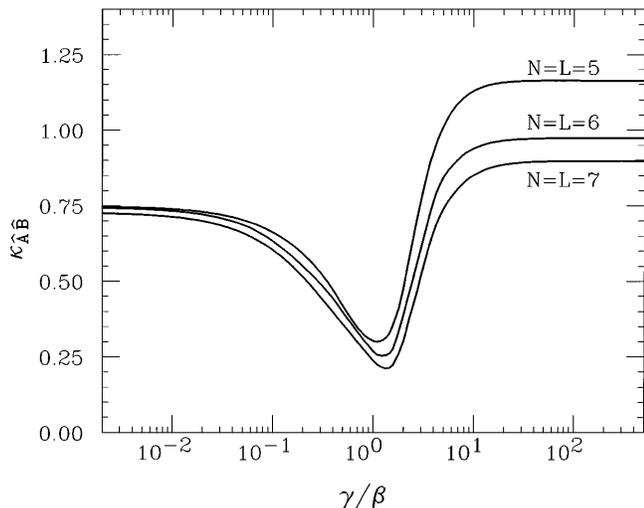
FIG. 2. Mixing indicator (5) at zero temperature for the system of Fig. 1 as a function of the ratio γ/β.

FIG. 3. Rescaled maximal Lyapunov exponent $\lambda\hbar/\gamma$ of the mean-field system (6) as a function of the ratio γ/β for $\alpha = 0$, $\beta = \eta$, $N = L = 5$, $\phi/\phi_0 = 0.3$, and periodic boundary conditions. The initial mean-field components $z_j(0)$ are arbitrary complex numbers with $|z_j(0)|^2 = 1/L$.

interaction strength γ. Nonlinear mean-field equations for the system (3) can be written as [15]

$$i\hbar \frac{d}{dt} z_j(t) = [\alpha_j + 2(N - 1)\gamma_j|z_j(t)|^2]z_j(t)$$
$$- \beta_{j-1}e^{i\theta}z_{j-1}(t) - \beta_j e^{-i\theta}z_{j+1}(t), \quad (6)$$

where $z_j(t)$ is the amplitude of the mean field in the site j. Conservation of the single-particle probability

$$\sum_{j=1}^{L} |z_j(t)|^2 = 1 \qquad (7)$$

and of the single-particle energy

$$\mathcal{E}[z, z^*] = \sum_{j=1}^{L} \{\alpha_j|z_j(t)|^2 + (N - 1)\gamma_j|z_j(t)|^4$$
$$- [\beta_{j-1}e^{i\theta}z_{j-1}(t) + \beta_j e^{-i\theta}z_{j+1}(t)]z_j^*(t)\}$$
$$\qquad (8)$$

is a crucial constraint for a correct numerical simulation of (6). The corresponding maximal Lyapunov exponent λ can then be numerically evaluated with negligible errors [14]. In order to use a dimensionless quantity we consider the rescaled exponent $\lambda\hbar/\gamma$ when the ratio γ/β is varied at fixed β. In fact, λ depends on both β and γ/β. The curve in Fig. 3 shows that $\lambda\hbar/\gamma$ has a pronounced maximum in the same region where $\kappa_{\hat{A}\hat{B}}$ has a minimum. This means that the tendency to chaoticity of the finite quantum system and the chaoticity of its c-number counterpart have the same qualitative behavior away from integrability points. This aspect can be analyzed in greater detail and will be discussed in a subsequent publication.

The numerical study of the quantum system (1) becomes prohibitive for values of D larger than a few thou-

sands. To get an idea of what happens when we increase further the number of particles, we make the reasonable hypothesis that the chaotic behavior increases if the same happens for the corresponding c-number system. The numerical evaluation of the maximal Lyapunov exponent of the mean-field dynamics is feasible also for large values of N and L. We now show that the chaotic behavior of the mean-field evolution of our system increases mono-
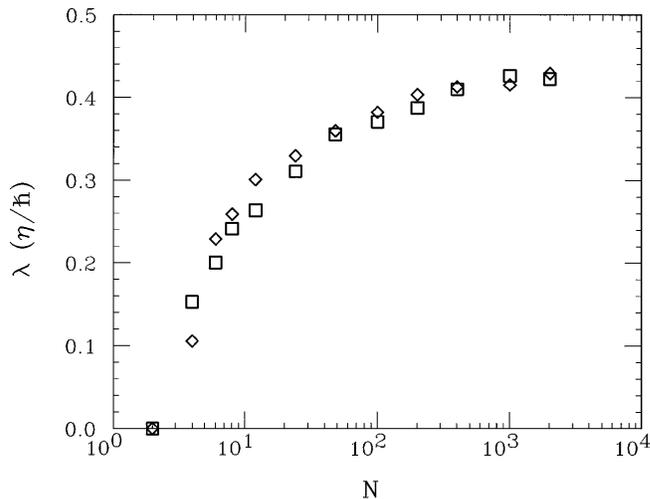
FIG. 4. Maximal Lyapunov exponent λ of the mean-field system (6) as a function of the number N of particles at constant density $N/L = 1$. We have $\alpha = 0$, $\beta = \eta$, and $\gamma = \eta L/(N - 1)$ with $\phi/\phi_0 = 0$ and Dirichlet boundary conditions (squares) and $\phi/\phi_0 = 0.3$ and periodic boundary conditions (diamonds). The initial mean-field components $z_j(0)$ are chosen in order to have the same single-particle energy for any value of N.

tonically and eventually becomes constant when the thermodynamic limit is approached. Figure 4 displays the behavior of the maximal Lyapunov exponent of (6) up to $N = 2000$ for $N = L$ and $\gamma \simeq \beta$, that is, in the region of maximal chaoticity. We have a satisfactory evidence that the maximal Lyapunov exponent reaches a limiting value which we assume to characterize the dynamics in the thermodynamic limit.

On the basis of these results we conclude that the maximal chaoticity of the quantum system should also increase steadily until the limit $\kappa_{\hat{A}\hat{B}} = 0$ is reached.

The approach that we have developed in this paper is clearly applicable to the study of the chaotic properties of any quantum system and is complementary to the usual search of quantum signatures of classical chaos.

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