Nonergodic behavior of interacting bosons in harmonic traps

Thomas Papenbrock and George F. Bertsch

Institute for Nuclear Theory, Department of Physics, University of Washington, Seattle, Washington 98195

(Received 29 July 1998)

We study the time evolution of a system of interacting bosons in a harmonic trap. In the low-energy regime, the quantum system is not ergodic and displays rather large fluctuations of the ground-state occupation number. In the high-energy regime of classical physics we find nonergodic behavior for modest numbers of trapped particles. We give two conditions that assure the ergodic behavior of the quantum system even below the condensation temperature. [S1050-2947(98)08612-0]

PACS number(s): 03.75.Fi, 05.30.Jp, 32.80.Pj

I. INTRODUCTION

The understanding of the formation and growth of atomic Bose-Einstein condensates [1–4] is of considerable interest and has been investigated experimentally and theoretically [5–9]. Bose-Einstein condensates may be formed while the trapped bosons are in contact with a heat bath and a particle reservoir (e.g., via evaporative cooling [10]) or from the evolution of a nonequilibrium state in an isolated system. In a recent experiment at MIT [11], harmonically trapped bosons were rapidly cooled below the transition temperature, and the subsequent relaxation towards a Bose-Einstein condensate was observed and measured. The existing theory uses the Boltzmann equation, which is fundamentally based on the ergodic Stoßzahlansatz. However, this assumption deserves closer scrutiny in the context of bosons in traps. In particular, the motion of two particles confined to a harmonic trap is integrable for any interaction potential that depends only on the distance. Closely related to ergodicity is the question about the fluctuations of the ground- state occupation number in an isolated interacting system. For the noninteracting system, these fluctuations have been calculated recently [12,13]. Fluctuations of the interacting system are first computed here.

The paper is organized as follows. The low-energy quantum Hamiltonian and observables of interest are introduced in the second section. In the third section, we present numerical results of the time evolution of the ground-state occupation number and its fluctuations for bosons in a harmonic and a square well potential, respectively. The comparison with a chaotic and ergodic random matrix model is presented in Sec. IV. The structure of classical phase space for a system of harmonically trapped hard-sphere particles is discussed in the fifth section. Finally, the results are summarized in the conclusion.

II. HAMILTONIAN AND OBSERVABLES

In this section we describe the quantum Hamiltonian and the observables that may indicate nonergodic behavior. We will consider interacting bosons confined to a harmonic potential or a square well potential. Magnetic traps, as used in recent experiments, are very well approximated by harmonic potentials. However, the square well potential is also of considerable interest, since many theoretical results were obtained for such traps and since the underlying classical system of hard-sphere bosons is chaotic and ergodic [14].

Independent of the specific trap potential, the Hamiltonian may be written

$$\hat{H} = \hat{H}_0 + \hat{V}. \tag{1}$$

Here

$$\hat{H}_0 = \sum_j E_j \hat{a}_j^\dagger \hat{a}_j \tag{2}$$

is the one-body trap Hamiltonian and

$$\hat{V} = \lambda \sum_{i,j,k,l} V_{ijkl} \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_k \hat{a}_l \tag{3}$$

is the two-body interaction. The operators $\hat{a}_j$ and $\hat{a}_j^\dagger$ annihilate and create one boson in the single-particle trap state $|j\rangle$ with energy E_j, respectively. They fulfill the usual bosonic commutation rules. In what follows, the interaction is chosen to be a contact interaction.

We will study the quantum dynamics of a N-body system of bosons using the occupation number representation. The basis of states is $|\alpha\rangle \equiv |n_0, n_1, \ldots, n_k\rangle$ with $\Sigma_{i=0,k} n_i = N$ and $\hat{a}_j^\dagger \hat{a}_j |n_0, n_1, \ldots, n_k\rangle = n_j |n_0, n_1, \ldots, n_k\rangle$. Here n_j denotes the occupation of the jth single-particle state $|j\rangle$. Obviously, the trap Hamiltonian is diagonal in this basis.

We also note that condensation occurs in d-dimensional harmonic traps for energies $E \approx N^{1+1/d} \hbar \omega$ [15,4], and this is the regime we are most interested in. No Bose-Einstein condensation occurs in square well potentials in two spatial dimensions.

A. Harmonic trap

To be specific, we now consider the case of an isotropic harmonic trap in two spatial dimensions. The single particle states are $|j\rangle \equiv |n_j, m_j\rangle$ with energy $E_j = n_j \hbar \omega$ and angular momentum $m_j \hbar$ $(m_j = -n_j, -n_j + 2, \ldots, n_j - 2, n_j)$. We denote the oscillator wave functions as $\phi_j(\vec{x}) \equiv \langle \vec{x} | j \rangle$. The ground-state energy is set to zero. In terms of the dimensionless coordinate $\vec{x} = \vec{r}/d_0$ (where $d_0 \equiv \sqrt{\hbar/m\omega}$ sets the length scale of the trap), the contact interaction (3) has matrix elements

$$V_{ijkl} = \int d^2x \, \phi_i^*(\vec{x}) \phi_j^*(\vec{x}) \phi_k(\vec{x}) \phi_l(\vec{x})$$

$$= \frac{\delta_{m_i+m_j}^{m_k+m_l}}{2} \int_0^\infty dx \, x^{-2} M_{(n_i+1)/2, \, |m_i|/2}(x)$$

$$\times M_{n_j+1/2, |m_j|/2}(x) M_{(n_k+1)/2, |m_k|/2}(x)$$

$$\times M_{(n_l+1)/2, |m_l|/2}(x). \tag{4}$$

Here $M_{\mu,\kappa}(x)$ denotes the Whittaker function [16] and the δ function ensures conservation of angular momentum. The coupling is given by $\lambda = 4\pi\hbar\omega a/d_0$, where a is the s-wave scattering length. Obviously, the total energy E and the total angular momentum M are conserved quantities. Furthermore, the motion of the center of mass decouples from the single-particle motion yielding a ladder of states spaced by $\hbar\omega$ for each spatial dimension [17]. Pitaevskii and Rosch have shown that Hamiltonian (1) possesses an additional SO(2,1) symmetry [18]. This leads to another conserved quantity B that can be associated with breathing modes. For fixed quantum numbers M and B the spectrum of Hamiltonian (1) consists of an infinite ladder with spacing $2\hbar\omega$. The contact interaction (3),(4) is valid in a dilute system at low energies $\sqrt{\hbar\omega/E} \gg a/d_0$, i.e., the scattering length is small compared to the wavelength.

One may think of the above model as a realization of a *three*-dimensional oblate trap with $\omega \ll \omega_z$ and $a/d_0 \ll a\sqrt{m\omega_z/\hbar} \ll 1$. Under these conditions, the Hamiltonian (1) provides a reliable approximation for a dilute gas of atoms confined in an oblate magnetic trap at sufficiently low excitation energy. The trap used by the JILA group is closest to such a trap.

We use in the numerical calculation a basis spanned by the eigenstates $|\alpha, E, M\rangle$ of the trap Hamiltonian (1) with total energy $E \le E_{max}$ and angular momentum M. (α accounts for the different states with quantum numbers E, M. Their number is $\Omega(E, M)$; in what follows we may suppress the dependence on E, M.) Within this basis, the matrix of the interaction (3) is set up as follows. After fixing the total angular momentum M and the maximal energy E_{max} we choose one (arbitrary) N-boson state $|\alpha, E, M\rangle$ with $E \le E_{max}$. We then act with the interaction (3) onto $|\alpha\rangle$ and onto all the states created by this procedure until the space with energies $E \le E_{max}$ and fixed angular momentum M is exhausted. The resulting matrix is sparse. As one checks on the numerics we note that the obtained spectra display ladders with spacings $2\hbar\omega$ or $\hbar\omega$ result from the breathing mode [18] or the center of mass motion [17], respectively. Results obtained after the exact diagonalization of Hamiltonian (1) were found to be in good agreement with mean-field theory even for rather small systems [19].

At fixed angular momentum, the spectrum of the trap (2) consists of equidistant shells of highly degenerate states with energy $E = 2K\hbar\omega$. The spacing between the shells is $2\hbar\omega$ [since even (odd) E_{max} requires even (odd) M]. We label the different shells by their energy quantum number K. Increasing the coupling λ shifts the entire spectrum towards higher energies and lifts the degeneracies partially. However, the spectrum still exhibits shell structure for not too large couplings and number of particles.

B. Square well trap

In case of a square well potential of width d_0, the creation operator $\hat{a}_j^\dagger$ creates a boson in the single-particle state $|j\rangle \equiv |n_{jx}, n_{jy}\rangle$ with energy $E_j = E_0(n_{jx}^2 + n_{jy}^2)$. Here, $E_0 = \hbar^2/2md_0^2$ sets the energy scale. n_{jx} and n_{jx} are the quantum numbers in the x and y directions, and the wave functions are $\phi_j(x,y) = 2\sin(n_{jx}\pi x)\sin(n_{jy}\pi y)$, where distances $0 \le x, y \le 1$ are measured in units of d_0. States may be characterized by their behavior under reflection at the axes $x = 1/2$, $y = 1/2$. (We do not specify the behavior under reflection $x \leftrightarrow y$.) The coupling is given by $\lambda = 4\pi E_0 a/d_0$ in terms of the s-wave scattering length a. In what follows we consider those states which have the same symmetry as the ground state. The Hamiltonian matrix is built up as for the harmonic trap. At zero coupling λ, the spectrum is highly degenerate and thus exhibits shell structure. With increasing coupling, most of the degeneracies are lifted, the entire spectrum is shifted towards higher energies, and the shells overlap very soon. This behavior is different from the harmonic trap where the shell structure persists even for relatively large values of the coupling.

C. Observables

Nonergodic behavior manifests itself in the difference between the time average of a dynamical observable and its ensemble average. The most interesting observable is the ground state occupation number, $\hat{n}_0 = \hat{a}_0^\dagger \hat{a}_0$. This observable has been measured, and its microcanonical fluctuations have been computed recently for the noninteracting system [12]. The time evolution for its expectation value with the trap eigenstate state $|\alpha\rangle$ is

$$n_0^{(\alpha)}(t) = \langle\alpha|\hat{U}^\dagger(t)\,\hat{n}_0\,\hat{U}(t)|\alpha\rangle. \tag{5}$$

Here

$$\hat{U}(t) = \exp[-i\hat{H}t/\hbar] \tag{6}$$

is the time evolution operator. In practice, we evaluate Eq. (5) by applying $U(\Delta t)$ with a suitable chosen Δt onto the initial state $|\alpha\rangle$ by using its Taylor expansion [20]. This procedure allows one to treat rather large matrices. The unitarity of $\hat{U}(t)$ was numerically ensured by an error of the norm $\langle\alpha\hat{U}^\dagger(t)|\hat{U}(t)\alpha\rangle$ that was smaller than 1%. The results are compared to the equilibrium value

$$\overline{n_0} \equiv \frac{1}{\Omega}\sum_{\alpha=1}^{\Omega} \langle\alpha|\hat{n}_0|\alpha\rangle. \tag{7}$$

In the case of the harmonic trap potential, this equilibrium value is the ensemble average over all $\Omega(E, M)$ states within one energy shell. Note that the states within this ensemble have different values of the conserved quantity B associated with the breathing mode. In the case of the square well potential the ensemble comprises all states within an energy layer $\delta E \approx 5\pi^2\hbar^2/2md_0^2$ around E that have the same symmetry as the ground state. δE is reasonably smaller than the ground-state energy $2N\pi^2\hbar^2/2md_0^2$ even for modest numbers of particles. Note that these ensembles differ from the
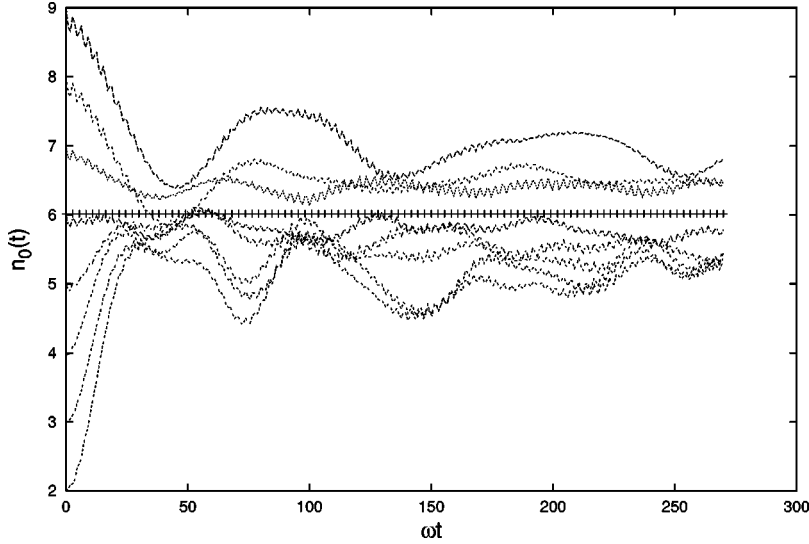
FIG. 1. Time evolution (thin lines) of the ground-state occupation number (5) for different initial states of the $(K=4)$ shell that are initially away from the equilibrium value (horizontal line of crosses). Results are obtained for a system of $N=10$ harmonically trapped bosons that interact via s-wave scattering. The coupling is $\lambda=0.15\hbar\omega$.

microcanonical ensembles that are determined by energy only and do not depend on additional quantum numbers. However, nonergodic behavior in a sector defined by additional quantum numbers implies nonergodic behavior in the entire energy shell.

A second and more quantitative indicator for nonergodic behavior is given by the fluctuations of the ground-state occupation number. These are defined by

$$\delta n_0^2(\lambda) = \frac{1}{\Omega}\sum_{\Psi} \langle\Psi|\hat{n}_0|\Psi\rangle^2 - \left(\frac{1}{\Omega}\sum_{\Psi} \langle\Psi|\hat{n}_0|\Psi\rangle\right)^2, \quad (8)$$

where $|\Psi(E,M)\rangle$ are the eigenstates of the interacting system. Note that the fluctuations (8) depend on λ.

For an ergodic system, these fluctuations should be very small since an expectation value should not depend on the particularly chosen state within an energy shell of Ω states. It is useful to compare the fluctuations for the interacting system with the fluctuations for the noninteracting system,

$$\delta n_0^2(0) \equiv \overline{n_0^2} - \overline{n_0}^2 = \frac{1}{\Omega}\sum_{\alpha} (\langle\alpha|\hat{n}_0|\alpha\rangle - \overline{n_0})^2. \quad (9)$$

To compute the fluctuations (8), we diagonalize the Hamiltonian (1) in the basis $|\alpha\rangle$ and obtain the eigenstates $|\Psi\rangle$.

III. NUMERICAL RESULTS

We describe the numerical results obtained for the harmonic trap and the square well potential.

A. Harmonic trap

We choose $\lambda=0.15\hbar\omega$, $N=10$ and $E_{max}=12\hbar\omega$. This space has a dimension of 1530 and according to the criterion given in Refs. [15] should exhibit condensation. Figure 1 shows $n_0^{(\alpha)}(t)$ for a few states of the $(K=4)$ shell that have initially $2 \leq n_0^{(\alpha)}(t=0) \leq N-1$. These states have occupation numbers that are initially different from the equilibrium

value $\overline{n_0}$ defined in Eq. (7). As shown in Fig. 1, for $n_0^{(\alpha)}(0) < \overline{n_0}$ [$n_0^{(\alpha)}(0) > \overline{n_0}$] the ground-state occupation number rises [falls] on a time scale involving many periods and saturates on a higher [lower] level. However, the saturation is lower [higher] than the equilibrium occupation number and is obviously different for different initial states. This indicates that the quantum system is not ergodic.

Figure 1 also shows that small amplitude oscillations of period $T/2$ are superposed on the time evolution. These oscillations result from the breathing mode. Their amplitude is small because the interaction yields only a small admixture of states belonging to different energy shells. The existence of large amplitude oscillations with periods $\tau \gg T$ seems to indicate that only a relatively small number of states within the considered $(K=4)$ shell contribute significantly to the time evolution. This picture is confirmed by the study of the ground-state fluctuations.

Table I shows the fluctuations (8) for different values of the coupling λ and $N=10$ bosons. Again, we have chosen

TABLE I. Fluctuations of the ground-state occupation number $\sqrt{\delta n_0^2(\lambda)}$ for different shells (labeled by K) and different values of the coupling λ. Systems of $N=10$ bosons are considered. For $\lambda =0$, the states of the Kth shell have the energy $E=2K\hbar\omega$. The shells comprise $\Omega(E=2K\hbar\omega,M=0)=9,31,109,339$ states for $K=2,3,4,5$, respectively. The last row shows results expected for an ergodic system.

	$K=2$	$K=3$	$K=4$	$K=5$
$\lambda=0.0\hbar\omega$	0.83	1.11	1.32	1.51
$\lambda=0.025\hbar\omega$	0.56	0.55	0.59	0.64
$\lambda=0.05\hbar\omega$	0.54	0.55	0.60	0.64
$\lambda=0.075\hbar\omega$	0.54	0.55	0.60	0.65
$\lambda=0.1\hbar\omega$	0.53	0.55	0.59	0.64
$\lambda=0.15\hbar\omega$	0.53	0.55	0.59	0.63
$\lambda=0.2\hbar\omega$	0.52	0.55	0.58	0.64
GOE	0.35	0.27	0.18	0.12

$E_{max} = 12\hbar\omega$. With increasing λ the spectrum is shifted towards higher energies but the shell structure persists. For nonzero λ the fluctuations are suppressed in comparison to the noninteracting case, and are practically independent of λ for $0 < \lambda \leq 0.2$. The last row of Table I presents the fluctuations one would expect in a ergodic system. These findings confirm the results obtained from the time evolution. They show that the quantum system is not ergodic in the regime of low energies and modest number of bosons.

We also consider the N dependence of the fluctuations. Fixing $\lambda = 0.025\hbar\omega$ and $E_{max} = 12\hbar\omega$, Table II shows the ratio $\sqrt{\delta n_0^2(\lambda)/\delta n_0^2(0)}$ for different numbers of particles. One observes that the fluctuations increase with increasing N and approach the fluctuations of the noninteracting system. This can be understood as follows. Since E_{max} has been fixed, the energy available per boson is decreasing with increasing numbers of bosons and thus the regime $N \gg 1$ corresponds to the low-temperature regime where most bosons are in the condensate. The interactions induce mostly scattering within the condensate, and this corresponds to the diagonal part of the interaction matrix (3), which does not yield any change in the eigenfunctions.

As shown in Sec. V the classical system becomes chaotic for $N^{5/2}(a/d_0)\sqrt{\hbar\omega/E} > 1$. Thus, the classical system is chaotic for the values $N = 40$, $\lambda = 0.025\hbar\omega$ and $E = 6\hbar\omega$ used in Table II. Nevertheless, this property of the classical system is not reflected by the quantum system.

B. Square well potential

We next consider a square well potential, keeping the same number of bosons ($N = 10$) as before. Figure 2 shows the fluctuations of the ground-state occupation number as a function of energy for different values of the coupling λ. With increasing values of λ the results have been shifted to lower energies, such that the average ground-state occupation number becomes (almost) independent of λ. Figure 2 shows that the fluctuations are relatively large even for the

TABLE II. Fluctuations of the ground-state occupation number $\sqrt{\delta n_0^2(\lambda)}$ normalized by the fluctuations of the noninteracting system $\sqrt{\delta n_0^2(0)}$ for different shells (labeled by K) and different numbers N of bosons. The coupling is fixed to $\lambda = 0.025\hbar\omega$. The shells comprise $\Omega(E = 2K\hbar\omega, M = 0) = 9, 31, 109, 339$ states for $K = 2,3,4,5$, respectively.

	$K=2$	$K=3$	$K=4$	$K=5$
$N=12$	0.71	0.56	0.51	0.46
$N=15$	0.77	0.65	0.58	0.54
$N=20$	0.83	0.73	0.68	0.63
$N=25$	0.86	0.78	0.73	0.69
$N=40$	0.91	0.85		

interacting system. Thus the quantum system is not ergodic at low energies. We recall that a classical system of hard-sphere particles confined to a square well is chaotic and ergodic [14]. This classical behavior is expected to be followed by the quantum system in the semiclassical limit [21,22] when the wavelength is sufficiently small compared to other length scales including the scattering length. However, our contact interaction demands the opposite limit of long wavelengths. One also recognizes in Fig. 2 that the fluctuations decrease with increasing λ. One may only speculate as to whether this behavior is tied to the ergodicity of the classical system.

Note that nonergodic behavior of a classically chaotic system is not unexpected in the low-energy quantum regime. The same observation has been made, e.g. for a system of one particle confined to the stadium billiard [23] or for anharmonic many-oscillator systems [24].

IV. RANDOM INTERACTIONS

We would now like to contrast the results presented in the last section with a quantum Hamiltonian that does display ergodic behavior. To this purpose, we restrict ourselves to the states within one energy shell and model the interaction by a $\Omega(E, M)$-dimensional random matrix that is drawn
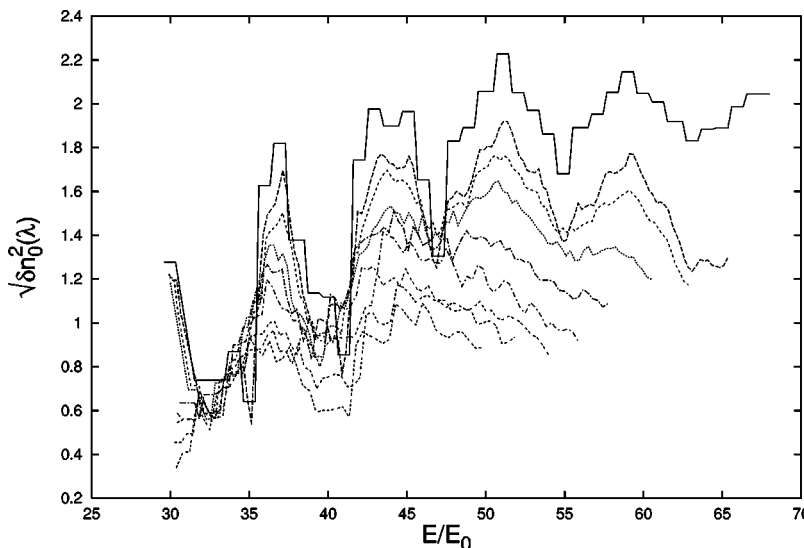

FIG. 2. Fluctuations of the ground-state occupation number $\sqrt{\delta n_0^2(\lambda)}$ for a system of $N = 10$ bosons confined to a square well and different values of the coupling λ. ($\lambda/E_0 = 0, \frac{1}{80}, \frac{1}{40}, \frac{3}{80}, \frac{1}{20}, \frac{5}{80}, \frac{3}{40}, \frac{7}{80}, \frac{1}{10}$ from top to bottom.) The energy is given in units of $E_0 = \pi^2\hbar^2/2md_0^2$.
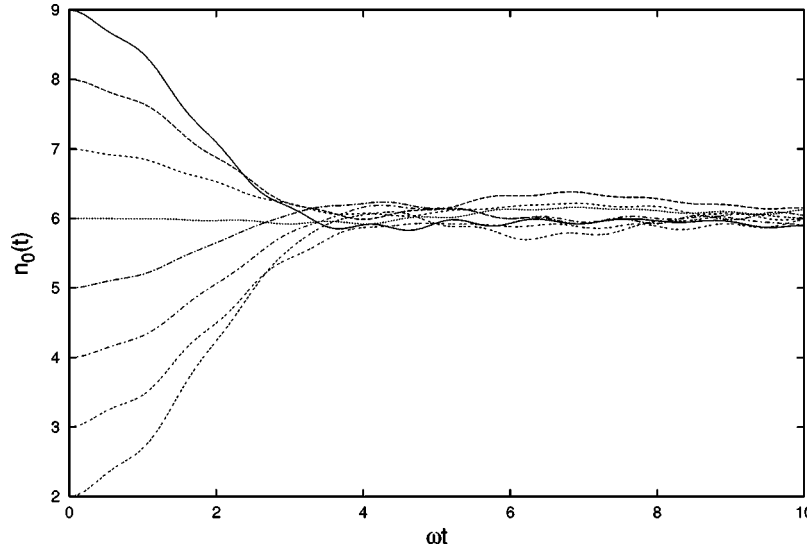
FIG. 3. Time evolution (thin lines) of the ground-state occupation number (5) for different initial states of the ($K=4$) shell that are initially away from the equilibrium value $\overline{n_0} \approx 6$. Results are obtained for a system of $N=10$ harmonically trapped bosons that interact via random interactions.

from the Gaussian orthogonal ensemble (GOE). Within one shell, the results depend only trivially on λ and the variance of the random matrix elements. Our random matrix model is motivated by the observation that, within the semiclassical regime, fluctuation properties concerning eigenvalues and wave functions of classically chaotic systems are universal and coincide with those of the Gaussian random matrix ensembles [25,21]. Thus, one would expect that a random interaction would yield ergodic behavior. The appropriate time evolution of the ground-state occupation number is shown in Fig. 3. As expected, the equilibrium is practically reached by every initial state, and the fluctuations are relatively small.

Using random matrix theory, we may also obtain analytical results for fluctuation of the ground-state occupation number. Let $|\Psi\rangle = \Sigma_\alpha c_\alpha |\alpha\rangle$ be an eigenvector of the random matrix Hamiltonian. Within the GOE the coefficients c_α are uniformly distributed over a Ω-dimensional sphere of unit radius. The normalized joint probability distribution for k coefficients is given by [26]

$$P_k(c_1, \ldots, c_k) = \pi^{-k/2} \frac{\Gamma(\Omega/2)}{\Gamma((\Omega-k)/2)}$$
$$\times \left(1 - \sum_{\alpha=1}^{k} c_\alpha^2\right)^{(\Omega-k-2)/2}. \quad (10)$$

To compute expectation values, the average over the energy shell is now replaced by the GOE average, and we denote the latter by brackets $\langle \cdot \rangle$. This is justified for $\Omega \gg 1$ since the GOE becomes ergodic in the limit of infinitely many levels; i.e., each of its members displays the same fluctuation properties as the ensemble [22]. The ground-state occupation number of the eigenstate $|\Psi\rangle$ is

$$n_0^{(\Psi)} \equiv \langle \Psi | \hat{n}_0 | \Psi \rangle = \sum_\alpha c_\alpha^2 n_0^{(\alpha)}, \quad (11)$$

and its GOE average is

$$\langle n_0^{(\Psi)} \rangle = \int_{-1}^{1} dc\, P_1(c)\, n_0^{(\Psi)} = \overline{n_0} \quad (12)$$

as expected. Using P_2 we obtain for the variance

$$\delta n_0^2(\text{GOE}) \equiv \langle (n_0^{(\Psi)} - \langle n_0^{(\Psi)} \rangle)^2 \rangle = \frac{2}{\Omega+2} \delta n_0^2(0), \quad (13)$$

where $\delta n_0^2(0)$ is the variance of the noninteracting system given in Eq. (9). This shows that random interactions lead to a tremendous suppression in comparison to the noninteracting case and vanish in the limit of infinitely many levels. Note that an expression similar to Eq. (13) holds for any one-body observable that commutes with the unperturbed Hamiltonian. Table III compares the fluctuations of the ground-state occupation number of the noninteracting system with the numerical results obtained with a random Hamiltonian and with the analytical result (13). Obviously, the fluctuations of the noninteracting system are much larger than those of the random Hamiltonian. One also recognizes that the agreement between the analytical result and the numerical simulation improves with increasing dimension of the random matrix. These results show that the interaction mediated by s-wave scattering is very different from a chaos simulating random many-body interaction.

TABLE III. Fluctuations of the ground-state occupation number in different shells labeled by K. Results are shown for the harmonic oscillator (HO), the harmonic oscillator with random interaction (RM), and the analytical result (13) derived from random matrix theory (GOE). The shells comprise $\Omega = 109,339,1039$ states for $K=4,5,6$, respectively.

	$K=4$	$K=5$	$K=6$
HO	1.32	1.51	1.64
RM	0.20	0.112	0.072
GOE	0.18	0.116	0.072

V. CLASSICAL PHASE SPACE

It would be interesting to investigate the ergodic properties also at higher energies. Unfortunately, a treatment of the full many-body system is very difficult outside the low-energy quantum regime. However, it is useful to study the classical many-body system in more detail. Within the semi-classical regime, where the wavelength is small compared to any length scale including the scattering length [i.e., $(a/d_0)\sqrt{E/\hbar\omega} \gg 1$ [27]], the quantum system is expected to reflect the properties of the underlying classical system [21,22]. Sinai has shown that the classical system of hard-sphere particles in a square well potential is ergodic and chaotic [14]. We therefore consider the classical dynamics of a dilute system of hard-sphere particles of radius a confined to a two-dimensional isotropic harmonic oscillator. At low energies, the corresponding quantum system is governed by the Hamiltonian (1). Of course, in the low-energy limit, *any* short-range two-body interaction with s-wave scattering length a would yield the quantum Hamiltonian (1), and there is no reason to choose a hard-sphere interaction. However, hard potentials induce more chaos than softer ones, and they are easier to treat. This justifies and motivates our specific choice. Nevertheless, most of the results derived below are valid for any two-body interaction that depends only on the distance and vanishes for distances larger than the scattering length.

Let us first consider the two-body system with coordinates and momenta $\vec{r}_i$ and $\vec{p}_i$ ($i = 1,2$), respectively. Introducing coordinates and momenta $\vec{q}_\pm = (\vec{r}_1 \pm \vec{r}_2)/\sqrt{2}$, $\vec{p}_\pm = (\vec{p}_1 \pm \vec{p}_2)/\sqrt{2}$ shows that the system is equivalent to a system of two nonidentical and noninteracting particles in a harmonic oscillator where the particle with coordinates $\vec{q}_-$ ''sees'' a spherical symmetric hard-core potential with radius $\sqrt{2}a$ in addition to the confining harmonic potential. In the new coordinate system, single-particle energies and single-particle angular momenta are conserved, which renders the system integrable. Obviously, scattering occurs only if the angular momentum of the particle with coordinates $\vec{q}_-$ is sufficiently low, i.e., $l_-^2 < 4\hbar^2(a/d_0)^2[E/\hbar\omega - (a/d_0)^2]$. Let us assume that the initial conditions of the two-body system are uniformly distributed over the shell of energy E. The probability of scattering is basically given by integrating $\Theta(4\hbar^2(a/d_0)^2[E/\hbar\omega - (a/d_0)^2] - l_-^2)$ over the energy shell in phase space. One obtains

$$P^{(2)}(\xi) = \begin{cases} 1, & 1 < \xi < 2, \\ \dfrac{24/5}{(\xi-1)^{1/2}} - \dfrac{9}{\xi-1} + \dfrac{8}{(\xi-1)^{3/2}} - \dfrac{3}{(\xi-1)^2} + \dfrac{1/5}{(\xi-1)^3}, & 2 < \xi, \end{cases} \qquad (14)$$

where $\xi = (d_0/a)^2 E/(\hbar\omega)$ is a dimensionless parameter. Note that $\xi \gg 1$ in the traps used in recent experiments. Obviously, the scattering probability is very small for two-body systems, and this is a consequence of the well-known fact that the periods do not depend on the energy in harmonic potentials. For the N-body system we may use Eq. (14) to compute the probability of having at least one scattering. We give an estimate. On average, any two particles have a fraction $2/N$ of the total energy. There are $N(N-1)/2$ different pairs of particles that may collide. Thus,

$$P^{(N)} \approx \frac{N(N-1)}{2} P^{(2)}(2\xi/N). \qquad (15)$$

A more accurate calculation of the leading term $\propto N^{5/2}\xi^{-1/2}$ in Eq. (15) confirms that the estimate is a good approximation. Note that Eqs. (15) and (14) are valid for any short-range two-body interaction that vanishes for distances larger than a. The absence of any scattering for some fraction of the energy shell is a consequence of the energy independence of the periods in the isotropic harmonic potential. Thus, the interacting classical system is not ergodic if the number of particles is not too large.

Let us also consider those regions of phase space that involve scattering among more than two particles. Starting trajectories in such regions, we computed the Lyapunov exponent [28] for systems with $2 < N < 25$ particles. As expected we found positive Lyapunov exponents. Thus, scattering between more than two particles yields chaotic dynamics in the corresponding fraction of phase space. As a rule of thumb, Eq. (15) shows that the classical system becomes chaotic for $N^{5/2}(a/d_0)\sqrt{\hbar\omega/E} > 1$.

Let us also discuss the case of a three-dimensional cylindrical symmetric trap with axial symmetry. In the absence of interactions the motion in the z direction decouples from the motion in the radial plane. Since a scattering in three dimensions also is a scattering of the particles in the radial plane, the results (14),(15) derived in this section also hold for three-dimensional axially symmetric traps provided the total energy is replaced by the *radial* energy. Our results are consistent with the recent theoretical observation that the quasiparticle motion of collective and single-particle excitations of Bose-Einstein condensates is only weakly chaotic [29].

VI. CONCLUSION

We have studied the ergodic properties of trapped bosons that interact via s-wave scattering. In the low-energy quantum regime we find nonergodic behavior for both the harmonic trap and the square well potential. The nonergodic behavior may be seen in the difference between time averages and ensemble averages and in rather large fluctuations of the ground-state occupation number. For modest numbers of harmonically trapped bosons the fluctuations are smaller

than for the noninteracting system and almost independent of exact magnitude of the s-wave scattering length. For larger numbers of harmonically trapped bosons the fluctuations of the interacting system approach the fluctuations of the noninteracting system in the low-temperature limit. This shows that even the many-body system is not ergodic at sufficiently low temperatures.

The analysis of the classical phase space structure shows that, unlike square well potentials, harmonic potentials do not necessarily lead to chaotic behavior of trapped interacting particles. Only for $N^{5/2}(a/d_0)\sqrt{\hbar\omega/E} > 1$ is a considerable fraction of classical phase space chaotic. This is achieved with the presently used traps if $N > 40$ particles are trapped at temperatures of the order of the condensation temperature ($E \approx N^{1+1/d}\hbar\omega$). The quantum system is expected to follow the classical system in the semiclassical regime where the wavelength is small compared to the scattering length. This is the case for $(a/d_0)\sqrt{E/\hbar\omega} \gg 1$, and $N \gg 3 \times 10^4$ or $N \gg 10^4$ atoms have to be trapped in $d=3$ or $d=2$ dimensions, respectively.

The parameter that compares the strength of the interaction with the kinetic energy is Na/d_0 [4]. For the experiments with rubidium at JILA [1], lithium at Rice University [2], and sodium at MIT [3], one has $Na/d_0 < 1$, $Na/d_0 > 1$, and $Na/d_0 \gg 1$, respectively. Our computations are restricted to the weakly interacting regime $Na/d_0 < 1$, and as one consequence we do observe shell structure. It is not obvious that this restriction is also responsible for the nonergodic behavior observed in this work. The results of Sec. IV show that any small random interaction may render the system ergodic since the noninteracting system is highly degenerate. Whether the quantum system is ergodic also in the low-energy quantum regime for $Na/d_0 > 1$ remains an open question. Given the fluctuations (13) for the system with random interactions on the one hand, and the results [12] for the noninteracting system on the other, experiments should be able to reveal how ergodic systems of trapped atoms really are.

We have considered the fluctuation of the ground-state occupation number as one observable that is sensitive to nonergodic behavior. Chaotic systems exhibit level repulsion within sectors of definite symmetry and may be distinguished from integrable ones by their level statistics [25,22]. Due to its SO(2,1) symmetry the two-dimensional harmonic trap with contact interaction is quite special. Sectors of definite symmetry (fixed angular momentum M and fixed value of B) are ladders of levels with spacing $2\hbar\omega$ [18] and are expected to display the same level statistics as a harmonic oscillator. The SO(2,1) symmetry prevents a mixing of the levels within one oscillator shell. Breaking this symmetry by a small perturbation would introduce some mixing of the levels within each oscillator shell. However, one would not expect that ergodicity might be restored in this way since the observed nonergodic behavior in the harmonic and the square well traps rather seems to be a wave phenomenon of the low-energy quantum regime.

It is also interesting to discuss the growth of the condensate in harmonic traps. As long as the shells do not overlap and first-order perturbation theory in λ is valid, the quantum mechanical time scale set by the interaction is given by the product $1/\lambda\omega$. This may be compared to an approach using the Boltzmann equation, where the time scale is proportional to $1/\lambda^2$ (when transition rates are obtained from Fermi's golden rule). Thus, for sufficiently small values of λ, the use of the Boltzmann equation in combination with transition rates resulting from Fermi's golden rule is inappropriate. It yields times for the condensate formation that are too large. This finding is a consequence of the high degeneracy of the harmonic trap spectrum.

[1] M.N. Anderson, J.R. Ensher, M.R. Matthews, C.E. Wieman, and E.A. Cornell, Science **269**, 198 (1995).

[2] C.C. Bradley, C.A. Sacket, J.J. Tollet, and R.G. Hulet, Phys. Rev. Lett. **75**, 1687 (1995).

[3] K.B. Davis, M.-O. Mewes, M.R. Andrews, N.J. van Druten, D.S. Durfee, D.M. Kurn, and W. Ketterle, Phys. Rev. Lett. **75**, 3969 (1995).

[4] For a review see, e.g., F. Dalfovo, S. Giorgini, L.P. Pitaevskii, and S. Stringari, e-print cond-mat/9805038.

[5] H.T.C. Stoof, e-print cond-mat/9805393.

[6] M. Holland, J. Williams, and J. Cooper, Phys. Rev. A **55**, 3670 (1997).

[7] H. Wu, E. Arimondo, and C.J. Foot, Phys. Rev. A **56**, 560 (1997).

[8] D. Jaksch, C.W. Gardiner, and P. Zoller, Phys. Rev. A **56**, 575 (1997).

[9] C.W. Gardiner, P. Zoller, R.J. Ballagh, and M.J. Davis, Phys. Rev. Lett. **79**, 1793 (1997); C.W. Gardiner, M.D. Lee, R.J. Ballagh, M.J. Davis, and P. Zoller, e-print cond-mat/9801027.

[10] For a review see, e.g., W. Ketterle and N.J. van Druten, Adv. At., Mol., Opt. Phys. **37**, 181 (1996).

[11] H.-J. Miesner, D.M. Stamper-Kurn, M.R. Andrews, D.S. Durfee, S. Inouye, and W. Ketterle, Science **279**, 1005 (1998).

[12] S. Grossmann and M. Holthaus, Phys. Rev. Lett. **79**, 3557 (1997).

[13] M. Gajda and K. Rzazewski, Phys. Rev. Lett. **78**, 2686 (1997).

[14] Ya.G. Sinai, Sov. Math. Dokl. **4**, 1818 (1963).

[15] S.R. de Groot, G.J. Hooman, and C.A. Ten Seldam, Proc. R. Soc. London, Ser. A **203**, 266 (1950); V. Bagnato, D.E. Pritchard, and D. Kleppner, Phys. Rev. A **35**, 4354 (1987).

[16] *Handbook of Mathematical Functions*, edited by M. Abramowitz and I.A. Stegun (Dover, New York, 1972).

[17] A.L. Fetter and D. Rokhsar, Phys. Rev. A **57**, 1191 (1998).

[18] L.P. Pitaevskii and A. Rosch, Phys. Rev. A **55**, R853 (1998).

[19] T. Haugset and H. Haugerud, Phys. Rev. A **57**, 3809 (1998).

[20] We have used a step size $\lambda\omega\Delta t \approx O(1/10)$ to assure a fast

convergence of the Taylor expansion.

[21] *Chaos and Quantum Physics,* edited by M.-J. Giannoni, A. Voros, and J. Zin-Justin (North-Holland, Amsterdam, 1991).

[22] T. Guhr, A. Müller-Groeling, and H.A. Weidenmüller, Phys. Rep. **299**, 189 (1998).

[23] F. Borgonovi, G. Casati, and B. Li, Phys. Rev. Lett. **77**, 4744 (1996).

[24] D.M. Leitner and P.G. Wolynes, Phys. Rev. Lett. **76**, 216 (1996).

[25] O. Bohigas, M.-J. Giannoni, and C. Schmit, Phys. Rev. Lett. **52**, 1 (1984).

[26] T.A. Brody, J. Flores, J.B. French, P.A. Mello, A. Pandey, and S.S.M. Wong, Rev. Mod. Phys. **53**, 385 (1981).

[27] This estimate is based on the assumption that one particle has the entire energy E. A more conservative estimate would use the fraction E/N for single-particle energies.

[28] G. Benettin, L. Galgani, and J.M. Strelcyn, Phys. Rev. A **14**, 2338 (1976).

[29] M. Fliesser, A. Csordás, and R. Graham, Phys. Rev. A **56**, 4879 (1997); M. Fliesser and R. Graham, e-print cond-mat/9806115.