Precision Monte Carlo test of the Hartree-Fock approximation for a trapped Bose gas

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We compare the semiclassical Hartree-Fock approximation for a trapped Bose gas to a direct path-integral quantum Monte Carlo simulation. The chosen parameters correspond to current ^{87}Rb experiments. We observe corrections to the mean-field density profile: the path-integral calculation reveals an increase of the number of condensed particles, which is of the same order as a previously computed result for a homogeneous system. We discuss the experimental observability of the effect and propose a method to analyze data of *in situ* experiments. [S1050-2947(99)02404-X]

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The experimental realization of Bose-Einstein condensation (BEC) in dilute atomic vapors [1–3] has generated extraordinary experimental and theoretical interest. From the viewpoint of quantum many-body physics, the trapped atomic vapors are peculiar. Well above the critical point, the gases are extremely dilute, and their description as noninteracting bosons is very accurate. As the condensation sets in, the trapped atoms are strongly compressed in real space. Then, interactions become much more important and even the simplest thermodynamic quantities (spatial distribution, condensate fraction, etc.) have to be obtained by the appropriate quantum many-body technique. At zero temperature, the Bogoliubov approach of weakly interacting Bose gases is well established [4]. There, the macroscopic condensate wave function is given by the Gross-Pitaevskii equation [5]. The effects of noncondensed particles at finite temperatures can be included via the Hartree-Fock-Bogoliubov equations, which have been solved in the Popov approximation [6] and in various simplified forms [7].

The equilibrium properties of Bose gases can also be directly computed by path integral quantum Monte Carlo (QMC) simulation [8]. Very importantly, the QMC calculation is free of systematic errors: apart from purely statistical fluctuations, it gives an exact numerical solution of BEC. For simulations corresponding to dilute atomic vapors, the QMC calculation can be performed directly for the large particle numbers ($\sim 10^4$–10^5) and the temperatures of experimental interest [9].

A subject of considerable interest in these systems is the detailed study of the critical region of the phase transition. The QMC approach was already used to show [9] that the trapped Bose gas with repulsive interactions has a lower critical temperature T_c and a smaller number N_0 of condensed particles below T_c than the free Bose gas, one of the predictions of mean-field theories [10,11]. This effect is intrinsic to the inhomogeneous trap potential, where the density is not fixed: The mean interaction of a given particle with the other particles, as well as with the external potential, changes the density profile with respect to the ideal Bose gas.

Although this leads to a shift of the critical temperature (even within mean-field theory), condensation sets in as soon as the phase-space density reaches (locally) the ideal gas limit: As for the ideal gas, mean-field theory predicts the occurrence of BEC for a degeneracy parameter in the center of the trap $\rho(0)\lambda_T^3 = 2.61\ldots$, where $\rho(0)$ denotes the density in the center of the trap and $\lambda_T = \hbar\sqrt{2\pi/mk_BT}$ is the thermal wavelength.

Up to now, the deviation of the degeneracy parameter from the ideal gas value due to interactions has not been determined. Only the homogeneous system has been studied, and has given contradictory results for the order of magnitude and even the sign of the critical temperature shift [12]. Relevant recent works are a QMC [13] and a renormalization group calculation [14] in the homogeneous case. Both predict a decreasing degeneracy parameter, which is equivalent to an increased critical temperature. The two calculations differ considerably in the amount of this shift.

The main point of this paper is to calculate corrections to mean-field theory of the trapped Bose gas directly in an experimental setting. It was proposed earlier to measure the local degeneracy parameter in the center of the trap, $\rho(0)\lambda_T^3$, precisely at the onset of condensation and to check whether it was smaller or bigger than the ideal gas value [15]. However, the total number of particles close to the center of the trap is necessarily small and large fluctuations in this number are inevitable. These large fluctuations prevent a precise measurement of the central density. A second obstruction to the direct measurement comes from the finite-size effects, which are far from negligible for current experimental setups. For finite systems, the critical point lacks a unique definition and finite-size scaling has to be performed. To circumvent these difficulties, we propose another scheme for detecting effects beyond mean-field theory: We compare the results of the exact QMC calculation with the Hartree-Fock

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(HF) mean-field approximation. Since both computations can be done for the same finite number of atoms, deviations lead to an estimate of the critical temperature shift, which will be largely independent of finite-size effects. The use of scaling arguments is thus avoided.

Besides extracting the effect of interactions on the critical temperature, we concentrate in this paper on a precision test of the HF calculation at finite temperatures. In this approximation, the local density is determined by the local trap potential and the mean interaction energy of the atoms in a self-consistent way. We have chosen this theory for several reasons: First, it is the simplest approach for an interacting Bose gas at finite temperature. Although collective modes and anomalous averages are neglected, we will show that it already gives a rather accurate description for static properties of the gas. Further, it provides an ideal reference system, since it corresponds to a *locally homogeneous* Bose gas. Thus the corrections to HF should be comparable to previous calculations in a homogeneous system, which predict an increased critical temperature [13,14]. One could therefore expect that the full QMC solution should give a higher condensate fraction than HF at identical temperatures close to the transition point. Since this effect also lies beyond the Bogoliubov and Popov description, there is no need to compare with these theories in this temperature regime. We prefer the HF approximation as a reference, since it is qualitatively easier to understand.

For a system closely corresponding to many experiments with ^{87}Rb, we find deviations from the HF density which are concentrated in the overlap region between the excited atoms and the condensate. The number of condensed particles N_0 is increased around the critical temperature by about 5%. For the quantitative analysis, we use a one-parameter fit to determine the condensate fraction. Our data analysis is based on reasonable physical assumptions and can also be used for a precision determination of the experimental temperature.

The QMC calculation is beset with statistical fluctuations. In fact, the noise of independent Monte Carlo configurations reproduces the sample-to-sample variations of repeated experimental measurements at the same temperature T and particle number N (or chemical potential). This allows us to discuss the experimental observability of these corrections to mean-field theory.

The Hamiltonian of N interacting particles in an *isotropic* harmonic trap with frequency ω is given by

$$H=\sum_{i=1}^{N}\left[\frac{p_i^2}{2m}+\frac{1}{2}m\omega^2 r_i^2\right]+\frac{1}{2}\sum_{i,j=1}^{N}V(r_{ij}), \qquad (1)$$

where V is the interatomic (pseudo) potential between two particles. Since we want to identify corrections beyond mean field we are very careful to assure the compatibility of QMC and HF on the level of the interparticle potential. In HF, the interaction is described by a single parameter, the s-wave scattering length a. In QMC, we have adopted a hard-core potential of diameter a. In HF, the interaction is described by the same parameter a, the s-wave scattering length. Notice that the s-wave scattering length of a hard-sphere potential coincides with its diameter, so that the low-energy collisions of both potentials are identical. Up to now there is no evidence that a more complex pseudopotential has to be used for ^{87}Rb.

The partition function Z of the system with inverse temperature $\beta=(k_BT)^{-1}$ is given by the trace of the symmetrized density matrix $\rho=e^{-\beta H}$ over all states. Z satisfies the usual convolution equation:

$$\begin{aligned} Z&=\frac{1}{N!}\sum_P\int dR\,\rho(R,R^P,\beta)\\ &=\frac{1}{N!}\sum_P\int dR\int dR_2\cdots\int dR_M\,\rho(R,R_2,\tau)\cdots\\ &\quad\times\rho(R_M,R^P,\tau). \end{aligned} \qquad (2)$$

Here $\tau=\beta/M$, R is the 3N-dimensional vector of the particle coordinates $R=(r_1,r_2,\ldots,r_N)$, and R^P denotes the vector with permuted labels: $R^P=(r_{P(1)},r_{P(2)},\ldots,r_{P(N)})$ [16]. As explained elsewhere [8], the QMC calculation relies on virtually exact formulas for the density matrices $\rho(R,R',\tau)$ at the higher temperature $1/\tau$ and performs the integral over $R,R_2,\ldots,R_M$ as well as the sum over all permutations P in Eq. (2) by Monte Carlo sampling. Special data-handling techniques allow us to cope with very large atom numbers N.

As in [9] we consider a model system of 10 000 particles, corresponding to a critical temperature of the ideal gas of $k_BT_c^0\simeq 20.25\hbar\omega$ and a hard-core potential with diameter $a=0.0043a_0[a_0=(\hbar/m\omega)^{1/2}]$. These values are typical for most ^{87}Rb experiments which are now in operation. We generally perform computations at different values of τ, and extrapolate to $\tau\to 0$, the limit in which the QMC formulas for the density matrices in Eq. (2) become manifestly exact. Notice that the convolution formula Eq. (2) is satisfied only for the *full* density matrix $\rho(R,R',\tau)$ but *not* for the s-wave contribution to $\rho(R,R',\tau)$. As τ becomes smaller, the region of applicability of the s-wave approximation for $\rho(R,R',\tau)$ shrinks, as higher angular momenta have to be taken into account. This is a ''lifetime'' effect, which stems from an increased collision rate with other particles. We can now understand that the corrections of the full QMC calculations with respect to the HF approximation can logically have two distinct origins: (i) the inapplicability of the s-wave approximation, (ii) the contribution of graphs (in the sense of a complete quantum many-body calculation), which are not contained in HF, but which are completely summed up by the Monte Carlo procedure.

Within our QMC simulation, we have explicitly studied the contributions of higher angular momenta ($l\geqslant 1$) to $\rho(R,R',\tau)$ and find them negligible. This allows us to affirm that the essential contributions from these graphs depend only on the low-energy scattering properties. Only the above point (ii) is realized.

In BEC, a single quantum state is occupied by a very large number of bosons. In the presence of interactions this state is a complicated many-body wave function. As far as one-particle properties are concerned it can, however, be described by a single-particle wave function $\psi_0(r)$ which describes the condensate. In HF theory, $\psi_0(r)$ is determined by the modified Gross-Pitaevskii equation

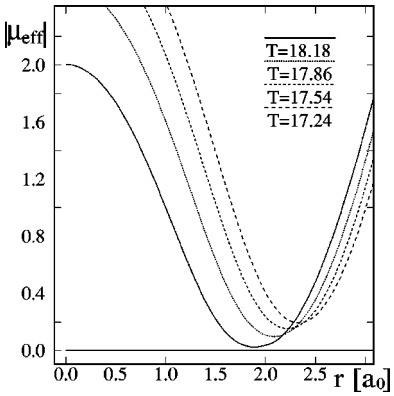

FIG. 1. Absolute value of the effective chemical potential $|\mu_{\rm eff}(r)|$ vs r/a_0 of the Hartree-Fock solution for different temperatures below the transition point ($\mu_{\rm eff}$ and T are in units of $\hbar\omega$). As the effective chemical potential approaches zero, the HF solution becomes instable.

$$\left(-\frac{\hbar^2\nabla^2}{2m}+\frac{m\omega^2}{2}r^2+U[n_0(\mathbf{r})+2n_T(\mathbf{r})]-\mu_0\right)\psi_0(\mathbf{r})=0, \tag{3}$$

where the densities of condensed particles $n_0(\mathbf{r})=N_0|\psi_0(\mathbf{r})|^2$ and of thermally excited particles $n_T(\mathbf{r})$ account for interactions between these particles. The interaction strength is given by $U=4\pi\hbar^2a/m$, where a denotes the s-wave scattering length, which coincides with the hard-core diameter. The factor of 2 in front of n_T accounts for the quantum-statistical exchange energy. In the semiclassical HF approximation, the thermal density is given by [10,11]

$$n_T(\mathbf{r})=\frac{1}{\lambda_T^3}g_{3/2}(e^{-[m\omega^2r^2/2+2Un(\mathbf{r})-\mu_T]/k_BT}). \tag{4}$$

Here, the thermal wavelength $\lambda_T=\hbar\sqrt{2\pi/mk_BT}$ and the Bose function $g_{3/2}(z)=\Sigma_{j=1}^{\infty}z^j/j^{3/2}$ have been used. In order to obtain the density distributions of the condensate and of the thermal component, Eqs. (3) and (4) have to be solved conjointly at the same chemical potential $\mu=\mu_0=\mu_T$ with the constraint of the fixed particle number N (different notations for the chemical potential appear for later convenience, cf. below). HF neglects the collective excitations of a more fundamental Bogoliubov theory. However, it was observed that these excitations do not contribute significantly to thermodynamic properties at temperatures well above the chemical potential [17]. On the other hand, collective excitations are fully included in our QMC calculation, as recently confirmed by a comparison of two-particle correlation functions at low temperatures [19].

The precise solution of the HF equation is quite difficult. We have obtained identical results both with an iterative procedure [17] and an interpolation-minimization routine cf. [9]. In a small window around the transition temperature, the HF equations have no solution. In fact, on approaching this window from below, the effective chemical potential $\mu_{\rm eff}(r)=-m\omega^2r^2/2-2Un(r)+\mu_T$ in Eq. (4) approaches zero as shown in Fig. 1. Since the Bose function $g_{3/2}(z)$ diverges for $z>1$, this causes a discontinuity of the HF solution. This problem is a finite-size effect which is related to the nonvanishing kinetic energy of the condensate wave function, and falls within the region of critical fluctuations [10,18,17].

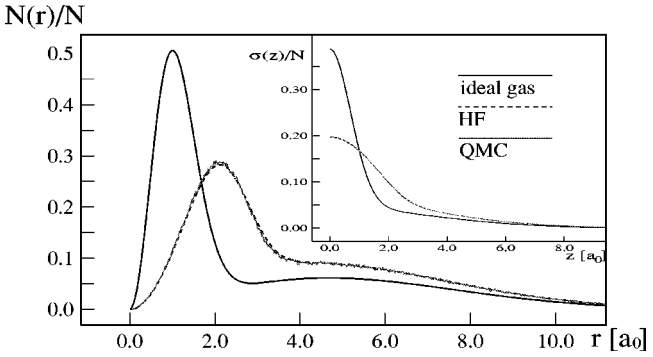

FIG. 2. Number density $N(r)/N$ from HF and the exact QMC calculations compared to the noninteracting Bose gas, both for $N=10\,000$ particles in an isotropic trap with $\beta=0.07/\hbar\omega(T\simeq 0.7\ T_c^0)$. The inset shows the corresponding cuts $\sigma(z)/N$ of the total density profile [20].

The raw output of our Monte Carlo simulations consists of histograms of the number density $N(r)$, where $N(r)dr$ describes the number of particles in a *spherical shell* between r and $r+dr$. The *density* $\rho(r)$ is given by $\rho(r)=N(r)/4\pi r^2$. Notice that the number density $N(r)$ is small near the center of the (isotropic) trap simply because the volume of the spherical shell goes to zero as $r\to 0$. A small value of $N(r)$ for $r\sim 0$ implies, however, that the fluctuations of this quantity $\sim\sqrt{N(r)}$ are necessarily large. As discussed above, this makes the *direct* measurement of the degeneracy parameter impractical. Of course, experiments measure neither $N(r)$, nor $\rho(r)$, but most often *cuts* of the total density profile $\sigma(z)=\int dx\int dy N'(x,y,z)$ or $\tilde{\sigma}(x,y)=\int dz N'(x,y,z)$, where $N'(x,y,z)dxdydz$ is the number of particles in the volume element at $\vec{r}=(x,y,z)$. This quantity is straightforward to calculate with the knowledge of the number density $N(r)$. However, the averaging process which obtains σ or $\tilde{\sigma}$ from $N(r)$ convolutes both the data and the noise, and it is therefore preferable to analyze the number density $N(r)$ directly.

In Fig. 2, we compare the QMC results for $N(r)$ with the HF solution far below the critical temperature, $T\simeq 0.7T_c^0$. We notice an excellent agreement between the two approaches. For comparison we also show the corresponding result for 10 000 noninteracting bosons at the same temperature. The cuts $\sigma(z)$ of the respective density profiles are shown in the inset. Both plots exhibit the two components which make up the particle distribution: one component in the region of the trap center, which belongs to the condensed atoms, and the second component of the thermal atoms with a much larger width. The cuts exhibit the customary peaks of BEC at $z=0$. In the plots of the number density $N(r)$, the condensate distribution is given by the profile of the inner peak. One can directly see that the peak height of the interacting solution (both for HF and QMC) is reduced with respect to the noninteracting case, whereas their distribution is widened. The last point corresponds to a shift of the position of the first peak to larger values in $N(r)$. The area underlying the first peak determines the condensate fraction, and one can deduce that the number of condensed particles is de-

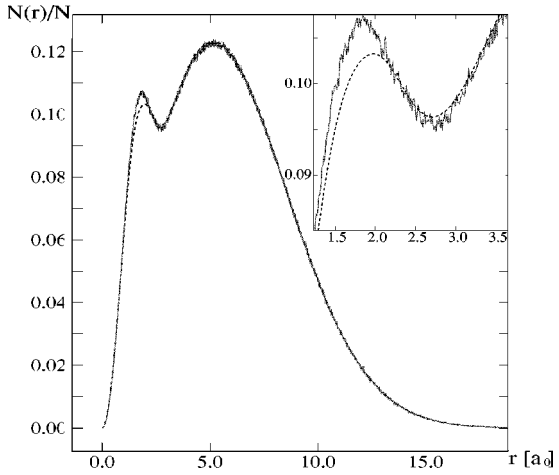

FIG. 3. $N(r)/N$ from HF and the exact QMC calculations for the same system as in Fig. 1, but at a higher temperature, $\beta = 0.056/\hbar\omega$ ($T \simeq 0.88 T_c^0$). The inset shows the two curves in the overlap region [20].

creased by the interaction. The second component of the distribution profile is built up by thermal atoms. Notice that even far away from the center of the trap the distribution of the interacting gas is quantitatively different from the ideal gas. Therefore a precise temperature determination within the ideal gas model is not feasible. We have attempted to fit the distribution of the wings to the semiclassical thermal density of the ideal gas, Eq. (4) with $U = \mu_T = 0$. A temperature determination within this model fails by up to 5%. At the very edge of the wings this error disappears, but the number of bosons found goes to zero, giving rise to the same measurement problem as discussed above. The determination of the temperature is much more successful if we fit the tails of the distribution with Eq. (4), where we replace the total density $n(\mathbf{r})$ with the density of thermal atoms $n_T(\mathbf{r})$ [21].

In Fig. 3, we show the data for the number density $N(r)$ for a temperature closer to the critical point, $T \simeq 0.88 T_c^0$. Here, the thermal component clearly dominates over the condensate contribution, as the majority of the atoms is thermal. The difference between QMC and HF becomes visible: The number of condensed particles in the exact numerical calculation is *increased* with respect to the mean field solution, as can be seen from the first peak. Qualitatively, this point agrees nicely with recent QMC [13] and renormalization group calculations [14] for the homogeneous case. These calculations indicate that the degeneracy parameter is changed by interaction effects beyond mean-field and that for a dilute gas the critical temperature is increased linearly in a/λ_T. The increased number of condensed particles is also reflected in the cuts $\sigma(z)$ which are not shown. However, the cuts are less sensitive and the peak at $z = 0$ is raised by less than 1% as compared to HF.

It might be suspected that this increase is a mere consequence of quasiparticle excitations. However, it has been shown within the Popov approximation that quasiparticles lead rather to a minute decrease of the critical temperature [17].

To analyze the data we extract the number of condensed particles as well as their distribution function from the QMC calculation. In Ref. [9] both were obtained from the permutation-cycle lengths (cf. also [22]). Strictly, the determination of the condensate fraction requires the computation of the off-diagonal elements of the one-particle density matrix. These elements are not obtained in the calculation, as Eq. (2) samples the diagonal terms only. The largest eigenvalue of the one-particle density matrix *defines* the number of condensed atoms, and the corresponding eigenvector the ground state wave function. At a difference with the case of ^{4}He, where the nondiagonal density matrix can be probed by neutron scattering (in the homogeneous sample), these elements seem to be experimentally inaccessible in the trap. In the present case, however, it is perfectly adequate to ''fit'' the QMC-generated histograms of $N(r)$ from a very large number of samples to smooth curves $n_0(r)$ and $n_T(r)$, as has been done to analyze experimental *in situ* measurements. We have found an excellent way of analyzing the data by using functional forms for $n_0(r)$ and $n_T(r)$ as given in Eqs. (3) and (4) with unrestricted ''chemical potentials'' μ_0 and μ_T. Equations (3) and (4) are used, but the data analysis is *not* a HF approximation in disguise: In the HF calculation, the single parameter μ allows us to satisfy the constraint on the total number of particles, but it also determines the condensate fraction. The HF solution, whenever it exists, usually is unique. With both μ_0 and μ_T, we have an additional parameter which allows us to vary the ratio between condensed and thermal atoms. This new parameter is fixed by the condition of minimizing the mean-square displacement between the data points and the interpolating function. Physically, this fit procedure corresponds to the assumption that the corrections to mean-field theory will not change the shape of the wave functions but rather their statistical weight, corresponding to the unrestricted ''chemical potentials'' μ_0 and μ_T in our fit. This assumption is also confirmed by a numerical diagonalization of the one-particle density matrix, obtained by a QMC calculation of trapped, interacting bosons including the nondiagonal elements [22]. Therefore, our data analysis is in the spirit of the common applications of the variational principle [16]: We take the best available functional form for the distribution function with one open parameter to minimize the deviations to the QMC results. This explains the extremely small value of the obtained χ^2 of the fit, which was compatible with purely statistical deviations for histograms containing more than 10^7 data points. We note in passing that the density $\rho(r) = N(r)/4\pi r^2$ and the component densities are obtained with very good precision *after* performing the fit of the raw-data histogram rather than from a direct rescaling of the data.

This fit could also provide a scheme for the accurate determination of T within experimental *in situ* measurements. In current experiments the temperature is mostly determined by a time-of-flight method. Due to collisions during the expansion and the noninstantaneous switch off of the trap this method limits the temperature determination to 5%, so that a more accurate determination of the critical temperature and the condensate fraction has not yet been possible [23,24].

The use of the fit allows us to compute N_0 vs temperature for the set of parameters chosen. The results, extrapolated to $\tau \to 0$, are plotted in Fig. 4 together with the HF result. The QMC calculation gives a consistently larger value of N_0 than HF at the same temperatures. It should be noticed that the

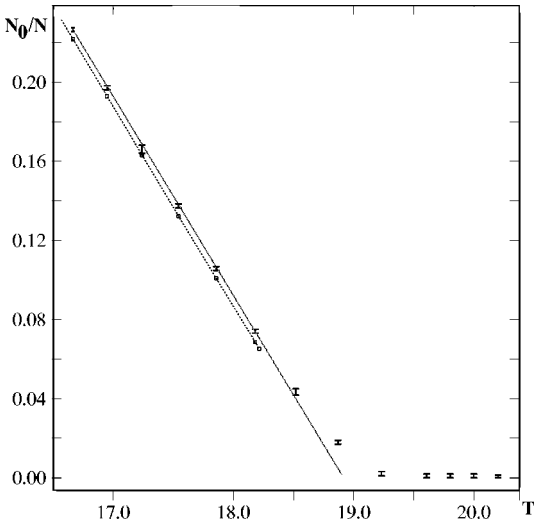

FIG. 4. Extrapolated condensate fraction N_0/N from HF (lower) and from QMC (upper) vs T in units of $\hbar\omega$. The gray line interpolates the QMC data. The inset illustrates the instability of the HF solution as the effective chemical potential $|\mu_{\rm eff}(r)|$ approaches zero.

HF equations, as mentioned above, have no solution for a range of temperatures close to T_c.

The correction to mean-field theory shown in Fig. 4 provides definite support for the scenario found in the spatially homogeneous Bose gas: Interaction effects beyond mean-field lead to an increased tendency towards Bose condensation [13,14]. There is, however, an important difference of context: in a homogeneous system the density at each point is fixed and unchanged by interactions, so that the shift in T_c corresponds directly to corrections to the homogeneous HF calculation. As we have seen in the present case, the trap is much more complicated since the finite-size effects, the mean field itself, and finally the corrections to mean field all influence the density profile and the condensate fraction. However, the finite-size effects and the mean field itself are already included in HF. Therefore the difference between QMC and HF becomes directly comparable to the corrections calculated for the homogeneous system. In Ref. [13], the following behavior is proposed: $\delta T_c/T_c^0=(T_c-T_c^0)/T_c^0 \simeq 0.34a\rho^{0.34}\simeq 0.46a/\lambda_{T_c^0}$, where T_c^0 is the critical temperature of a homogeneous Bose gas. In our case we would expect a change of the critical temperature $\delta T_c\sim 0.065\hbar\omega$. This corresponds roughly to the apparently constant offset in T of the two lines in Fig. 4.

It has been suggested [15] that a direct measurement of the density in the center of the trap $\rho(r=0)$ would be useful to determine the deviation of the degeneracy parameter from the mean-field result, $\rho(0)\lambda_{T_c}^3=2.61$. Even though we are able to extract $\rho(0)$ from QMC or from experimental data very precisely, the onset of condensation is not very sharp and the finite-size effects prevent a precise determination of the critical degeneracy parameter [25]. We repeat that a direct comparison between HF (which is available for finite systems) and the data is much more promising.

It is evident from an experimental point of view that the observation of these corrections necessitates a high resolution for T and for $N(r)$. Naturally, a single observation of a condensate will not result in a smooth curve for the histograms: even for ideal experiments there are intrinsic quantum-statistical fluctuations which may prevent the precision measurement of $N(r)$, necessary to determine the deviations from mean-field theory. Within QMC, we have determined these fluctuations from repeated measurements of the *complete* distribution of one whole sample. We find that an average of at least 50 independent samples has to be taken in order to detect that there is a difference between HF and the exact result in the sense of a Kolmogorov-Smirnov test [26]. For a precise evaluation (as in Fig. 3) a much larger data pool is necessary. Experimentally this seems to require a nondestructive measurement scheme, where the needed configuration averages must be accumulated by a time average over many thermal relaxation times. A detailed quantitative prescription for this effect is beyond the scope of this paper.

In conclusion, we have shown that the Hartree-Fock approximation succeeds in giving an accurate description of static properties in current BEC experiments. Moreover, we have computed the *corrections* to this mean-field theory by using numerically exact quantum Monte Carlo methods. Experimental access to the mean-field corrections will be of fundamental theoretical interest [27]. Comparison between theory and experiment on the level treated in this paper is very difficult but, we hope, conceivable.

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