Bose-Einstein condensation in two dimensions: A quantum Monte Carlo study

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A path-integral quantum Monte Carlo method is used to calculate finite temperature properties of up to 1000 hard-core bosons in a two-dimensional isotropic harmonic-oscillator potential. If the interatomic repulsions are sufficiently short range, an abrupt increase in the condensate fraction and a hump in the specific heat occur close to the critical temperature of ideal bosons. The critical temperature and the condensate fraction are in general lowered by an increase in the hard-core radius a. If a is decreased below a certain level, the condensate fraction becomes indistinguishable from the corresponding value of the ideal bosons. For up to 1000 particles, this occurs when $\ln^{-1}(1/na^2) \lesssim 0.1$, where n is the average particle density. [S1050-2947(98)04812-4]

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Bose-Einstein condensation (BEC) [1–3] of magnetically confined, weakly interacting atomic gases has now been observed in several laboratories [4–7]. Those achievements have provoked considerable theoretical interest, much of which has concentrated on bosons trapped in one or two dimensions [8–13]. It appears that the inclusion of the interactions between particles might have a profound effect on the BEC transition [14,15]. We therefore study both noninteracting (ideal) bosons and weakly interacting bosons with a hard core of radius a in a two-dimensional (2D) harmonic-oscillator potential. The emphasis is on the difference and similarity between the ideal and hard-core systems when a is varied.

BEC in one and two dimensions was initially ruled out by Hohenberg's theorem [16]. Widom [17] later pointed out that this theorem applies specifically to homogeneous systems, and proved that BEC phase transitions occur in a 2D rotating gas and a one-dimensional (1D) gas in the presence of a gravitational field. Further examples include an attractive δ-impurity system in any number of dimensions [18], a general 2D power-law trap, and a 1D power-law trap more confining than parabolic [19].

The system that we consider here consists of N particles, interacting via a pure hard-core potential of radius a and confined to move in a 2D harmonic-oscillator potential. The potential energy of the N particles is given by

$$V(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N)=\sum_{i=1}^{N} U(\mathbf{r}_i)+\sum_{i<j} V_I(|\mathbf{r}_i-\mathbf{r}_j|), \quad (1)$$

where $\mathbf{r}_i$ is the 2D position vector of the ith particle,

$$U(\mathbf{r}_i)=\frac{m}{2}\omega^2(x_i^2+y_i^2) \quad (2)$$

is the confinement potential on the ith particle, and

$$V_I(r)=\begin{cases}\infty & \text{for} \quad r<2a \\ 0 & \text{otherwise}\end{cases} \quad (3)$$

is the interaction potential between any two particles separated by a distance r. In Eq. (2), ω is the classical oscillator frequency and m is the mass of a particle. The harmonic-oscillator length scale is characterized by $l\equiv\langle r^2\rangle_0^{1/2} \equiv\sqrt{\hbar/m\omega}$. An ideal Bose gas in a 2D harmonic-oscillator potential has been studied in some detail [11–13,19]. Generally speaking, BEC is anticipated when the thermal de Broglie wavelength

$$\Lambda_T=\sqrt{2\pi\hbar^2/mk_BT} \quad (4)$$

becomes comparable with the average spacing between particles, so that the average particle density $n\sim\Lambda_T^{-2}$. For ideal bosons in a harmonic-oscillator potential, the BEC transition occurs at the critical temperature

$$T_c^0=\frac{\sqrt{6N}}{\pi}\frac{\hbar\omega}{k_B}, \quad (5)$$

with the average boson density given by $n\sim l_c^{-2}$. Here $l_c \sim l/N^{1/4}$ is a length scale that characterizes the critical density of the ideal bosons in a harmonic-oscillator potential.

In the thermodynamic limit, BEC can occur in 1D and 2D systems only if the particle density somewhere in the system can increase without bound. Of course this is impossible if interparticle repulsions are present. So strictly speaking, there can be no phase transition to a Bose-condensed state for nonideal bosons in a 2D harmonic-oscillator potential [14,15]. However, the noncondensed system is said to become unstable at the critical temperature and to make a transition to some non-BEC state. The possibility of a Kosterlitz-Thouless transition [20] has been proposed [14], with the transition to the superfluid state occurring very close to the condensation temperature for the ideal gas.

The thermodynamic limit is somewhat removed from typical experimental conditions, for which questions of density divergence never arise. A given d-dimensional system of interacting bosons for $d\geqslant 3$ is generally expected to exhibit essentially the same behavior as its noninteracting counterpart as long as the particular diluteness criterion is satisfied. In general, corrections to the behavior of an ideal gas will be small when $na^d\ll 1$, where $n\sim\Lambda_T^{-d}$. In two dimensions, the condition for diluteness is in fact given by a logarithmic relation [14]

$$\ln^{-1}(1/na^2)\ll 1, \quad (6)$$

which is obtained by requiring that the interaction energy is negligible compared to the kinetic energy and holds for a homogeneous gas [21] as well as for all types of power-law confinement, although there is no phase transition in the ideal limit of the former case. Considering BEC of bosons in a 2D harmonic-oscillator potential, in which case $n \sim N^{1/2}/l^2$, the diluteness condition of Eq. (6) is satisfied only for extremely small values of the parameter $aN^{1/4}/l$. If $aN^{1/4}/l$ is not extremely small, then the diluteness parameter $\ln^{-1}(1/na^2)$ approaches unity and the correction $\Delta T_c = T_c - T_c^0$ is expected to be significant. ΔT_c is expected to be negative for a hard-core Bose gas in a harmonic-oscillator potential in both two [13,14] and three dimensions [22,23], and positive for harmonically interacting bosons in a 2D harmonic-oscillator potential [24].

The system that we simulate is strictly 2D. In an experiment, a trap could be made effectively 2D by making ω_z, the confinement frequency in the perpendicular direction, much greater than ω, the confinement frequency in the other two directions. More precisely, the requirement is $\hbar\omega_z \gg k_B T_c^0$ so that $\omega_z \gg N^{1/2}\omega$, where T_c^0 is given by Eq. (5). Possible experimental configurations for trapping an atomic Bose gas in two dimensions are described in Ref. [19] and more recently in Ref. [25]. In the latter case, a method for trapping atoms above a magnetic surface using the Zeeman effect is proposed, resulting in a very strong confinement perpendicular to the surface.

We apply the path-integral quantum Monte Carlo method for bosons [26,27], specifically following the formulation of Ref. [27]. The path-integral quantum Monte Carlo scheme has recently been used to simulate BEC for a hard-sphere gas in two [13] and three dimensions [23,28]. The method relies on the fact that the partition function $\mathcal{Z} = \mathrm{Tr}\,\rho$ of a many-body system can be written in the form of a path integral [29] if the density operator $\rho = e^{-\beta(H_0+H_1)}$ is decomposed according to the Trotter formula

$$e^{-\beta(H_0+H_1)} = \lim_{M\to\infty} (e^{-\beta H_0/M} e^{-\beta H_1/M})^M, \qquad (7)$$

where $H_0 = -(\hbar^2/2m)\Sigma_i^N \nabla_i^2$ and $H_1 = V(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N)$ are, respectively, the kinetic and potential energy operators of the system. For bosons, a sum over permutations of all the particles is necessary in order to symmetrize the density matrix [26,27]. In practice, this means that the Monte Carlo simulation consists of permutation moves as well as coordinate moves.

A simple procedure for treating hard-core interactions in a 1D simulation was described in Ref. [30]. In two dimensions, we use a similar, albeit slightly more involved method. A 2D grid of square cells, each of side $\sqrt{2}a$, is defined. We are thus permitted to reject any move that places a particle into an already occupied cell. In the case that the cell is otherwise vacant, it is only necessary to compute interparticle separations between the moved particle and those in up to 20 nearby cells. The move is rejected if any separation is smaller than $2a$.

Particles on the same permutation cycle are in the same quantum state, so the particle permutations can be used to estimate the condensate fraction N_0/N. By comparing the results of our Monte Carlo simulations for ideal bosons with already known exact results, we find that the average maximum length of extended permutation cycles provides a lower bound close to N_0. Shorter exchanges can contribute to N_0 also, but since for finite N there is in general significant condensation into the first excited single-particle energy level near $T = T_c^0$ [9], inclusion of these is bound to result in an overestimation of N_0. Hence, we have calculated the average maximum length of extended permutation cycles in order to estimate the number of condensate particles in our interacting system.

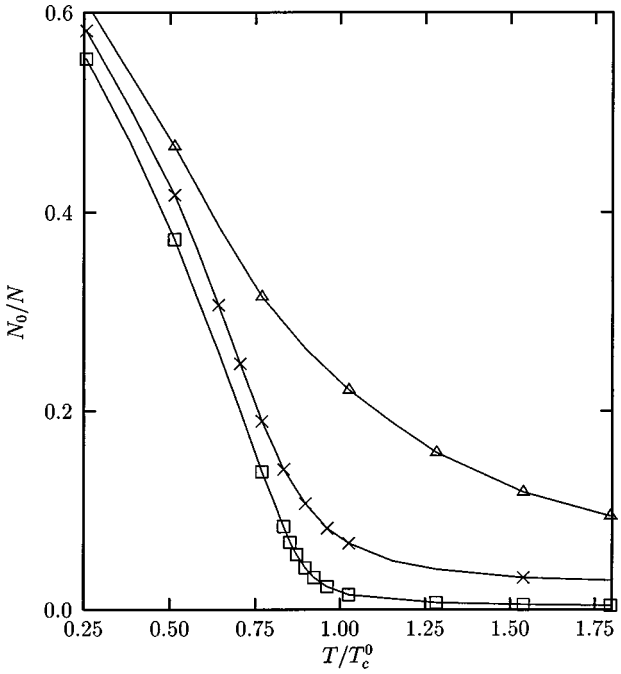

FIG. 1. The condensate fraction N_0/N as a function of T/T_c^0 with hard-core radius $a/l = 0.01$. Results are shown for $N = 10$ (triangles), 100 (crosses), and 1000 (boxes). Lines connecting data points provide a visual guide only.

We have carried out simulations for various N (10, 100, and 1000). In each case, we have obtained precise results by ensuring convergence with respect to the Trotter number M as well as the number of Monte Carlo iterations. The simulation of 10 and 100 atoms required relatively little CPU time with our available resources, so that in those cases it was possible to practically eliminate random errors from the estimation of thermal averages. The $N = 1000$ simulation required several days per data point to reduce the random errors to a reasonable level. We were unable to obtain reliable results for higher N within a reasonable amount of computing time. Our initial results are obtained with $a/l = 0.01$. Taking the case of ^{23}Na as one example, that would correspond to a confinement frequency of $\omega/2\pi = 5.1$ kHz [31]. The diluteness condition stated above does not appear to be satisfied by this value of a/l because for each N, the diluteness parameter is roughly $\ln^{-1}(1/na^2) \sim 0.1$. Of course, the situation would only worsen if we approached the typical experimental regime of higher N. Nevertheless we find that there is an abrupt increase in N_0/N just below $T = T_c^0$. The curves in Fig. 1 show phenomena qualitatively similar to the behavior of N_0/N for ideal bosons, with the onset of condensation becoming quite abrupt for $N = 1000$.

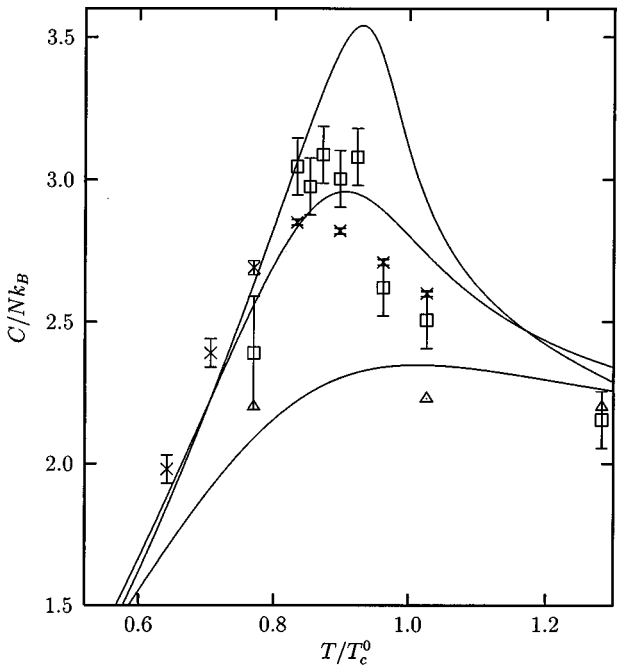

FIG. 2. The specific heat C/Nk_B as a function of T/T_0^c with hard-core radius $a/l=0.01$. Results are shown for $N=10$ (triangles), 100 (crosses), and 1000 (boxes). The solid lines represent the exact values for 10 (lowest peak), 100, and 1000 (highest peak) ideal bosons.

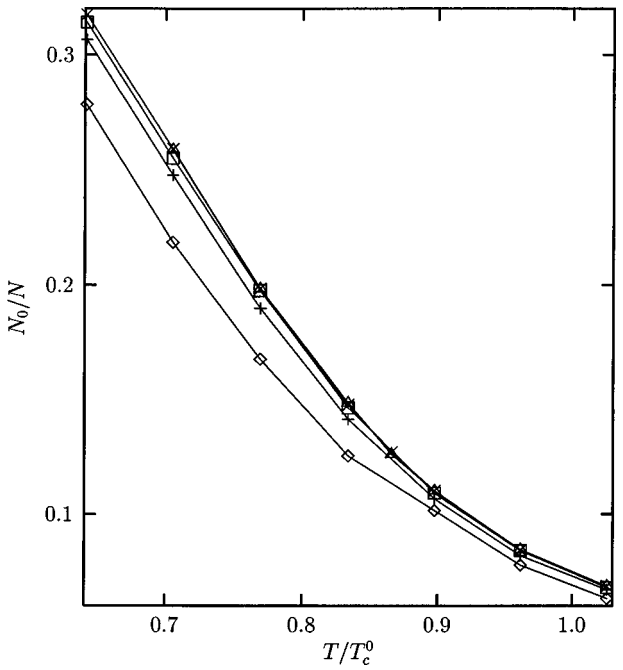

FIG. 3. N_0/N for various hard-core radii a with $N=100$. The individual points represent $a/l=0.02$ (diamonds, bottom curve), 0.01 (vertical crosses), 0.005 (boxes), 0.0025 (diagonal crosses), and 0.001 25 (triangles). Results for the smallest two values of a are virtually identical. Lines connecting data points provide a visual guide only.

The specific heat, shown in Fig. 2, approaches the classical value of noninteracting particles, $C/Nk_B=2$, for large enough T. As T is decreased toward the condensation temperature, a hump develops. This result is qualitatively similar to the case of ideal bosons [11], which is represented by the solid lines. However, the hump is considerably more pronounced in that case and develops into a sharp peak as N approaches infinity. In the present case, the positions of the peaks are shifted down in temperature with respect to the ideal case, indicating that the transition temperature is lowered by interactions.

Now we ask whether it is possible to recover the behavior of the finite system of ideal bosons by decreasing the size of the hard-core radius a. For 100 bosons, we have studied the depletion of the condensate as a function of a/l. Figure 3 shows that the value of N_0/N stops changing when a/l is decreased to 1.25×10^{-3}. In other words, the condensate fraction for interacting bosons coincides with the condensate fraction for ideal bosons when a/l reaches some small finite value. This result seems reasonable because this value of a/l is quite small compared with the average distance between particles in the trap. As a is increased from this value, N_0/N decreases, indicating that the transition temperature decreases with increasing a.

The density increases with the number of particles in our fixed trap, so the required value of a that reaches the noninteracting limit is bound to depend on N. This is illustrated in Fig. 4. The graph shows the difference $\Delta N_0/N=N_0(a=0)-N_0(a\neq0)$ between the condensate fractions for ideal and interacting bosons, plotted as a function of $aN^{1/4}/l$. We show results for a single temperature below the transition point: $T=0.77T_c^0$. We have confirmed that the choice of temperature does not have a significant effect on the rate (with respect to changes in a) that the noninteracting limit is approached, which is evident for $N=100$ in Fig. 3. For all three values of N studied, the ideal and interacting values of N_0/N

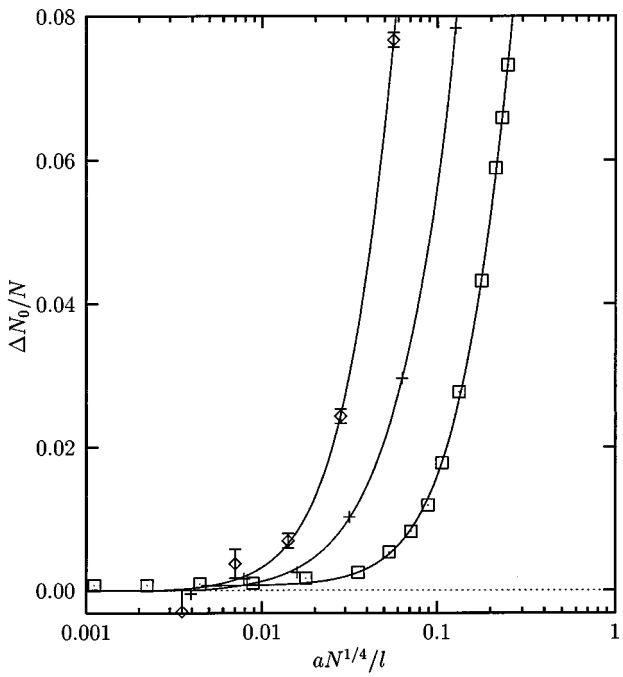

FIG. 4. The difference between the values of N_0/N for ideal and interacting bosons, plotted as a function of $aN^{1/4}/l$ (in logarithmic scale) for temperature $T=0.77T_c^0$. Points correspond to $N=10$ (diamonds), $N=100$ (crosses), and $N=1000$ (boxes). Lines connecting data points provide a visual guide only.

become almost indistinguishable when $aN^{1/4}/l$ goes below about 0.01 although as N increases, smaller $aN^{1/4}/l$ is required to reach the noninteracting limit. From this result, the diluteness condition can be approximated (for the values of N considered here) as $\ln^{-1}(1/na^2) \lesssim 0.1$. However, consistent with the absence of BEC for $a>0$ in the thermodynamic limit, the curves in Fig. 4 shift towards $a \to 0$ as N is increased. In other words, as N becomes very large, very small values of a are required to avoid total depletion of the condensate. As $N \to \infty$, $aN^{1/4}/l \to 0$ is required because the presence of interactions prevents the density divergence that is necessary for BEC to occur. Results for higher N than 1000 would be required to obtain a definite picture of what happens as the thermodynamic limit is approached.

In a recent path-integral quantum Monte Carlo simulation [13], the condensate fraction was calculated for 1000 hard-core bosons in the same type of trap. For the values of a and T used there, a heavier depletion of the condensate was obtained, compared with the equivalent case studied here. In that case, a slightly different approach was used to extract N_0/N from the simulation data.

Future experiments might use gases of ^{87}Rb or ^{23}Na as in the three-dimensional case. In fact ^{23}Na was Bose condensed in three dimensions at a critical temperature $T_c \sim 2$ μK [6]. If a 2D gas containing 1000 ^{23}Na atoms were Bose condensed in a trap whose confinement frequency was chosen such that the critical temperature $T_c \sim 2$ μK, it is straightforward to obtain from Fig. 4 that $\Delta N_0/N \sim 0.02$ at $T = 0.77 T_c^0$. Using the fact that the shift in the condensate fraction is roughly constant over a finite temperature range below the critical point, we are also able to estimate the shift in the critical temperature. For the present example of 1000 ^{23}Na atoms, we estimate a relative decrease in the critical temperature: $\Delta T_c/T_c^0 \sim -0.02$. Alternatively, if experimental capabilities were such that the ^{23}Na gas could be cooled to the nanokelvin temperature scale, then a much smaller ω would be used and the diluteness condition could in principle be satisfied so that the relative shift in the critical temperature would be practically zero.

The results presented here have been obtained by simulating various numbers of atoms in a single fixed trap. We find that the required value of a becomes very small as N is increased. As long as a lower ω was used, condensation close to T_c^0 could presumably be achieved for some values of higher N with a realistic value of a. A defining characteristic of BEC is the sudden increase in N_0/N at some finite critical temperature T_c. In two dimensions, the difference between the N_0/N curves for $N=1000$ and $N \to \infty$ is quite small for ideal bosons so satisfactory results may be obtained even without resorting to very large N.

As demonstrated elsewhere [13], it appears that the experimental observation of BEC in two dimensions is an attainable goal. The difference between the results of ideal and hard-core Bose gases virtually disappears if the range of interactions is small enough. It is anticipated that under typical experimental conditions, the critical temperature would be slightly lower than the critical temperature for ideal bosons.

For a given 2D power-law trap $U(\mathbf{r}_i) \propto r_i^{\eta}$, the magnitude of ΔT_c depends on the value of the exponent η. For $\eta \gtrsim 1$, this correction to the transition temperature is proportional to the ηth root of the diluteness parameter so it has been proposed that traps more confining ($\eta \simeq 1$, for example) than parabolic could provide the most promising confinement geometry [14]. On the other hand, T_c^0 depends both on η and on the average boson density n [19]. If the trap size is kept fixed, then T_c^0 will increase rapidly with η for a large enough N, implying that a high η is favorable. Even so, the diluteness condition might be difficult to satisfy—especially for large η—in such a high density limit. It should be straightforward to evaluate the transition temperature of interacting bosons for different η with the simulation method used here. Those results would be especially interesting from the experimental viewpoint.

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