Kosterlitz-Thouless Transition of the Quasi-Two-Dimensional Trapped Bose Gas

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We use quantum Monte Carlo methods to compute the density profile, the nonclassical moment of inertia, and the condensate fraction of an interacting quasi-two-dimensional trapped Bose gas with up to $N \sim 5 \times 10^5$ atoms and parameters closely related to recent experiments. We locate the Kosterlitz-Thouless temperature T_{KT} and discuss intrinsic signatures of the onset of superfluidity in the density profile. Below T_{KT}, the condensate fraction is macroscopic even for our largest systems and decays only slowly with system size. We show that the thermal population of excited states in the transverse direction changes the two-dimensional density profile noticeably in both the normal and the superfluid phase.

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Recent experiments have opened the way for detailed microscopic studies of the Kosterlitz-Thouless phase transition [1] in quasi-two-dimensional quantum gases [2–5]. These systems are particularly interesting because the external potential—a pancake-shaped harmonic trap with a tightly confining transverse direction—places them in the vicinity of two distinct phase transitions. Interactions, on the one hand, drive the Kosterlitz-Thouless transition from the normal state to a superfluid state with a vanishing condensate fraction in the infinite system [6]. The modification of the free density of states through the two-dimensional trap, on the other hand, drives a conventional Bose-Einstein condensation at finite temperature, but only for the noninteracting gas [7,8]. However, due to the mesoscopic size of trapped quantum gases, the clear distinction between the Kosterlitz-Thouless and the Bose-Einstein transition necessitates finite-size extrapolation to the thermodynamic limit.

Experimental evidence for a Kosterlitz-Thouless transition in quasi-two-dimensional quantum gases was provided by interference studies revealing thermally activated vortices [3] and quasi-long-range coherence [4]. Initially, strong deviations of the measured critical temperature with respect to known results in strictly two dimensions seemed to point towards effects beyond mean-field theory even in the high-temperature normal phase [5]. However, in the quasi-two-dimensional regime, the population of several excited states in the tightly confined direction must be taken into account [8]. As we will show, the latter is important for a proper description of the density profiles above and below the critical temperature.

In this Letter, we apply quantum Monte Carlo (QMC) methods [10–13] to simulate a very large number N of dilute interacting bosons in trap geometries directly relevant to the experiments. These methods allow us to determine thermodynamic properties. We consider three-dimensional trapped bosons interacting with an s-wave pseudopotential in a harmonic trap with frequencies $\omega = \omega_x = \omega_y \ll \omega_z$. Our particle numbers range from $N = 2000$ to $N = 576\,000$, the latter exceeding current experiments with $\sim 40\,000$ atoms [5] by more than 1 order of magnitude. The diagonal many-particle density matrix yields the density profile and the nonclassical moment of inertia. Both allow us to locate the phase transition. We also determine the condensate fraction explicitly from the largest eigenvalue of the reduced off-diagonal one-particle density matrix. We can distinguish between condensatelike and Kosterlitz-Thouless–like behavior by studying finite-size effects of the condensate.

The trapped ideal strictly two-dimensional Bose gas shows a Bose-Einstein transition [7] at a temperature $T_{\mathrm{BEC}}^{\mathrm{2d}} = \sqrt{6N}\hbar\omega/\pi$. In the quasi-two-dimensional regime, for finite $\tilde{\omega}_z = \hbar\omega_z/T_{\mathrm{BEC}}^{\mathrm{2d}}$, the Bose-Einstein temperature is decreased [8]. It occurs at a temperature $T_{\mathrm{BEC}}^{\mathrm{q2d}} = 0.78 T_{\mathrm{BEC}}^{\mathrm{2d}}$ for the experimental value $\tilde{\omega}_z = 0.55$ [5]. In the strongly anisotropic trap, at temperatures around $T_{\mathrm{BEC}}^{\mathrm{q2d}}$, and at finite $\tilde{\omega}_z$, the extension of the density profile in z is comparable to the de Broglie wavelength $\lambda = \sqrt{2\pi\hbar^2/mT}$, so that the gas is essentially two dimensional.

In the many-body density matrix, the z dependence is dominated by a (normalized) single-particle contribution, $\rho(z, z')$, which separates out, and the effective two-dimensional interaction strength is given by

$$g = \frac{4\pi\hbar^2 a_0}{m} \int dz [\rho(z, z)]^2, \tag{1}$$

where a_0 is the three-dimensional s-wave scattering length. For particles distributed in z according to the ground state of the harmonic oscillator, Eq. (1) reduces to $g = \tilde{g} \equiv a_0\sqrt{8\pi\omega_z\hbar^3/m}$. For our simulations, we have

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used the experimental value $m\tilde{g}/\hbar^2 = 0.13$ [5]; however, the actual value of g can be obtained directly from the computed density profile in the z direction using Eq. (1).

Numerical calculations [14] have determined the critical density n_c at the Kosterlitz-Thouless transition in the weakly interacting two-dimensional homogeneous Bose gas of density n,

$$n_c\lambda^2 \simeq \ln\frac{380\hbar^2}{mg}. \tag{2}$$

The interaction g enters this expression only logarithmically, and the differences between g and $\tilde{g}$, of the order of 40% at T_{KT}, results in only a 6% shift in the critical density.

In the trapped Bose gas, within the local-density approximation, the transition takes place when the central density $n(0)$ equals the critical density of the homogeneous gas, in our case $n_c(0)\lambda^2 \simeq 8$. Within strictly two-dimensional mean-field theory [6], the Kosterlitz-Thouless transition is somewhat below$T_{\mathrm{BEC}}^{\mathrm{2d}}$:

$$\frac{T_{\mathrm{KT}}^{\mathrm{2d}}}{T_{\mathrm{BEC}}^{\mathrm{2d}}} = \left(1 + \frac{3mg}{\pi^3\hbar^2}[n_c(0)\lambda^2]^2\right)^{-1/2} \simeq 0.75, \tag{3}$$

where we used Eq. (2). In the quasi-two-dimensional regime, the Kosterlitz-Thouless temperature can also be computed. For $\tilde{\omega}_z = 0.55$, one obtains $T_{\mathrm{KT}}^{\mathrm{q2d}} = 0.69 T_{\mathrm{BEC}}^{\mathrm{2d}}$ [8].

In Fig. 1, we show the two-dimensional density profile $n(r)$ with $r = \sqrt{x^2 + y^2}$ from our QMC calculations at $T = T_{\mathrm{BEC}}^{\mathrm{2d}}$ for $N = 576\,000$. We also illustrate the large deviations from the strictly two-dimensional ideal Bose gas. As already noticed in the experiments [5], the profile also deviates strongly from the strictly two-dimensional mean-field theory and it is closer to that of ideal quantum Boltzmann particles described by the density matrix of the harmonic oscillator. However, it is virtually indistinguishable from the quasi-two-dimensional mean-field theory proposed in Ref. [8].

In Fig. 2, we show the analogous density profile at temperature $T/T_{\mathrm{BEC}}^{\mathrm{2d}} = 0.5$, again for $N = 576\,000$ particles. The central density is now well in excess of the critical value of Eq. (2). We may define a "critical radius" r_c, which separates the "inner region" of the trap, with $r < r_c$ and $n(r) > n_c$, from an "outer region" with $r > r_c$ and $n(r) < n_c$. In the local-density approximation, the inner region is in the superfluid phase, whereas the outer region is normal. At the critical radius, the density is at the Kosterlitz-Thouless temperature. In the inner region, $n(r)$ is very well described by a Thomas-Fermi profile

$$n(r) = n(0) - \frac{1}{g}\frac{m\omega^2 r^2}{2}, \qquad r < r_c, \tag{4}$$

with the effective two-dimensional interaction parameter at this temperature $mg/\hbar^2 = 0.107$, obtained, via Eq. (1), directly from the density profile in z (see inset of Fig. 2). The latter is wider than the ground state distribution of the harmonic oscillator, so that g is smaller than $\tilde{g}$. The density profile in r, whose width depends linearly on g^{-1}, is more sensitive to the detailed value of the interaction than the transition temperature, which decreases with the logarithm of g.

In Fig. 3, we plot the central density $n(0)\lambda^2$ and also the (central) curvature $\kappa = -\partial n(r)\lambda^2/\partial(\beta m\omega^2 r^2)|_{r=0}$. The

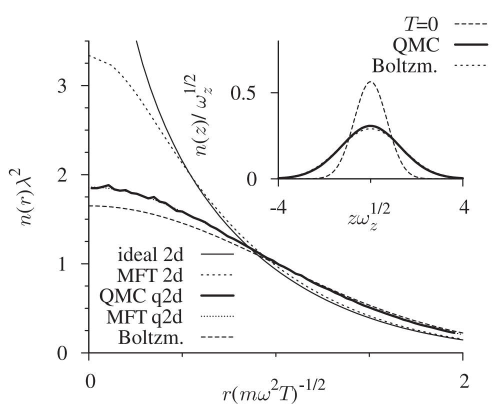

FIG. 1. Two-dimensional density profile $n(r)\lambda^2$ at $T = T_{\mathrm{BEC}}^{\mathrm{2d}}$ for $N = 576\,000$, compared to that of the strictly two-dimensional ideal Bose gas, the ideal gas of distinguishable particles, and strictly two-dimensional mean-field theory (MFT). The QMC data are virtually indistinguishable from the results of quasi-two-dimensional mean-field theory [8]. The inset compares the density profile in z to the ground state distribution of the harmonic oscillator and to the ideal gas of distinguishable particles.

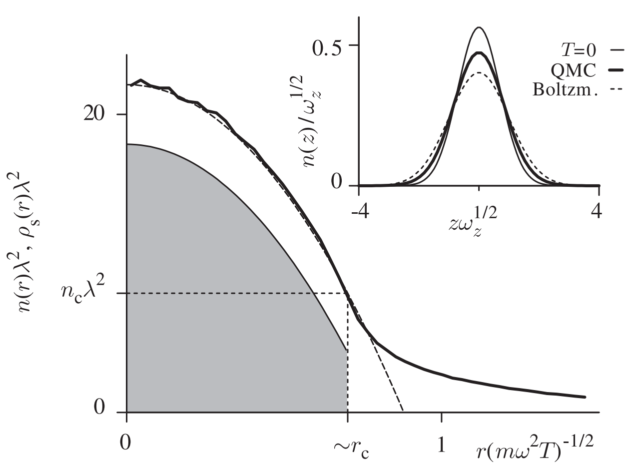

FIG. 2. Two-dimensional density profile $n(r)\lambda^2$ at temperature $T = 0.5T_{\mathrm{BEC}}^{\mathrm{2d}}$ for $N = 576\,000$ (thick line), compared to the Thomas-Fermi profile of Eq. (4) (with $mg/\hbar^2 = 0.109$, dashed line). The ansatz of Eq. (5) for the superfluid density $\rho_s(r)$, with the universal jump at $r = r_c$, corresponds to the shaded region. The inset compares the density profile in the tightly confined z direction to the ground state distribution of the harmonic oscillator and the distribution of an ideal gas of distinguishable particles.

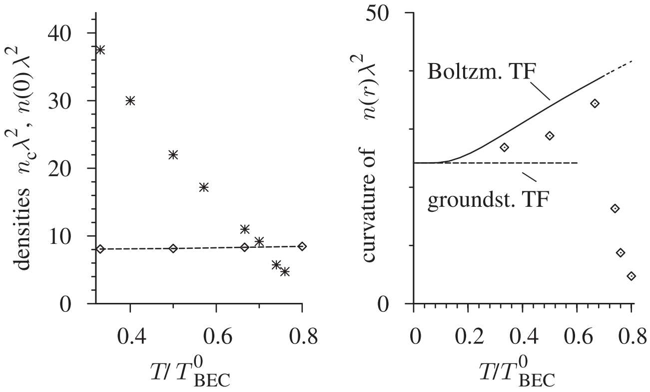

FIG. 3. Left panel: Densities $n_c\lambda^2$ and $n(0)\lambda^2$ vs $T/T^{2\mathrm{d}}_{\mathrm{BEC}}$ for the quasi-two-dimensional gas with $N = 576\,000$. The intersection of both curves leads to a transition temperature $T_{\mathrm{KT}} \simeq 0.70$. Right panel: Central curvature κ compared to the ground state Thomas-Fermi (TF) curvature, Eq. (4), with $g = \tilde{g}$ and with g corresponding to an ideal gas of distinguishable particles. The central curvature changes slope at T_{KT}.

curvature of the Thomas-Fermi profile [in Eq. (4)] is $\kappa = \pi\hbar^2/(mg)$ with $g = \tilde{g}$ at very low temperature. The curvature increases (the profile becomes narrower) with T because particles spread out farther in the z direction. Above the critical temperature, however, the curvature decreases (the profile becomes wider), as is natural for a thermal gas, with $\kappa \propto n(0)\lambda^2$. The curvature plot provides an intrinsic signature of the phase transition, at a temperature $T/T^{2\mathrm{d}}_{\mathrm{BEC}} \simeq 0.70$, which agrees nicely with the temperature at which the central density passes the critical value Eq. (2). We have also studied smaller systems (with $N = 2250$, 9000, 36 000, and 144 000) at unchanged values of $T/T^{2\mathrm{d}}_{\mathrm{BEC}}$ and $\tilde{\omega}_z = 0.55$, but found only very small variations in the density profiles. Our value for the critical temperature $T_{\mathrm{KT}} \simeq 0.70T^{2\mathrm{d}}_{\mathrm{BEC}}$ agrees reasonably well with the mean-field value $T^{\mathrm{q2d}}_{\mathrm{KT}} = 0.69T^{2\mathrm{d}}_{\mathrm{BEC}}$ of the Kosterlitz-Thouless transition in the quasi-two-dimensional trapped Bose gas [8].

From Fig. 1, we see that the density profile deviates from the thermal distribution with a single Gaussian component as soon as $n(r)\lambda^2 \gtrsim 1$. The temperature determination from the tails of the density profile therefore suffers from a poor signal-to-noise ratio. Indeed, a direct comparison of our data with the experimental density profiles [9] showed that a proper temperature calibration of the experimental data accounts for the difference between our transition temperature and the original experimental value of Ref. [5]. Alternatively, the experimental temperature in the high-temperature phase can be calibrated conveniently using quasi-two-dimensional mean-field theory [8,9].

The low-temperature phase below the Kosterlitz-Thouless transition is a superfluid. For a homogeneous system, the superfluid fraction can be probed through the response to boundary conditions [10]. Likewise, a trapped superfluid does not respond to an infinitely slow rotation

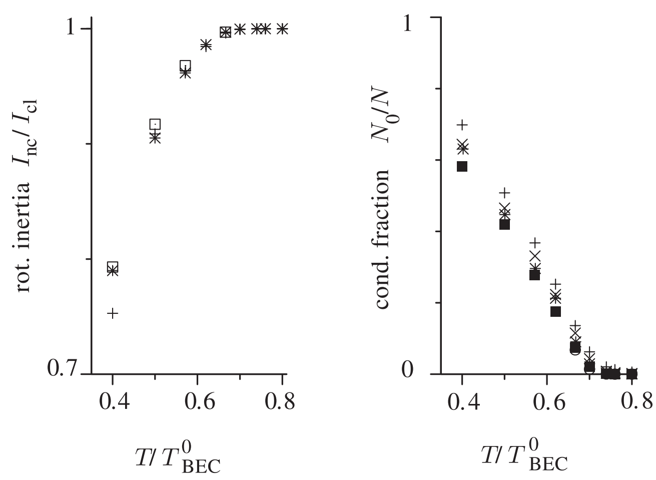

FIG. 4. Left panel: Nonclassical moment of inertia $I_{\mathrm{nc}}/I_{\mathrm{cl}}$ vs $T/T^{2\mathrm{d}}_{\mathrm{BEC}}$ for $N = 9000$ (crosses) and $N = 144\,000$ (stars) compared to the ansatz of Eq. (5) (squares). Right panel: Condensate fraction for particle numbers ranging from $N = 2250$ (crosses) to $N = 144\,000$ (squares).

of a trap leading to a nonclassical moment of inertia, I_{nc}, which is smaller than the classical value $I_{\mathrm{cl}} = \int d\mathbf{r} r^2 n(r)$. The nonclassical moment of inertia can be computed from the diagonal elements of the density matrix [15]. In a homogeneous system, the ratio of the nonclassical moment to the classical moment equals the normal fraction. In Fig. 4, we show that a superfluid phase emerges below $T \simeq 0.70T^{2\mathrm{d}}_{\mathrm{BEC}}$, and that $I_{\mathrm{nc}}/I_{\mathrm{cl}}$ remains different from unity, independent on system size.

To interpret our data for the nonclassical moment of inertia, we observe that in an infinite homogeneous system, at the Kosterlitz-Thouless transition, the superfluid density develops a universal jump [16], $\Delta\rho_s = 2mT_{\mathrm{KT}}/(\pi\hbar^2)$, and the superfluid mass and the moment of inertia are both discontinuous. In the trap, the spatial structure smears out these discontinuities [6], but in local-density approximation, as mentioned, the gas is critical at the critical radius r_c. Therefore, we expect a normal phase beyond r_c, and a superfluid for $r < r_c$, with a jump of the superfluid density taking place at this radius and the superfluid density vanishing for $r > r_c$. For our parameters, the superfluid fraction at the critical radius is $\rho_s(r_c)/n(r_c) = 2mT/(n(r_c)\pi\hbar^2) \simeq 0.5$. We can continue the superfluid density $\rho_s(r)$ into the inner region by a Thomas-Fermi profile:

$$\rho_s(r) = \begin{cases} m\omega^2 r_c^2(1 - r^2/r_c^2)/2g + 2mT/(\pi\hbar^2) & \text{for } r \leq r_c, \\ 2mT/(\pi\hbar^2) & \text{for } r \to r_c^-, \\ 0 & \text{for } r > r_c. \end{cases} \tag{5}$$

(See Fig. 2.) The nonclassical moment of inertia $I_{\mathrm{nc}} = \int d\mathbf{r} r^2[n(r) - \rho_s(r)]$, computed using Eq. (5) and the computed density profile $n(r)$, agrees excellently with our data (see Fig. 4).

In an inhomogeneous system, the ground state eigenfunction of the one-body density matrix is fixed by symmetry alone. Still, in the rotationally symmetric trap the one-body density matrix is block diagonal with respect to the Fourier components l of the angle between $\mathbf{r}$ and $\mathbf{r}'$. Projection onto the Fourier components yields one-dimensional matrices, $\rho_l^{(1)}(r, r'; \beta)$, which can be discretized more easily than the bigger matrix $\rho^{(1)}(\mathbf{r}, \mathbf{r}'; \beta)$. The condensate fraction, N_0/N, corresponds to the largest eigenvalue with $l = 0$ [17]. Figure 4 shows that the condensate fraction of our quasi-two-dimensional system is rather large, but it decays algebraically with system size: $N_0/N \sim N^{-\eta(T)/2}$. The exponent $\eta(T)$ depends on the temperature; we obtain $\eta(0.70T_{\mathrm{BEC}}^{\mathrm{2d}}) \approx 0.5$ and $\eta(0.67T_{\mathrm{BEC}}^{\mathrm{2d}}) \approx 0.2$. Precisely at the critical temperature, we expect $\eta(T_{\mathrm{KT}}) \simeq 1/4$ from the homogeneous Kosterlitz-Thouless theory [1] which implies that the critical temperature is between $0.67T_{\mathrm{BEC}}^{\mathrm{2d}}$ and $0.70T_{\mathrm{BEC}}^{\mathrm{2d}}$. This value is compatible with our more precise estimate based on the nonclassical moment of inertia. The algebraic decay of the condensate fraction with the system size strongly supports the Kosterlitz-Thouless character of the transition with a vanishing condensate in the thermodynamic limit.

Notably, in the trap, the characteristic universal jump in the superfluid density at the critical temperature of the Kosterlitz-Thouless transition does not induce a significant discontinuity in the inertial response, as in two-dimensional films [19]. Nevertheless, the universal jump determines $\rho_s(r)$ at the radius $r = r_c$ where the gas is locally critical. Based on the local-density approximation, we proposed a superfluid density profile, Eq. (5), which continues the $\rho_s(r)$ from $r = r_c$ into the superfluid inner region. It depends on a single parameter r_c whose value can be determined directly from the density profile. The nonclassical moment of inertia calculated from the superfluid density profile, Eq. (5), is in excellent agreement with a direct computation of this quantity. Further, it is remarkable that in the finite Kosterlitz-Thouless system, the condensate fraction, which must vanish for an infinite system, is still rather large, even close to the transition temperature. The fact that the ground state wave function of size $\sim r_c$ remains macroscopically occupied for systems with particle number $N \lesssim 10^6$ implies that the coherence of the atoms is neither destroyed by interparticle interactions nor by fluctuations, essential for building continuous and coherent sources of matter waves in lower dimensions [20].

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