

Semiclassical theory of the quasi–two-dimensional trapped Bose gas

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Abstract – We discuss the quasi–two-dimensional trapped Bose gas where the thermal occupation of excited states in the tightly confined direction is small but remains finite in the thermodynamic limit. We show that the semiclassical theory describes very accurately the density profile obtained by quantum Monte Carlo calculations in the normal phase above the Kosterlitz-Thouless temperature T_{KT} , but differs strongly from the predictions of strictly two-dimensional mean-field theory, even at relatively high temperature. We discuss the relevance of our findings for analyzing ultra-cold–atom experiments in quasi–two-dimensional traps.

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For many years, the physics of two-dimensional quantum gases has been under close experimental and theoretical scrutiny. The quest for quantum phase transitions in two-dimensional atomic Bose gases has started with experiments on spin-polarized atomic hydrogen adsorbed on liquid ^4He surface reaching the quantum degenerate regime (see, *e.g.*, [1,2]) and observing quasi-condensation [3]. The Kosterlitz-Thouless transition [4] was observed recently in trapped atomic gases of ultra-cold ^{87}Rb atoms in an optical lattice potential with a tightly confined z -direction [5].

In contrast to experiments with liquid ^4He films [6], where the Kosterlitz-Thouless transition is realized directly, the typical extension in the z -direction in the experiments on two-dimensional gases is much larger than the three-dimensional scattering length. For this reason, the effective two-dimensional interaction strength remains sensitive to the density distribution in z [7]. Nevertheless, the gas is kinematically two-dimensional because of the strong out-of-plane confinement.

In this letter, we consider the quasi–two-dimensional regime of the trapped Bose gas, where the temperature T is of the order of the level spacing in z . This corresponds to the experimental situation with small, but not completely

negligible, thermal occupation of a few excited states of the tightly confining potential [5,8]. The quasi–two-dimensional regime crosses over to the three-dimensional and the strictly two-dimensional Bose gases as the potential in the z -direction is varied.

Semiclassical theory cannot describe the Kosterlitz-Thouless transition, but it is expected to describe accurately the spatial distribution of a trapped dilute gas in the normal high-temperature phase. At the transition, only the particles in the very center of the trap are critical, and it was argued that the mean-field profile should still hold down to this temperature [9]. However, it was noticed in experiments [8,10] and in direct quantum Monte Carlo calculations [11] that the density profile of the gas deviates strongly from strictly two-dimensional mean-field theory, even at relatively high temperature. Originally, these deviations were thus attributed to effects beyond mean field [8]. We point out in the present paper that they are rather accounted for by a quasi–two-dimensional mean-field theory which incorporates the thermally activated states in the tightly confined direction.

We first discuss Bose-Einstein condensation of the ideal gas in strongly anisotropic harmonic traps, and we define the quasi–two-dimensional regime where the ideal-gas critical temperature is always lower than that of the strictly two-dimensional ideal gas. By including

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interactions on the level of mean field, we obtain the density profiles in the semiclassical approximation and solve the self-consistent mean-field equations directly. Remarkable agreement of the semiclassical density profiles with the results of quantum Monte Carlo calculations is obtained in the high-temperature normal phase down to the Kosterlitz-Thouless temperature. The profiles should be very convenient for calibrating the temperature in experiments of quasi-two-dimensional Bose gases. Comparison of experimental density profiles with quantum Monte Carlo data has already removed the original discrepancy of the Kosterlitz-Thouless temperature between calculation and experiment [10].

We consider an anisotropic trap with oscillator frequencies $\omega \equiv \omega_x = \omega_y \ll \omega_z$. At temperature $T \sim \hbar\omega_z$, the motion is semiclassical in the coordinates x, y and in the momenta $\hbar k_x, \hbar k_y$, whereas the quantization in the z -direction is best described through the energy levels $\nu\hbar\omega_z$ ($\nu = 0, 1, \dots$) of the corresponding harmonic oscillator. Semiclassically, the number dN of particles per phase-space element $dk_x dk_y dx dy$ in the energy level ν is given by [12]

$$dN = \frac{1}{(2\pi)^2} \frac{dk_x dk_y dx dy}{\exp[\beta(\frac{\hbar^2 k^2}{2m} + v(r) + \nu\hbar\omega_z - \mu)] - 1}, \quad (1)$$

where $\beta = 1/T$, $k^2 = k_x^2 + k_y^2$, and where $v(r)$ is an arbitrary two-dimensional potential energy (with $r^2 = x^2 + y^2$).

Equation (1) can be integrated over all momenta and summed over all oscillator levels to obtain the two-dimensional particle density

$$n(r) = \sum_{\nu} \int_0^{\infty} \frac{dk^2}{4\pi} \frac{1}{\exp(\beta(\frac{\hbar^2 k^2}{2m} + v(r) + \nu\hbar\omega_z - \mu)) - 1} = -\frac{1}{\lambda^2} \sum_{\nu=0}^{\infty} \ln\{1 - \exp[\beta(\mu - v(r) - \nu\hbar\omega_z)]\}, \quad (2)$$

where $\lambda = \sqrt{2\pi\hbar^2\beta/m}$ is the thermal wavelength. The potential $v(r)$ can itself contain the interaction with the density $n(r)$, so that eq. (2) is in general a self-consistency equation. The integral of $n(r)$ over space yields the equation of state, that is, the total number of particles as a function of temperature and chemical potential.

Let us first consider the ideal gas, where the potential energy $v(r) = m\omega^2 r^2/2$ is due only to the trapping potential, so that the rhs of eq. (2) is independent of the density $n(r)$. We get

$$N = -\frac{\pi}{\lambda^2} \sum_{\nu=0}^{\infty} \int_0^{\infty} d(r^2) \ln\left[1 - e^{\beta(\mu - \nu\hbar\omega_z - m\omega^2 r^2/2)}\right] = \frac{T^2}{\hbar^2\omega^2} \sum_{\nu=0}^{\infty} F_2(-\mu\beta + \nu\beta\hbar\omega_z), \quad (3)$$

where we have defined

$$F_s(x) = \sum_{n=1}^{\infty} \frac{e^{-nx}}{n^s}.$$

The saturation number $N_{\text{sat}}(T)$ is the maximum number of excited particles (reached at $\mu = 0$) at a given temperature. We have

$$N_{\text{sat}}^{\text{q2d}} = \frac{T^2}{\hbar^2\omega^2} \sum_{\nu=0}^{\infty} F_2(\nu\beta\hbar\omega_z). \quad (4)$$

The above relation between the saturation number and the temperature defines the dependence of the Bose-Einstein condensation temperature on the particle number N . As mentioned before, the strictly two-dimensional limit is characterized by the limit $\beta\hbar\omega_z \rightarrow \infty$ (the level spacing in z is much larger than the temperature). In this limit, only the first term in eq. (3) contributes. Using $F_2(0) = \pi^2/6$, we find

$$N_{\text{sat}}^{\text{2d}}(T) = \frac{T^2}{\hbar^2\omega^2} \frac{\pi^2}{6} \Leftrightarrow T_{\text{BEC}}^{\text{2d}}(N) = \frac{\sqrt{6N}\hbar\omega}{\pi}. \quad (5)$$

In the quasi-two-dimensional case, with finite $\beta\hbar\omega_z$, the occupation of the oscillator levels $\nu = 1, 2, \dots$ increases the saturation number and therefore lowers the critical temperature. It is convenient to express in units of $T_{\text{BEC}}^{\text{2d}}$ both the temperature $t = T/T_{\text{BEC}}^{\text{2d}}$ and the oscillator strength $\tilde{\omega}_z = \hbar\omega_z/T_{\text{BEC}}^{\text{2d}}$, and to write $\tilde{\mu} = \beta\mu$. Using eq. (5), we may rewrite the equation of state, eq. (3), as a relation between the temperature t , the chemical potential $\tilde{\mu}$, and the oscillator strength $\tilde{\omega}_z$,

$$t = f(t, \tilde{\mu}, \tilde{\omega}_z), \quad (6)$$

with

$$f(t, \tilde{\mu}, \tilde{\omega}_z) = \left(\frac{6}{\pi^2} \sum_{\nu=0}^{\infty} F_2(-\tilde{\mu} + \nu\tilde{\omega}_z/t) \right)^{-1/2}. \quad (7)$$

Equation (6) is solved numerically by iterating $t_{n+1} = f(t_n)$ from an arbitrary starting temperature t_0 to the fixed point. The critical temperature $t_{\text{BEC}} = T_{\text{BEC}}^{\text{q2d}}/T_{\text{BEC}}^{\text{2d}}$ (as a function of $\tilde{\omega}_z$) of the quasi-two-dimensional ideal Bose gas is the solution for $\tilde{\mu} = 0$ (see fig. 1). The reduction with respect to the strictly two-dimensional case is notable for systems of experimental interest. For example, we find $t_{\text{BEC}} = 0.78$ for the experimental value $\tilde{\omega}_z = 0.55$ [5,8] considered in the quantum Monte Carlo calculations [11].

We can expand eq. (7) for small and for large $\tilde{\omega}_z$ and find

$$t_{\text{BEC}} \sim \begin{cases} \left[\frac{\zeta(2)}{\zeta(3)} \right]^{1/3} \tilde{\omega}_z^{1/3} - \frac{1}{6} \frac{\zeta(2)}{\zeta(3)} \tilde{\omega}_z, & \text{for } \tilde{\omega}_z \ll 1, \\ 1 - \frac{1}{2\zeta(2)^{3/2}} \exp(-\tilde{\omega}_z), & \text{for } \tilde{\omega}_z \gg 1, \end{cases} \quad (8)$$

where we have used $\zeta(s) \equiv F_s(0)$ (note that $\zeta(2) = \pi^2/6$ and $\zeta(3) \simeq 1.202$). The expansions are indicated in fig. 1. They give the critical temperature to better than 1.2% for all values of $\tilde{\omega}_z$ (the low- $\tilde{\omega}_z$ expansion is used for $\tilde{\omega} < 1.8$ and the high- $\tilde{\omega}_z$ expansion for $\tilde{\omega} > 1.8$). The first term in the small- $\tilde{\omega}_z$ expansion of eq. (8) corresponds to the three-dimensional gas. Indeed, $t_{\text{BEC}} \sim [\zeta(2)/\zeta(3)]^{1/3} \tilde{\omega}_z^{1/3}$

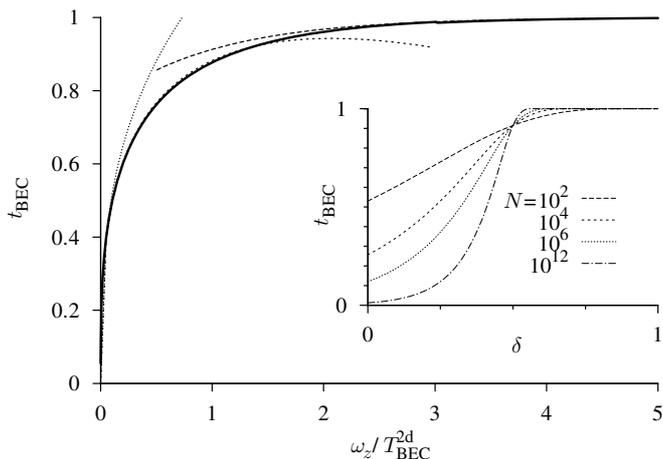


Fig. 1: Bose-Einstein condensation temperature t_{BEC} of the ideal quasi-two-dimensional gas in a harmonic trap with $\omega_z/\omega \propto N^{1/2}$ (expansions from eq. (8)). The inset shows t_{BEC} for scaling $\omega_z/\omega = N^\delta$ as a function of δ for different N . At $\delta = 0$, the critical temperature $T_{\text{BEC}}^{\text{3d}} = [N/\zeta(3)]^{1/3}$ of the ideal gas in a three-dimensional isotropic trap is recovered.

is equivalent to

$$T_{\text{BEC}} \sim \left[\frac{\zeta(2)}{\zeta(3)} \right]^{1/3} (\hbar\omega_z)^{1/3} (T_{\text{BEC}}^{\text{2d}})^{2/3} \sim \left[\hbar^3 \omega_z \omega^2 / \zeta(3) \right]^{1/3} N^{1/3}, \quad (9)$$

the well-known condensation temperature for the three-dimensional Bose-Einstein gas in an anisotropic trap [13]. Equation (9) also follows directly from eq. (4) by replacing the sum over the oscillator levels by an integral. Likewise, the first term in the large- $\tilde{\omega}_z$ expansion of eq. (8) represents the strictly two-dimensional gas.

The inset of fig. 1 further analyzes the expansions of eq. (8). Indeed, we can choose a scaling $\omega_z/\omega \sim N^\delta$ different from the quasi-two-dimensional case $\delta = 1/2$. Any choice of $\delta < 1/2$ corresponds to $\tilde{\omega}_z \rightarrow 0$ for $N \rightarrow \infty$ so that asymptotically the three-dimensional regime is reached. Analogously, $\delta > 1/2$ corresponds to $\tilde{\omega}_z \rightarrow \infty$ for $N \rightarrow \infty$, driving the transition into the strictly two-dimensional regime. The rescaled transition temperatures are plotted for $\omega_z/\omega = N^\delta$ where the case $\delta = 0$ corresponds to the three-dimensional isotropic trap¹.

In order to describe interaction effects in the quasi-two-dimensional Bose gas, we now add a semiclassical contact term to the potential energy of eq. (2):

$$v(r) = m\omega^2 r^2/2 + 2g[n(r) - n(0)]. \quad (10)$$

We have subtracted the central density, so that the potential still vanishes at the origin. As discussed earlier [11], the effective interaction $g = 4\pi a\hbar^2/m \int dz [\rho(z)]^2$ is proportional to the three-dimensional s -wave scattering length

¹The inset of fig. 1 is evaluated from the asymptotic expansion eq. (8). Very similar results for T_c follow from the exact saturation numbers at finite N .

a and to the integral of the squared density distribution in z , described by the normalized diagonal density matrix $\rho(z)$. In the temperature range of interest, this density distribution is well described by the single-particle harmonic-oscillator density matrix in z , leading to

$$g = a\sqrt{\frac{8\pi\omega_z\hbar^3}{m}} \sqrt{\tanh[\tilde{\omega}_z/(2t)]}. \quad (11)$$

The effective interaction thus decreases with temperature from its zero-temperature value $\tilde{g} = a\sqrt{8\pi\omega_z\hbar^3/m}$. To keep the interaction strength fixed, we must keep g (or equivalently \tilde{g}) constant in the quasi-two-dimensional thermodynamic limit which requires a fixed value of the scaled scattering length $a\sqrt{\omega_z} \propto a\omega^{1/2}N^{1/4}$.

The mean-field density $n(r)$, on the lhs of eq. (2), depends on the variable r only via the potential $v(r)$. In the space integral over the particle density, we can thus change the integration variable from r to v . This allows us to determine the equation of state explicitly:

$$N = \pi \int_0^\infty d(r^2) n(r) = \pi \int_0^\infty dv \left[\frac{\partial(r^2)}{\partial v} \right] n(v) = \frac{2\pi}{m\omega^2} \int_0^\infty dv \left[1 - 2g \frac{\partial n}{\partial v} \right] n(v) = \frac{T^2}{\hbar^2\omega^2} \left(\sum_{\nu=0}^\infty F_2(-\tilde{\mu} + \nu\beta\hbar\omega_z) + \frac{mg}{2\pi\hbar^2} [n(0)\lambda^2]^2 \right), \quad (12)$$

where the central density,

$$n(0)\lambda^2 = - \sum_{\nu=0}^\infty \ln \{ 1 - \exp(\tilde{\mu} - \nu\tilde{\omega}_z/t) \}, \quad (13)$$

is directly expressed in terms of $\tilde{\mu}$, independently of the interaction, due to the subtraction performed in our effective potential, eq. (10). (Note that the first integral on the second line of eq. (12) has already appeared in eq. (3) and that the second integral is a total derivative.) The equation of state can be written in terms of the temperature t . This yields the following generalization of eq. (7) to the mean-field gas:

$$t = \left(\frac{6}{\pi^2} \left[\sum_{\nu=0}^\infty F_2 \left(-\tilde{\mu} + \nu \frac{\tilde{\omega}_z}{t} \right) + \frac{mg}{2\pi\hbar^2} [n(0)\lambda^2]^2 \right] \right)^{-1/2}. \quad (14)$$

An iteration procedure $t_{n+1} = f(t_n)$ again obtains the temperature $t = T/T_{\text{BEC}}^{\text{2d}}$ as a function of the chemical potential $\tilde{\mu}$ for given parameters $\tilde{\omega}_z$ and g . (The central density is computed using eq. (13) during each iteration.)

The mean-field density profile is obtained in two steps by first calculating the density profile as a function of the scaled effective potential $\tilde{v} = \beta v$,

$$n(\tilde{v})\lambda^2 = - \sum_{\nu=0}^\infty \ln \{ 1 - \exp(\tilde{\mu} - \tilde{v} - \nu\tilde{\omega}_z/t) \},$$

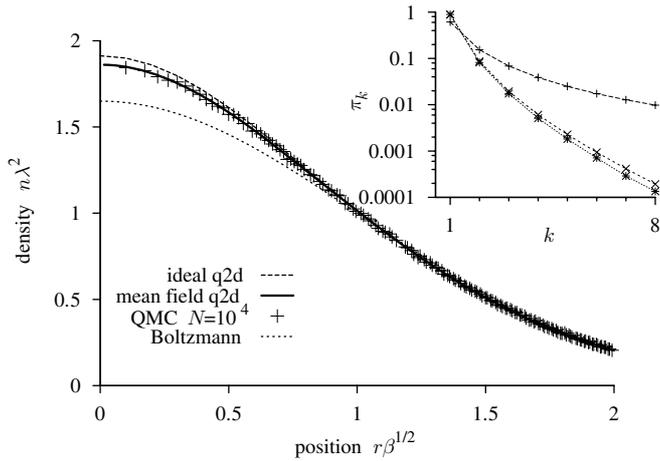


Fig. 2: Two-dimensional density profile $n(r = \sqrt{x^2 + y^2})\lambda^2$ at temperature $T = T_{\text{BEC}}^{2\text{d}}$ in a trap with $\omega_z = 0.55T_{\text{BEC}}^{2\text{d}}$, in the ideal Bose gas and for $m\tilde{g}/\hbar^2 = 0.13$ according to mean-field theory, compared to quantum Monte Carlo simulations at $N = 10000$, and for ideal distinguishable particles (first term in eq. (16)). The inset shows the cycle weights π_k for the strictly two-dimensional and the quasi-two-dimensional ideal Bose gas, and for the quantum Monte Carlo simulations (from above).

and then by inverting eq. (10) to obtain $r(n)$ (thus $n(r)$) for the given \tilde{v} and $n\lambda^2$:

$$r(n\lambda^2, \tilde{v}) = \sqrt{\frac{2T}{m\omega^2} \left(\tilde{v} - \frac{mgn\lambda^2}{\pi\hbar^2} \right)}. \quad (15)$$

In fig. 2, we show the remarkable agreement of the quasi-two-dimensional mean-field profile with the one obtained by quantum Monte Carlo simulations as in ref. [11], for $N = 10000$ bosons for parameters $\tilde{\omega}_z = 0.55$, $t = T/T_{\text{BEC}}^{2\text{d}} = 1$, and $m\tilde{g}/\hbar^2 = 0.13$. The simulations take into account the full three-dimensional geometry, and particles interact via the three-dimensional s -wave scattering length a (see ref. [14] for a more detailed description of finite-temperature simulations of trapped Bose gases). Comparison with the ideal quasi-two-dimensional gas is also very favorable.

The mean-field density is extremely well represented by a sum of Gaussians,

$$n(r)\lambda^2 = \frac{\pi^2}{6t^2} \sum_{k=1}^N k\pi_k \exp \left[-\frac{m\omega^2(r\sqrt{k\beta})^2}{2} \right], \quad (16)$$

whose variances correspond to the density distribution of the harmonic oscillator at temperature $k\beta$. The prefactors in eq. (16) contain the cycle weights π_k . These weights give the probability of a particle to be in a cycle of length k in the path-integral representation of the Bose gas, where the density matrix must be symmetrized through a sum of permutations [15,16]. For the ideal Bose gas, the π_k are easily computed for any choice of the three-dimensional oscillator frequencies. Mean-field theory modifies these weights, without essentially changing the functional form of eq. (16). In the distinguishable-particle

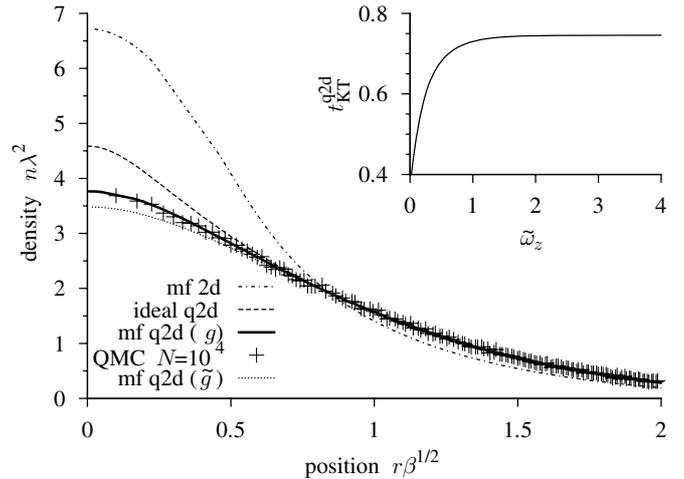


Fig. 3: Two-dimensional density profile $n(r = \sqrt{x^2 + y^2})\lambda^2$ at temperature $T = 0.8T_{\text{BEC}}^{2\text{d}}$ in a trap with $\omega_z = 0.55T_{\text{BEC}}^{2\text{d}}$, in the ideal Bose gas and for $m\tilde{g}/\hbar^2 = 0.13$ according to strictly two-dimensional and quasi-two-dimensional mean-field theory (using g and \tilde{g}), compared to quantum Monte Carlo simulations with $N = 10000$. The inset shows the Kosterlitz-Thouless temperature within modified mean-field theory as a function of $\tilde{\omega}_z$ (the strictly two-dimensional limit is $t_{\text{KT}}^{2\text{d}} = 0.745$ (from eq. (18)).

limit, at infinite temperature, only cycles of length $k = 1$ contribute ($\pi_1 = 1$), whereas the Bose-Einstein condensate is characterized through contributions of cycles of length $k \propto N$. The cycle weights π_k are shown in the inset of fig. 2 for small k . Only very short cycles contribute, and the density profile can thus be described by a very small number of Gaussians. The exact cycle-weight distribution of the quantum Monte Carlo calculation does not rigorously correspond to a profile as in eq. (16), although the corrections are negligible in our case.

Figure 3 considers the temperature $t = 0.8$ in the interval between the Kosterlitz-Thouless temperature of the quasi-two-dimensional interacting gas (at $t = t_{\text{KT}} \simeq 0.70$ for these parameters [11]) and the strictly two-dimensional Bose-Einstein condensation temperature. Again, the agreement of the quasi-two-dimensional mean field with the exact density profile obtained by quantum Monte Carlo calculation is remarkable. At this temperature, the deviations with the ideal quasi-two-dimensional profile and with the strictly two-dimensional mean field are important. To illustrate the temperature dependence of the effective interaction, we also show the mean-field profile computed with the zero-temperature interaction parameter \tilde{g} instead of the true effective two-dimensional interaction g (see eq. (11)). We note in this context that the difference in eq. (11) between g and \tilde{g} was determined under the condition that the interaction leaves the density distribution in z unchanged. Whenever this condition is violated, the density distribution in z must be computed by other means, as for example by quantum Monte Carlo methods (see [11]). The importance of changes of the

density profile in z in the low-temperature regime of a quasi-condensed Bose gas has already been pointed out in the context of spin-polarized hydrogen absorbed on helium surfaces [17].

Let us finally discuss the Kosterlitz-Thouless transition into the low-temperature phase, which is not contained in mean-field theory. The semiclassical quasi-two-dimensional gas does not Bose-condense because the particle number in eq. (12) diverges at $\tilde{\mu} = 0$ (it saturates at a finite value in the ideal Bose gas). This divergence is due to the logarithmic divergence of the central density (see eq. (13)). However, interaction effects beyond mean-field drive a Kosterlitz-Thouless phase transition [4] from the high-temperature normal phase to a superfluid one below T_{KT} .

As discussed previously [9,11], the Kosterlitz-Thouless transition occurs when the central density $n(0)\lambda^2$ reaches the critical value of the two-dimensional homogeneous gas, which has been determined numerically [18] for $g \rightarrow 0$:

$$n(0)\lambda^2 \simeq n_c\lambda^2 \simeq \log \frac{380\hbar^2}{mg}. \quad (17)$$

We can introduce (by hand) the concept of a critical density into mean-field theory by selecting among the solutions $t(\tilde{\mu})$ of eq. (14) the one satisfying eq. (17). For the interaction parameters used in ref. [11], $m\tilde{g}/\hbar^2 = 0.13$, we find a mean-field critical temperature $t_{\text{KT}}^{\text{q2d}} = T_{\text{KT}}^{\text{q2d}}/T_{\text{BEC}}^{\text{2d}} = 0.69$. This value is in excellent agreement with the Monte Carlo data. The inset of fig. 3 shows the variation of this mean-field critical temperature as a function of $\tilde{\omega}_z$ (for $m\tilde{g}/\hbar^2 = 0.13$).

The calculation of the mean-field critical temperature simplifies further in the strictly two-dimensional Bose gas, because the chemical potential in eq. (13) is then an explicit function of the critical density, and can be entered into eq. (12). With $\tilde{\mu}_c = \ln \{1 - \exp(-n_c\lambda^2)\} \simeq -mg/(380\hbar^2)$, and by again transforming the equation for N vs. central density into a relation between critical temperatures [9,11], we obtain

$$t_{\text{KT}}^{\text{2d}} = \frac{T_{\text{KT}}^{\text{2d}}}{T_{\text{BEC}}^{\text{2d}}} = \left[1 + \frac{3mg}{\pi^3\hbar^2} \left(\ln \frac{380\hbar^2}{mg} \right)^2 \right]^{-1/2}, \quad (18)$$

where we have neglected small corrections of order $\tilde{\mu}_c \log |\tilde{\mu}_c|$. The strictly two-dimensional limit $t_{\text{KT}}^{\text{2d}} = 0.745$ for $m\tilde{g}/\hbar^2 = 0.13$ agrees with the data shown in the inset of fig. 3 in the large $\tilde{\omega}_z$ limit.

In conclusion, we have considered in this letter the semiclassical description of the quasi-two-dimensional trapped Bose gas. We have compared this description with quantum Monte Carlo data and have shown that the density profiles are accurately reproduced in the normal phase down to the Kosterlitz-Thouless temperature. The thermal occupation of excited states in the out-of-plane direction quantitatively explains the large deviations of the density profiles from strictly two-dimensional mean-field theory, which was recently noticed in the experiment [8]. Originally, it was speculated that the

emerging almost-Gaussian density profiles could be attributed to effects beyond mean field [8,10]. However, even though the thermal occupation of the excited states in the tightly confined direction is clearly noticeable for the experimental parameters, the transition itself is still of the Kosterlitz-Thouless type as revealed by the experimental coherence patterns [5] and confirmed by numerical calculations of the algebraic decay of the condensate density with system size [11].

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