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Superfluid to normal phase transition in strongly correlated bosons in two dimensions

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Abstract. Using quantum Monte Carlo simulations, we investigate the finite-temperature phase diagram of hard-core bosons (XY model) in two-dimensional lattices. To determine the phase boundaries, we perform a finite-size-scaling analysis of the superfluid stiffness in two different ways and find that both approaches provide results of comparable accuracy. Furthermore, we discuss how such a phase diagram can be determined by measuring the occupancy of the zero momentum mode in homogeneous and trapped systems. The latter approach can be used in current experiments with ultracold gases.

1. Introduction

Systems of interacting bosons are of interest in a vast range of physical contexts such as in experiments with superfluid helium [1], Josephson-junction arrays [2], elementary excitations in magnetic insulators that can be understood as bosonic quasiparticles [3], and more recently in experiments with ultracold gases loaded in optical lattices [4, 5]. Specifically, the latter ones offer a unique opportunity to study models that are widely considered in statistical and condensed matter physics with unprecedented experimental control over the parameters which, in turn, determine the Hamiltonian describing such systems. The Bose-Hubbard model [6, 7] is perhaps the most successful example of such systems where the match between experiment and theory has been corroborated in widely diverse situations. More concretely, the Mott-insulator transition has been experimentally observed in such a model and in various effective dimensionalities [8, 9, 10, 11]. Despite the fact that it has received considerably less attention, the superfluid to normal transition in the Bose-Hubbard model has been realized in a two-dimensional lattice of Josephson-coupled Bose-Einstein condensates [12, 13], and in experiments with ultracold atoms in two- and three-dimensional optical lattices [14, 15].

One important aspect that determines the nature of the physical phases and their associated order parameters is the dimensionality d . Mermin, Wagner, and Hohenberg rigorously proved that at any nonzero temperature, continuous symmetries cannot be spontaneously broken in systems with sufficiently short-range interactions in dimensions $d \leq 2$ [16, 17]. This implies that, at finite temperature, Bose-Einstein condensation (BEC) cannot occur in one and two dimensions. Two-dimensional Bose systems, however, are marginal in the sense that fluctuations are strong enough to destroy the fully ordered state but are not so strong as to suppress superfluidity. Thus critical behavior develops in the Berezinskii-Kosterlitz-Thouless

(BKT) transition [18, 19], where a superfluid phase with quasi-long-range order competes with thermal fluctuations and induces a continuous phase transition to the normal fluid as the temperature is increased. It was found that the mechanism for the transition in two dimensions is markedly different from the usual finite-temperature phase transitions because it does not involve any spontaneous symmetry breaking. Kosterlitz and Thouless predicted that superfluid transition occurs through the formation of vortex-antivortex pairs in the quasi-long-range ordered superfluid phase that are instead free in the normal phase. Because of the absence of a local order parameter in the low-temperature phase and because of the essential singularity in the divergence of the correlation length, the numerical detection of the superfluid transition in two dimensions is very subtle. However, it was also predicted that in such a transition, the superfluid stiffness jumps from zero to a finite value at the critical temperature. Taking advantage of that observation, several approaches that measure the superfluid stiffness have been introduced. Since most numerical work is based on simulations of finite-sized clusters, several schemes, mainly based on the renormalization group theory of such transition, have been introduced in the literature in order to perform size-scaling analysis of the superfluid stiffness [20, 21, 22].

Our goal here is to focus on the superfluid to normal transition in a system of strongly interacting bosons in two-dimensional lattices. Specifically, we consider the Bose-Hubbard model in the limit of infinite on-site repulsion, i.e., the hard-core boson limit. By the use of exact quantum Monte Carlo simulations, we compute the finite-temperature phase diagram as a function of chemical potential. Accurate results are obtained through finite-size scaling of the the superfluid stiffness. To perform the finite-size scaling, we used two different but related schemes and we show that the results of both methods are consistent. Furthermore, we introduce and test a method to detect such transition that is based on the measurement of the zero-momentum occupation, which can be applied to both homogeneous and inhomogeneous systems. This method can be used in experiments with ultracold atoms even in the presence of unavoidable confining potentials that, in such setups, are needed in order to contain the gas. We note that, in the presence of a confining potential, domains of different phases can coexist in the trap both at zero [23, 24, 25] and finite [26, 27, 28, 29] temperature. A related and more extensive discussion on work discussed here, including an analysis of the three-dimensional case, can be found in Ref. [30].

The paper is organized as follows. In Sec. 2, we introduce the model and its phase diagram in two dimensions. Section 3 is devoted to the discussion of the techniques to obtain the phase boundaries. Finally, in Sec. 4, we draw our conclusions.

2. Model and phase diagram

We consider a system of hard-core bosons on a two-dimensional lattice with L^2 sites. The Hamiltonian can be written as

$$\hat{H} = -t \sum_{\langle i,j \rangle} \left(\hat{a}_i^\dagger \hat{a}_j + \text{H.c.} \right) - \mu \sum_i \hat{n}_i, \quad (1)$$

where $\hat{a}_i^\dagger$ ($\hat{a}_i$) is the boson creation (annihilation) operator at a given site i , and $\hat{n}_i = \hat{a}_i^\dagger \hat{a}_i$ is the particle number operator at site i . The hard-core boson creation and annihilation operators satisfy the constraint $\hat{a}_i^{\dagger 2} = \hat{a}_i^2 = 0$, which prohibit multiple occupancy of lattice sites. The first term in equation (1) is the kinetic energy, where t is the hopping amplitude between neighboring sites i and j ($\langle i, j \rangle$). The second term contains the chemical potential μ that controls the total number of particles in the system. In what follows, positions will be given in units of the lattice spacing a and the energy will be given in units of the hopping amplitude t .

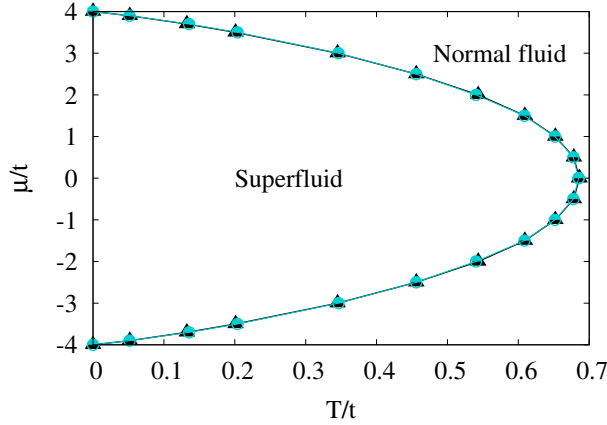


Figure 1. (Color online) Finite temperature phase diagram in two dimensions as obtained by two different size scaling procedures.

We recall that the Hamiltonian in equation (1) can be exactly mapped to the broadly studied quantum XY model [31]

$$\hat{H} = -2t \sum_{\langle i,j \rangle} \left(S_i^x S_j^x + S_i^y S_j^y \right) - \mu \sum_i S_i^z, \quad (2)$$

where S_i^α is the α th component of the spin-1/2 spin operator at site i . In the spin language, the term proportional to t describes a ferromagnetic exchange interaction, while the one proportional to μ describes a magnetic field in the z -direction.

We study the Hamiltonian in equation (1), at finite temperature T , by means of the stochastic series expansion (SSE) quantum Monte Carlo (QMC) method with operator-loop updates [32, 33, 34]. The determination of the phase diagrams is carried out through a finite size scaling of the superfluid stiffness ρ_s using periodic boundary conditions. The numerically exact (QMC) phase diagram in two dimensions (2D) is presented in figure 1. The finite-temperature phase diagram comprises a low-temperature quasi-ordered superfluid lobe surrounded by a high-temperature normal phase with exponentially decaying correlation functions. Specifics on the procedure to obtain the phase boundaries are discussed in the following section.

3. Superfluid to normal phase transition in two dimensions

3.1. Superfluid stiffness and the Kosterlitz-Thouless transition

Our results for the two-dimensional phase diagram in figure 1 are based on the fact that the model in equation (1) undergoes a BKT transition as a function of the temperature. This phase transition has been studied in great detail the context of the two-dimensional quantum XY model in equation (2) in the absence of a magnetic field [35, 36, 37, 21]. Kosterlitz and Thouless predicted that the superfluid stiffness ρ_s jumps from zero to the value $(2/\pi)T_c$ at the critical temperature. Thus, we consider measurements of the superfluid stiffness ρ_s for different system sizes L as a function of temperature. Within the SSE method, the superfluid stiffness is computed by measuring the fluctuations of the winding number W [38]; they are connected through the relation $\rho_s = \langle W^2 \rangle / 2\beta$, where $\beta = 1/T$ is the inverse temperature.

Figure 2(a) shows results for the superfluid stiffness of 2D hard-core bosons at $\mu = 0$ [or equivalently the spin stiffness of the 2D XY model in equation (2)] as a function of T for several system sizes. The observed slow approach of the superfluid stiffness to the characteristic jump expected for the infinite system is due to strong finite-size effects at the BKT transition. Finite-size scaling relations for the superfluid stiffness can be derived by integrating the Kosterlitz

renormalization-group equations [see, for instance, Refs. [21, 39, 20]. This procedure yields

$$\begin{aligned}\frac{\rho_s(T, L) \pi}{2T} - 1 &= c \coth 2c (\ln L + l_0), \quad T < T_c \\ \frac{\rho_s(T_c, L) \pi}{2T} - 1 &= \frac{1}{2 (\ln L + l_0)}, \quad T = T_c \\ \frac{\rho_s(T, L) \pi}{2T} - 1 &= c \cot 2c (\ln L + l_0), \quad T > T_c\end{aligned}\quad (3)$$

where c measures the distance from the critical point and l_0 depends only weakly on temperature. Close to the critical point $c \sim \sqrt{|T - T_c|}$. In the limit $2c (\ln L + l_0) \ll 1$, a scaling form for the superfluid stiffness based on equation (3) can be written as

$$\frac{\rho_s(T, L) \pi}{T} - 2 = \frac{1}{\ln L + l_0} F \left[(\ln L + l_0)^2 (T - T_c) \right]. \quad (4)$$

From equation (3) in the limit $2c (\ln L + l_0) \ll 1$, $F(x) = 1 - (4/3)x$. One can find the scaling function F and critical temperature T_c by computing $x_L = (\ln L + l_0)^2 (T - T_c) / t$ and $y_L = \rho_s(T, L) \pi / T - 2$ based on our Monte Carlo simulations for different L and T . The adjustment of the constant l_0 and critical temperature T_c , such that the data produce the best possible collapse, yields a numerical estimate of the scaling function F and the critical temperature itself. The result of the determination of the scaling function F is reported in figure 2(b), where a plot of y_L as a function of x_L is presented. Notice that, as expected, the value of F is very close to one for $x_L = 0$ and that the function is, to a very good approximation, a straight line with negative slope similar to $4/3$. Our result $T_c/t = 0.685 \pm 0.001$ is consistent with the best value reported in Ref. [21], for which $T_c/t = 0.6846 \pm 0.0006$. An analogous procedure to the one just described is carried out for different values of the chemical potential to complete the two-dimensional phase diagram in figure 1 (drawn with green empty circles).

Based on the relations in equation (3) at the critical temperature, one can also use the following scaling Ansatz for the superfluid stiffness as a function of system size and temperature [22]

$$\rho_s(T, L) = \left(1 + \frac{1}{2 [\ln L + l_0]} \right) F'(\xi/L), \quad (5)$$

which is expected to be a good approximation in the vicinity of the critical temperature $T \rightarrow T_c^+$. When dealing with equation (5), we assume the essential singularity of the correlation length $\xi \sim e^{b/(T-T_c)^{1/2}}$, where b is a chemical-potential dependent scaling factor. [Note that equation (5) is, strictly speaking, inconsistent with renormalization-group arguments, which lead to equation (4).] F' is a scaling function that, after taking the logarithm of the argument, can be replaced by another function f . Hence, equation (5) can be written as

$$\rho_s(T, L)^* = f(x'_L), \quad (6)$$

where $x'_L = \ln L - b/(T - T_c)^{1/2}$ and $\rho_s(T, L)^* = \rho_s(T, L) \left(1 + \frac{1}{2 [\ln L + l_0]} \right)^{-1}$. The scaling hypothesis in equation (6) is consistent with the fact that the rescaled superfluid stiffness $\rho_s(T, L)^*$ becomes system-size independent at the critical temperature where the correlation length diverges. The scaling function f can be obtained numerically by finding the constants b and c , as well as the critical temperature T_c , that produce the best possible collapse of the data in the normal phase where the correlation length is finite. The result of the estimation of the scaling function f is portrayed in figure 2(c), where a plot of the rescaled superfluid stiffness as a function of x'_L is presented. As expected, the data is seen to coalesce to a unique curve

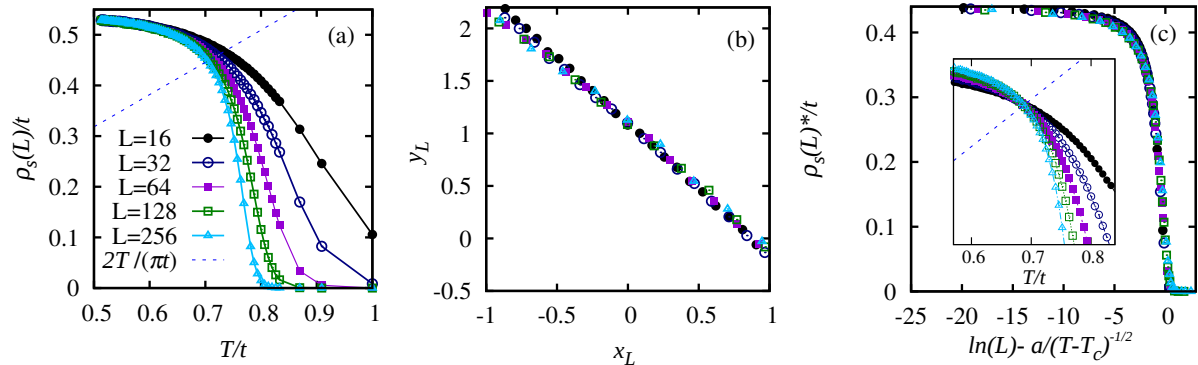


Figure 2. (Color online) (a) Superfluid stiffness for $\mu = 0$ and several values of L . The error bars (not shown) are smaller than the point size used in the plot. (b) Data collapse according to the relation in equation (4). (c) Numerical determination of the scaling function f based on equation (6). The inset in (c) shows the rescaled superfluid stiffness vs T .

representing $f(x'_L)$, which makes apparent the relevance of the scaling relation in equation (6) to the region close to the critical point. As argued before, one expects from equations (3) and (5) that a plot of the rescaled superfluid stiffness $\rho_s(T, L)^*$ as a function of the temperature T should become system-size independent at the critical temperature T_c . This observation is confirmed in the inset of figure 2(c). Remarkably, those curves intersect with the line $(2/\pi)T$ right at the critical temperature, in agreement with the BKT scenario. Our result $T_c/t = 0.687 \pm 0.002$ is again consistent with the values reported in Ref. [21] and with the value obtained through equation (4). This procedure is carried out for different values of the chemical potential to complete the two-dimensional phase diagram in figure 1 (green empty dots). Note that, in figure 1, the two scaling procedures lead to almost identical phase diagrams.

Finally, we should mention that equation (3) predicts the value of the superfluid stiffness in an infinite system at the critical temperature to be $\rho_s(T_c)/T_c = 2/\pi$. However, in Ref. [40], it was shown that the superfluid stiffness at the transition temperature is $\rho_s(T_c)/T_c \simeq 0.63650$, which is very close (and indistinguishable within the present study) to the result based on equation (3) [$2/\pi \simeq 0.63662$].

3.2. Zero-momentum occupation and trapped systems

We now turn our attention to the behavior of the occupation of the zero momentum state [$n_{k=0} \equiv n_0$] in the critical region, and address the determination of the transition temperature from it. As mentioned in the introduction, thermal fluctuations in two dimensions prevent the emergence of a Bose-Einstein condensate, which means that the zero-momentum occupation is not macroscopic. Nevertheless, as the critical temperature is approached from the normal phase, n_0 diverges [see figure 3(a)]. From the Fourier transform of the one-body density matrix in the long-distance limit $\langle \hat{a}_i^\dagger \hat{a}_{i+r} \rangle \propto r^{-1/4} \exp(-r/\xi)$, one can precisely understand the way n_0 diverges as T_c is approached,

$$n_0 \sim \xi^{7/4}. \quad (7)$$

From equation (7), it follows that not only does n_0 diverge at T_c , but also its derivative with respect to T does,

$$\frac{dn_0}{dT} \sim -\frac{\xi^{7/4} \ln^3 \xi}{b^2} \quad (8)$$

In finite clusters, however, when T is close to T_c , the role of the correlation length is taken over by L when $\xi \gtrsim L$. This occurs at a temperature $T^*(L)$ determined by the critical temperature

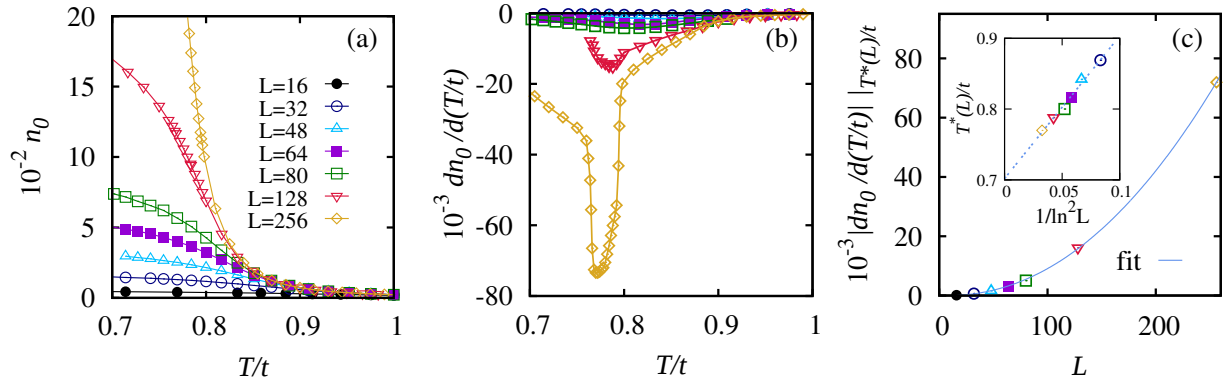


Figure 3. (Color online) (a) Zero-momentum occupation n_0 vs T . (b) Derivative of the zero-momentum occupation n_0 with respect to the temperature for different values of L . (c) Finite-size scaling of the height of the negative peak in dn_0/dT . The continuous line is a fit to the function $g(L) = a_0 + a_1 L^{7/4} \ln^3(a_2 L)$. The inset shows the finite-size scaling of $T^*(L)$.

and the size of the system under consideration, it is given by

$$T^*(L) = T_c + b'/\ln^2 L, \quad (9)$$

where b' is a related to b . At that temperature, the derivative in equation (8) scales with the system size as

$$\left. \frac{dn_0}{dT} \right|_{T^*(L)} \sim -\frac{L^{7/4} \ln^3 L}{b^2}. \quad (10)$$

Below $T^*(L)$, n_0 cannot vary as fast as right above $T^*(L)$ because the exponential increase of the correlation length is truncated by L . Below $T^*(L)$, the variation of n_0 comes mainly from the temperature dependence of the anomalous exponent, which is not as strong as the variation due to the exponential behavior of the correlation length. Accordingly, dn_0/dT should exhibit a sharp minimum at the size-dependent temperature $T^*(L)$. Additionally, in a finite system, n_0 cannot grow indefinitely as the temperature is reduced. In the limit $T \rightarrow 0$, n_0 must come closer to its (finite) $T = 0$ value, which implies that the derivative with respect to temperature should eventually vanish for any given finite cluster.

Figure 3(b) shows the derivative of the n_0 for different system sizes as a function of T . The divergence of dn_0/dT is clearly observed. A sharp minimum develops and its location $T^*(L)$ approaches T_c as the system size increases. This is expected from the finite-size relation in equation (9). The scaling of the height of this minimum is studied in figure 3(c), where we plot the absolute value of $dn_0/dT|_{T^*(L)}$ vs L . The data follows the scaling relation in equation (10), as made evident by a fit to the function $g(L) = a_0 + a_1 L^{7/4} \ln^3(a_2 L)$. In the inset in figure 3(c), we show the finite-size scaling of $T^*(L)$. We observe that $T^*(L)$ is consistent with the scaling relation in equation (9), which we use to obtain the critical temperature in the thermodynamic limit. We find $T_c/t = 0.701 \pm 0.007$. This value is compatible with the one found by performing the finite-size scaling of the superfluid stiffness. While this approach is obviously less accurate than the one discussed before for ρ_s , among other things because a numerical derivative is involved, the fact that it works very well is important for current trapped ultracold gases experiments where n_0 can be measured while the superfluid density cannot.

If an additional confining potential is added to the system, the reasoning we have just presented remains valid. The effect of the confining potential can be taken into account by replacing the second term in equation (1) with a spatially varying chemical potential as

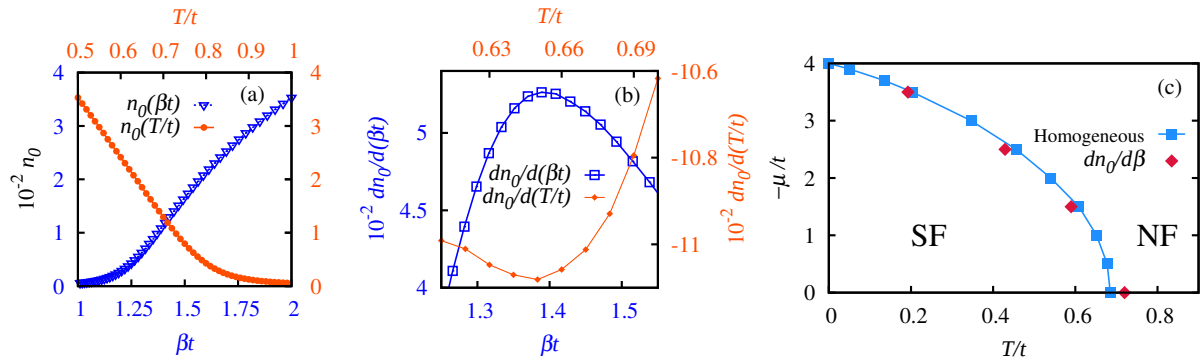


Figure 4. (Color online) (a) n_0 as a function of T and β in a trapped 2D system with $V_0/t = 0.00125$, $\mu = 0$ in the center of the trap, and $L = 128$. (b) Derivatives of n_0 with respect to β and with respect to T . (c) Estimate of the critical points based on the derivative of the zero-momentum occupation with respect to β (red diamonds based on a system with $L = 128$). The phase diagram of the homogeneous system is also shown for comparison.

$\mu \sum_i \hat{n}_i \rightarrow \sum_i \mu_i \hat{n}_i$. Here, $\mu_i = \mu - V_0 r_i^2$, where V_0 quantifies the strength of the harmonic potential and μ plays the role of the overall chemical potential. At fixed chemical potential ($\mu \leq 0$), when lowering T , the normal-to-superfluid crossover in the trapped system proceeds through the appearance and enlargement of a superfluid region in the center of the trap. Hence, the zero-momentum state becomes increasingly populated. Exactly as it was argued for finite homogeneous systems, it is expected that as $T \rightarrow T_c^+$ for the normal-to-superfluid transition in the center of the system, the rate of growth of n_0 will increase. Below T_c , on the other hand, dn_0/dT will eventually decrease because of the finite extend of the system imposed by the confining potential. If T is lowered well below T_c , almost the entire system will become superfluid and the observables will saturate their (finite) zero-temperature values. This means that the derivative dn_0/dT is expected to exhibit a minimum very close to the critical temperature.

Therefore, a similar approach to detect criticality can be utilized in confined systems. Provided that the trapping potential is weak enough, the accuracy of the estimations based on trapped systems should be comparable with the accuracy obtained in the homogeneous case. Figure 4(a) depicts the evolution of n_0 vs T , as well as vs the inverse temperature β , for a harmonically confined 2D system with $V_0/t = 0.0015$ ($L = 128$) and $\mu = 0$ in the center of the trap. In figure 4(b), we show dn_0/dT which, as expected, exhibits a minimum located at $T/t = 0.66 \pm 0.02$. This temperature is compatible with the value of T_c/t obtained for the homogeneous case where, after a finite-size scaling, we obtained $T_c/t = 0.685 \pm 0.001$. Our estimate derived from the study of a single trapped system is about 4% off the value of the homogeneous system.

The same analysis based on measurements of n_0 , but now as a function of the inverse temperature β , can be carried out; in that case, one expects a maximum in the derivative $dn_0/d\beta$ instead of a minimum. Generally, for finite and not very large systems, the position of such maximum β_c will not coincide with $1/T_c$ obtained from the minimum of dn_0/dT [30]. Overall, we find that, for the system sizes available to our QMC simulations, the analysis based on $dn_0/d\beta$ provides more accurate estimates of the critical temperature than the one based on dn_0/dT . This follows from the fact that, the maximum found in $dn_0/d\beta$ is consistently sharper and better defined when compared to the minimum found for dn_0/dT , which instead is shallower and broader, thus leading to results with lower accuracy. Based on measurements of $dn_0/d\beta$ presented in figure 4(b) on the same system with $V_0/t = 0.0015$ ($L = 128$), $\mu = 0$, we find $T_c/t = 0.72 \pm 0.02$. This value is also very close to the critical temperature of the homogeneous

system. When the maximum is sharply defined, in the limit of very shallow traps with large numbers of bosons, the two approaches should coincide (i.e., their difference is due to finite size effects) [30]. Therefore, for the determination of the phase diagram based on measurements in harmonically confined systems, we consider only measurements based on $dn_0/d\beta$.

In figure 4(c), we summarize our results for the determination of the critical parameters with the derivative of the zero-momentum occupation with respect to β , and contrast them with the phase diagram of the homogeneous system. In spite of the small differences and the fact that the peaks in $dn_0/d\beta$ are shallower than those of the homogeneous system, the agreement in the calculations of the phase diagram based on both the homogeneous and the trapped systems is remarkably good. We mention that at the tip of the superfluid lobe, where the size effects are expected to be the strongest, we observed that as the size of the system is increased (or the strength of the trap is decreased), keeping constant the chemical potential in the center of the trap, the estimate of the critical temperature decreases approaching the result in homogeneous systems.

4. Conclusions

We have presented a detailed study of the finite temperature phase diagram of strongly correlated bosons in the hard-core limit (or the XY model) in two dimensions. The critical parameters were determined through a finite-size scaling analysis of the superfluid stiffness. Two methods to determine the critical temperature have been used. The first method follows directly from the integration of the Kosterlitz-Thouless renormalization group equations while the second one is based on an Ansatz that is justified only in the vicinity of the critical temperature. The validity of the second method has been, nevertheless, empirically confirmed by the quality of the collapse obtained in our analysis. Both methods provided results with comparable accuracy and the phase diagrams obtained are consistent with each other.

We introduced an approach to estimate the critical temperature from measurements of n_0 in finite systems. It makes use of the behavior of the derivative dn_0/dT and we derived finite-size scaling relations that can be used to extrapolate the results to the thermodynamic limit. This approach can be applied to systems that exhibit a diverging zero-momentum occupation in any dimension, irrespective of the universality class to which the transition belongs to. When an additional confining potential is introduced, we considered measurements of the critical temperature based on measurements of the zero-momentum occupation, out of which we obtained a phase diagram that is in good agreement with the homogeneous counterpart.

Acknowledgments

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