Universal scaling of three-dimensional bosonic gases in a trapping potential

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We investigate the critical properties of cold bosonic gases in three dimensions, confined by an external quadratic potential coupled to the particle density, and realistically described by the Bose-Hubbard (BH) model. The trapping potential is often included in experiments with cold atoms and modifies the critical finite-size scaling of the homogeneous system in a non trivial way. The trap-size scaling (TSS) theory accounts for this effect through the exponent $\theta$.

We perform extensive simulations of the BH model at the critical temperature, in the presence of harmonic traps. We find that the TSS predictions are universal once we account for the effective way in which the trap locally modifies the chemical potential $\mu$ of the system. The trap exponent for the BH model at $\mu = 0$ is the one corresponding to an effective quartic potential. At positive $\mu$, evidence suggests that TSS breaks down sufficiently far from the centre of the trap, as the system encounters an effective phase boundary.

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I. INTRODUCTION

A key aspect of the theory of critical phenomena is universality: the relevant properties of physical systems at criticality depend only on some global features, such as the dimensionality and the invariance symmetries of the underlying Hamiltonian, while the microscopic details of the interaction play no role to this end. The different physical systems can then be catalogued into universality classes, according to their critical behaviour. Consequently, models in the same class share the values of the critical exponents, as well as the shape of scaling functions. Moreover, simplified theoretical models have predictive power on the universal properties of complex experimental systems, as long as they fall in the same universality class.

In recent years, thanks to the great improvements in the experimental capabilities of handling ultra-cold atoms, it has become possible to create many-body systems which quite closely realise the theoretical models commonly studied in condensed matter physics. In particular, cooling techniques and optical lattices led to the experimental observation of the Bose-Einstein condensation (BEC) and of the superfluid to Mott-insulator transition, in the language of the renormalisation group (RG) theory, it constitutes a new relevant field, to which the trapping interaction must be added. In this framework, the trap modifies the critical behaviour of the gas: most notably, the correlation length $\xi$, which usually diverges at phase transitions, is bound to remain finite by the confining potential, so that the (homogeneous) phase transition gets suppressed in the (inhomogeneous) real system. Only in the limit $v \to 0$, in which the trap is switched off, a true phase transition is expected to be seen.

It is then evident that a correct modelling of the experimental setup must include the effect of the confinement and, to this end, the trapping interaction must be added to the fundamental Hamiltonian of the systems under investigation. Since this interaction rules out the phase transition, in the presence of a trap is the trap-size scaling (TSS) theory. In this framework, the

$$V(\mathbf{r}) = v^p \rho^p,$$

where the parameter $v$ is related to the strength of the confinement and $p$ is a positive integer. Generally, parabolic traps are used ($p = 2$). The presence of the trap modifies the critical behaviour of the gas: most notably, the correlation length $\xi$, which usually diverges at phase transitions, is bound to remain finite by the confining potential, so that the (homogeneous) phase transition gets suppressed in the (inhomogeneous) real system. Only in the limit $v \to 0$, in which the trap is switched off, a true phase transition is expected to be seen.

The Bose-Hubbard (BH) model provides a realistic description for these experimental systems. It is defined by the Hamiltonian

$$H_{BH} = -\frac{J}{2} \sum_{(xy)} \left( b_{x,y}^{\dagger} b_{y,x} + b_{y,x}^{\dagger} b_{x,y} \right) - \mu \sum_{x} n_x + \frac{U}{2} \sum_{x} n_x(n_x - 1),$$

where $n_x = b_{x,x}^{\dagger} b_{x,x}$ is the particle density operator, $b_{x,y}^{\dagger}$ is the bosonic creation operator and $(xy)$ indicates nearest neighbour sites on a cubic lattice. The chemical potential $\mu$ acts as a control parameter coupled to the particle density and $U > 0$ is the strength of the contact repulsion between particles. In the following, we take the hard-core (HC) limit $U \to \infty$. In this way the local particle number operator is restricted to the values $\{0, 1\}$ only.

In the spirit of universality, this change only affects the strength of the interaction among atoms, and it is not expected to change the universal behaviour of the model near phase transitions.

The theory of phase transitions generally applies to homogeneous systems in the thermodynamic limit, so that the comparison with experiments may not be immediate. In particular current experiments almost always include a trapping potential to keep the atoms confined on a limited region of the optical lattice. The shape of the trap is usually well approximated by a power-law profile of the form

$$V(\mathbf{r}) = v^p \rho^p,$$
We discuss the main results of the present work. The distance from the centre of the trap increases in the direction of the arrow. Notice how the line (b) crosses the phase boundary at $\mu = -2$. The dashed lines represent the local effective potential which belongs to the homogeneous 3D XY universality class, in the HC limit and at the finite-temperature phase transition from a normal fluid to a superfluid (see phase diagram in Fig. [1]). The physical problem we want to analyse in this paper concerns the issue of the universality of the modified critical behaviour. Following the RG ideas, we expect that the critical properties of trapped systems, summarised in the exponent $\theta$, depend only on some global and general features, such as the way the potential is coupled to the critical modes of the unconfined system, the shape of the potential and the homogeneous universality class. To this end, we analyse the three-dimensional (3D) BH model, which belongs to the homogeneous 3D XY universality class, in the HC limit and at the finite-temperature phase transition from a normal fluid to a superfluid (see phase diagram in Fig. [1]). The order parameter of this transition is the phase of the condensate wave function, which is related to superfluid density. The critical exponents for this transition are $\nu = 0.6717(1)$ and $\eta = 0.0381(2)$.

We recall that phase transitions at $\mu = 0$ are driven by quantum fluctuations, whose ultimate origin is the Heisenberg uncertainty principle. On the other hand, finite-$T$ transitions are always classical in nature: the occupation number of the states corresponding to the critical modes diverges, so that classical statistics may apply. The universality class of the $U(1)$-invariant quantum BH model at finite-$T$ is then the one of the classical XY model.

When the confining potential is turned on, we consider the full system Hamiltonian

$$H = H_{\text{BH}} + \sum_x V(x)n_x,$$

where the trapping potential is coupled to the particle density. A standard RG analysis within the TSS framework leads to the result

$$\theta(p) = \frac{p\nu}{1 + p\nu},$$

for the relevant critical exponent $\theta$. The TSS of the 3D HC BH model has been investigated in Ref. [12] for the range $-3 < \mu < 0$. At $\mu = -2$ it was found $T_c = 0.7410(1)$ and the scaling functions of the microscopic degrees of freedom are ruled by the exponent $\theta = 0.57327(4)$, which was obtained from the basic RG prediction [3] using the known value of $\nu$ from Ref. [11]. In a recent work on the 2D HC BH model [13], we proposed that the universal critical features of phase transitions in a trapped system do not only depend on the bare shape of the confining potential but also on the particular way in which the trap locally modifies the control parameter $\mu$. The actual local phase space position of the system can then be tracked by means of an effective chemical potential $\mu_{\text{eff}}(r)$. In the following we show that the TSS scaling of the 3D HC BH model for a chemical potential $\mu \neq 0$ follows the standard $\theta(p)$ behaviour whereas the correct scaling at $\mu = 0$ is given by $\theta(2p)$. Furthermore, the scaling functions are different depending on the sign of the chemical potential. In particular, in the $\mu > 0$ conditions, the system falls in an effective superfluid phase up to a distance $r_{\text{bd}}$ from the centre of the trap, at which TSS breaks down.

The paper is organised as follows. For the study of criticality in the presence of a trap, a very precise determination of the homogeneous parameters at the phase transition point is needed. This is because we want to analyse the emergence of the known homogeneous behaviour in the limit $l \to \infty$ which removes the trap. The measurement of the transition temperature at $\mu = 0$ is reported in detail in Sec. [II]. In Sec. [III] we examine the model in the presence of the external trapping potential: we verify our findings by performing a trap-size scaling (TSS) analysis of the correlation function and a finite-size trap-size scaling (FTSS) study of suitable observables, both at zero chemical potential and for the $\mu > 0$ case. Finally, in Sec. [IV] we discuss the main results of the present work and draw our conclusions.

II. HOMOGENEOUS SYSTEM

In order to perform a detailed FSS analysis of the homogeneous model and determine its critical temperature, we consider the helicity modulus $\Upsilon$ and the second moment correlation length $\xi$. 

![Figure 1: (Colour online) A qualitative sketch of the phase diagram of the three-dimensional hard-core Bose-Hubbard model.](image-url)
The helicity modulus $\Upsilon$ is defined as

$$\Upsilon \equiv -\frac{1}{L} \frac{\partial^2 Z(\phi)}{\partial \phi^2} \bigg|_{\phi=0},$$

(6)

where $Z$ is the partition function under a twist $\phi$ of the boundary conditions in one direction. In our QMC simulations the quantity $\Upsilon$ is simply related to the linear winding number $W$ through the relation

$$\Upsilon = \frac{(W^2)}{L}.$$  

(7)

The two-points Green function $G_b(x,y)$ is defined as

$$G_b(x,y) = \langle b^\dagger_x b_y \rangle.$$  

(8)

The homogeneous system with periodic boundary conditions is translation invariant, so that the Green function only depends on the separation $r = x - y$ between the two points. We can thus restrict the study to $G_b(r) \equiv G_b(\mathbf{r}, 0)$. Finally, we denote the lattice Fourier transform of $G_b(r)$ as $\tilde{G}_b(p)$. The second moment correlation length $\xi$ is then defined as

$$\xi^2 \equiv \frac{1}{4 \sin^2(\pi/L)} \frac{\tilde{G}_b(0) - \tilde{G}_b(p)}{\tilde{G}_b(p)},$$

(9)

where $p = (2\pi/L, 0, 0)$.

The quantities $R_\Upsilon = Y L$ and $R_\xi = \xi/L$ are dimensionless and RG invariants. For small $\tau \equiv T/T_c - 1$, they follow the universal scaling relation

$$R = f(\tau L^{1/\nu}) + L^{-\omega} f_\omega(\tau L^{1/\nu}).$$

(10)

A. FSS analysis for the homogeneous system

We performed quantum Monte Carlo (QMC) simulations of the 3D HC BH model, for lattice sizes up to $L = 32$. Within the stochastic series expansion framework, we use the directed operator-loop algorithm. More details on our implementation of the QMC can be found in Refs. 19,20. Our simulations for the homogeneous system are approximately $4 \times 10^6$ Monte Carlo steps (MCS) long. We decorrelated the data by applying the blocking method and the errors are calculated through a jackknife analysis. For a discussion of the self-correlation times of the data, see Appendix A.

Close to the asymptotic regime, Eq. (10) can be expanded as a Taylor series about $\tau = 0$:

$$R = R^* + \sum_{i=1}^n a_i \tau^i L^{i/\nu} + L^{-\omega} \sum_{j=0}^m b_j \tau^j L^{j/\nu}.$$  

(11)

The asymptotic values for the helicity modulus and the correlation length are known from previous works.

$$R_\Upsilon^* = 0.516(1), \quad R_\xi^* = 0.5924(4).$$

(12)

Figure 2: (Colour online) Estimates of $T_c$ obtained from the FSS analysis of $R_\Upsilon$ and $R_\xi$, considering data with $L \geq L_{\text{min}}$. as the exponents $\nu$ and $\omega$,

$$\nu = 0.6717(1), \quad \omega = 0.785(20).$$  

(13)

The data for $R_\Upsilon$ and $R_\xi$ at different $L$ and $T$ can then be fitted against the first few terms of this expansions. The optimal number of terms to use in the fit (i.e. $m$ and $n$ in Eq. (11) is determined by progressively adding more terms to the series and looking for the stabilisation of the fit parameters and to when the residuals start degrade. Residual corrections to scaling are assessed by repeating the fit discarding the data for lattice sizes $L < L_{\text{min}}$ while progressively increasing $L_{\text{min}}$.

For the fit of $R_\Upsilon$ data, we found optimal to use $n = 1$ and $m = 0$, while the analysis of $R_\xi$ requires higher order corrections $O(L^{-2\omega})$. The data used in the analyses was chosen in a self-consistent way, by only retaining the data points satisfying

$$|R/R^* - 1| \leq 0.1.$$  

(14)

The limit of 10% deviation from the asymptotic value in the formula above was set by requiring that the $\chi^2$ be acceptable. The results of the fits on $R_\Upsilon$ and $R_\xi$ are reported in Table 1 and plotted in Fig. 2. The scaling ansatz of Eq. (11) accurately accounts for subleading corrections to scaling. This, together with the self-consistent choice of the fitting window, Eq. (14) allows us to obtain a precise estimate of the critical temperature with simulation data on relatively small lattice sizes.

The analyses on both observables converge to a common value. Our final estimate for the critical temperature of the 3D HC BH model at $\mu = 0$ is

$$T_c^{(\mu=0)} = 1.00801(4).$$  

(15)

We consider the value of $T_c$ extracted from the fit on $R_\Upsilon$ to be more reliable, due to the stability of the observable and to the residual $\chi^2$ obtained. The results
from $R_c$ are a cross-check and we use them to better estimate the error on $T_c$. The latter must also take into account the uncertainties on the other parameters entering in Eq. 11, namely those reported in Eqs. 12 and 13. A standard bootstrap analysis shows that the error introduced by these quantities is not negligible, yet it decreases for increasing lattice size. For the fits on $R_T$ (resp. $R_c$) data and lattice sizes $L \geq 10$ this error ranges between $1.5 \times 10^{-5}$ (resp. $0.5 \div 0.3 \times 10^{-5}$). The quoted error $\Delta T_c = 4 \times 10^{-5}$ accounts for all of these effects.

Our value of $T_c$ agrees with the previous estimates of Ref. 21 and Ref. 22, quoting respectively $T_c = 1.008(3)$ and $T_c = 1.00835(25)$.

### III. TRAPPED SYSTEM

The question we want to address in this paper is related to the universality of the TSS theory. The trap exponent $\theta$ depends on the power $p$ of the trapping potential, cf. Eq. 2. We suggested in Ref. 13 that the trap exponent $\theta$ predicted by TSS is indeed universal throughout the 3D XY universality class. However, the particular shape of the BH phase diagram leads to a modified TSS behaviour when $\mu = 0$. In this condition, the trap exponent is the one corresponding to a trapping potential of power $2p$.

We recall that the trap-size limit is defined as the limit in which $r, l \to \infty$ while keeping the ratio $\zeta = r/l^{1-\theta}$ fixed. In this limit the argument of the trapping potential $r/l = \zeta/l^{1-\theta}$ vanishes, since $\theta < 1$, so that only the short range behaviour is relevant for the scaling features of the model.

The trapping potential couples to the density operator, and can thus be thought as a local effective chemical potential

$$\mu_{\text{eff}}(r) = \mu - V(r).$$

Calling $T_c(\mu)$ the critical temperature of the inhomogeneous system, we can define an effective temperature $T_{\text{eff}}(r) \equiv T_c(\mu_{\text{eff}}(r))$. This is the temperature at the phase transition of a homogeneous system whose chemical potential is set to the value of $\mu_{\text{eff}}$ at site $r$ of the inhomogeneous system. We argue that the critical modes of the inhomogeneous system can be described by means of the local control parameter

$$\tau_{\text{eff}}(\mu, r) \equiv T_c(\mu) - T_{\text{eff}}(r).$$

One should keep in mind that the system is considered at equilibrium at the critical temperature. Here $\tau_{\text{eff}}$ should be considered as an effective distance from the phase boundary, much in the same way as is $\tau$ [defined before Eq. 17]. However, $\tau$ bears a precise physical meaning, whereas $\tau_{\text{eff}}$ is only a practical tool to describe the trapped critical behaviour.

Recalling that in the trap-size limit only the short-$r$ behaviour of the trapping potential is relevant, we can expand the function $T_{\text{eff}}$ in Eq. 17 around $\mu$, obtaining the general expression

$$\tau_{\text{eff}}(\mu, r) \approx T_c'(\mu)V(r) - \frac{1}{2}T_c''(\mu)V(r)^2.$$  

For $\mu \neq 0$, the first term, of order $r^p$, dominates the expansion. We then expect the TSS behaviour of the 3D BH to agree with that of the trapped 3D XY universality class with the same trapping exponent $\theta(p)$. However, for $\mu = 0$, the phase diagram of Fig. 1 tells us that the first derivative vanishes, and the second term, of order $r^{2p}$, becomes dominant. For this reason we expect that, at $\mu = 0$, the critical behaviour be ruled by the exponent

$$\theta(2p) = \frac{2p\nu}{1 + 2p\nu},$$

i.e., the system behaves as a classical 3D XY model trapped by a potential $U \sim r^q$ with exponent $q = 2p$.

In the presence of a trapping potential, the translational invariance is broken. Due to the spherical symmetry of the potential, it is then natural to replace the two-point function $G_b$ with the correlation function with respect to the centre of the trap,

$$G_b(0, r) \equiv \langle b^\dagger_0 b_r \rangle \approx l^{-(1+\eta)\theta} G_b(r l^{-\theta_\eta} r^{(1+\eta)/2}).$$

where $G_b$ is a universal function. The inhomogeneous susceptibility is defined as

$$\chi_t = \sum_x G_b(0, x)$$

and the second moment correlation length as

$$\xi_t^2 \equiv \frac{1}{6\chi_t} \sum_x |x|^2 G_b(0, x).$$

Note that $\chi_t$ is related only to the integral of the correlation with the centre of the trap, and thus differs from the usual definition of the susceptibility for the homogeneous system.

In our simulations of trapped systems, the trap is enclosed within a hard walled cubic box. The size of the

| $L_{\text{min}}$ | $T_c^{(T)}$ | $\chi_{\text{isol}}^{(T)}$ [dof] | $T_c^{(\xi)}$ | $\chi_{\text{isol}}^{(\xi)}$ [dof] |
|---|---|---|---|---|
| 5 | 1.007984(4) | 8.5[31] | 1.007980(6) | 2.9[39] |
| 6 | 1.008001(4) | 2.4[27] | 1.007975(6) | 2.1[34] |
| 8 | 1.008008(5) | 1.8[23] | 1.007972(8) | 2.1[29] |
| 10 | 1.008015(5) | 1.8[19] | 1.007978(1) | 2.2[24] |
| 12 | 1.008015(6) | 1.8[15] | 1.007980(1) | 2.2[19] |
| 16 | 1.008021(7) | 1.7[11] | 1.008002(2) | 2.8[14] |
| 20 | 1.008027(9) | 1.9[7] | 1.007995(5) | 1.6[7] |
| 24 | 1.008010(1) | 1.2[3] | – | – |
Figure 3: (Colour online) Scaling at $\mu = 0$ and $T = T_c^{\mu=0}$ of the two-point function between the centre of the trap and points at distance $r$. The exponents $\theta_1$ (top) and $\theta_2$ (bottom) are used. The homogeneous scaling (dashed line) holds close to the centre of the trap.

Figure 4: (Colour online) Finite-size trap-size scaling at $\mu = 0$ and $T = T_c^{\mu=0}$ for $\xi_t/L$ (top) and saturation curve of $\xi_t$ (bottom).

Box $L$ is always an odd integer, so that the centre of the trap falls exactly on top of the central site of the cubic box. The size of the trap $l$ and that of the box $L$ both affect the critical properties of the system, requiring a simultaneous finite-size and trap-size analysis. The following behaviours for the correlation length and the susceptibility are expected:

$$\xi_t = LR(\tau^{\theta_0/\nu}, L/l^{\theta_0}), \quad \chi_t = L^{2-\eta}\mathcal{X}(\tau^{\theta_0/\nu}, L/l^{\theta_0}). \quad (23)$$

As discussed above, the exponent $\theta$ in these equations is

$$\theta_2 \equiv \theta(2) = 0.57327(4) \quad \text{at } \mu \neq 0, \quad (24)$$

$$\theta_4 \equiv \theta(4) = 0.72876(3) \quad \text{at } \mu = 0. \quad (25)$$

A. TSS at $\mu = 0$

We simulated the model at $\mu = 0$ and at the homogeneous critical temperature of Eq. (15) for different trap sizes $l$ and lattice sizes $L$. In the asymptotic condition $L \gg l^{\theta_0}$ it is possible to perform a pure TSS study of the two-point correlation function $G_b(r)$. The latter is a standard physical observable where it is possible to check the validity of our reasoning. In Figure 3 we plot the data for $G_b(r)$ using the TSS ansatz (20), in which we set $\tau = 0$. The data were generated keeping $L/l^{\theta_0} \approx 7$ (justified below) and runs of approximately $(0.6 \div 1) \times 10^6$ MCS were used. Here and below, the analysis method is analogous to the one used in the homogeneous case discussed in Sec. II, as are the considerations related to self-correlation times. Notice that, for $r \to 0$, the trap is locally flat, hence we expect to recover the homogeneous scaling, while only for $r > l^{\theta_0}$ does the effect of the trap becomes evident. In this region, the rescaling of the correlation function plotted in Fig. 3 nicely supports the scaling with exponent $\theta_4$ (top panel) against $\theta_2$ (bottom).

To further check our scaling predictions, in Figures 4-5 we show the FTSS analyses. The data presented in these figures come from QMC runs approximately $2 \times 10^5$ MCS long. Figure 4-(top panel) shows the rescaling of $\xi_t/L$: all the data fall onto a single universal curve when using the predicted exponent $\theta_4$. The data for the observ-
able $\chi_t/L^{2-\eta}$ confirm our claims and are shown Figure 5. Both Fig. 4 and Fig. 5 show small corrections to scaling for low values of $L/l^0$. The source of these discrepancies is to be found in the non-analytic corrections due to irrelevant perturbations. In Figure 4 (bottom) we plot $\xi_l$ normalised with its asymptotic value: $s_l \equiv \xi_l(L)/\xi_l(\infty)$. Operatively, we simulated the system at fixed trap size $l$ and increased the lattice size $L$ until saturation; at this point, the value of the observable at the largest $L$ was used as $\xi_l(\infty)$ to fix the normalisation. From this figure we observe that the data saturate for $L/l^0 \gtrsim 6$, indicating that, for larger lattice sizes $L$ (as was the case for the previous analysis of $G_b$), the hard-walled box does not influence the scaling inside the trap. The data for $\chi_t$ agree with these considerations. Both the data for $\xi_l/L$ and $\chi_t/L^{2-\eta}$, when rescaled with the wrong exponent $\theta_2$, do not collapse onto a single curve, similarly to what is shown in Fig. 4 (bottom). We conclude that our QMC results are consistent with the scaling prediction of the preceding section and discriminate between the two exponents, $\theta_2$ and $\theta_4$.

To conclude this section, we point out that similar scaling relations hold for the density-density correlator. However, this correlator is significantly different from zero only in a very narrow region around the centre of the trap. To have acceptable signal to noise ratios, larger values of $l$ are needed, whose computational cost makes them impractical to simulate.

B. FTSS at $\mu > 0$

Having verified that the exponent at $\mu = 0$ is the one expected for the effective quartic potential, we now need to check that at $\mu \neq 0$ the scaling behaviour is determined by the exponent $\theta_2$ corresponding to the harmonic trap. A previous work\textsuperscript{13} investigated the model at $\mu = -2$ and already confirms the theory. In that case, moving away from the centre of the trap, i.e. decreasing the effective chemical potential $\mu_{\text{eff}}$, the gas locally falls into the normal liquid phase and the effective distance from the phase transition point increases (see dashed line (a) in Fig. 5).

In order to check the theory at $\mu > 0$, we simulate the BH model at $\mu = 2$. The choice of this specific value for the chemical potential is driven by two competing requirements: on the one hand, we need $\mu$ be sufficiently large so that $T'_c(\mu)$ be significantly different from zero, thus making the quadratic trapping potential the dominant perturbation to the homogeneous system; on the other hand, the different nature of the zero-temperature quantum phase transition at the endpoint of the $\mu > 0$ transition line means that we must keep $\mu$ sufficiently below $\mu = 3$. The value $\mu = 2$ is in this sense a good compromise.

Thanks to the symmetry of the phase diagram of the

![Figure 5: (Colour online) Finite-size trap-size scaling of $\chi_t$ at $\mu = 0$ and $T = T_{\text{c}}^{\mu=0}$.](image)

![Figure 6: (Colour online) FTSS plots of $\xi_l/L$ (a) and $\chi_t/L^{2-\eta}$ (b) at $\mu = 2$ and $T = T_{\text{c}}^{\mu=2}$ using the predicted exponent $\theta_2$. The curves, especially those for $\xi_l/L$ (a), are affected by large corrections to scaling. For large $L/l^0$, each fixed-$l$ curve tends to abandon the asymptotic curve, indicating the break down of the FTSS close to the effective phase boundary crossing (c).](image)
HC model, the transition temperature is known from previous works at $\mu = -2$ and its value reads $T_{\mu=2}^c = 0.7410(1)$. Contrary to the $\mu \leq 0$ case, moving out of the trap along a radius at $\mu > 0$, the system locally falls into the superfluid (low temperature) phase (cf. dashed line (b) in Fig. I). At large distances, however, we also expect the system to cross again the phase boundary on the opposite side of the phase diagram, i.e., when $\mu_{\text{eff}}(r) = -2$.

According to our previous considerations, we expect Eq. (22) to hold at most as long as all the sites in the system belong to the same effective phase (in our case, the superfluid phase). This requirement can be cast in the form

$$\mu_{\text{eff}}(r_{\text{max}}) > -2,$$

where $r_{\text{max}}$ is the distance of the farthest point from the centre of the trap. In a 3D cube, $r_{\text{max}} = \sqrt{3}L/2$, i.e., half of the length of the diagonal of the box. Using the definition for $\mu_{\text{eff}}$, for a harmonic trap at $\mu = 2$, we expect to observe finite-size and trap-size scaling behaviour at most up to

$$L_{\text{bd}} = \frac{4l}{\sqrt{3}}. \tag{27}$$

In Figure 6 we show the FTSS analyses on the data obtained at the homogeneous critical temperature corresponding to $\mu = 2$. The QMC runs are approximately $1 \cdot 10^6$ MCS long. The simulations substantially confirm the proposed scaling scenario. The data of Fig. 6(a,b) collapse on a universal curve characterized by the trap exponent $\theta_2$, even though sizeable corrections to scaling are present (see discussion below). At a sufficiently large value of $L/l^p$, the data fall out of the universal curve (see Fig. 6c). Quantifying the exact value of $L/l^p$ at which FTSS breaks down is a difficult task, since we cannot sample the curve in more points. In our simulations, in fact, $L$ must be odd, so that the minimum step for the data points in the figure is $2/l^p$ for any given $l$. However, we can qualitatively say that the corresponding value of $L/l$ is close to 2, which is in good agreement with the forecast value of $4/\sqrt{3} \approx 2.3$.

We conclude this section by discussing in some detail the origin of the scaling corrections. We identify two main sources of corrections: the irrelevant operators already present in the homogeneous system and the presence of the $O(V^2)$ term in Eq. (15). We can provide a rough quantitative estimate for the relative weights of the $O(V)$ and $O(V^2)$ contributions by approximating the critical boundary $T_c(\mu)$ with an ellipse with semi-axes fixed by the critical temperature at $\mu = 0$ and the endpoint at $\mu = \pm 3$:

$$T_c(\mu) \approx T_c^{\mu=0} \sqrt{1 - \left(\frac{\mu}{3}\right)^2}. \tag{28}$$

This ansatz reproduces the measured critical temperature at $\mu = 2$ within a few percent. We can then evaluate the coefficients $a$ of $V$ and $b$ of $V^2$ in Eq. (16) to find that they are of the same order of magnitude, with $b/a \approx \frac{1}{2}$. The scaling corrections due to the potential $V^2 \sim (r/l)^{2p}$ are expected to be of order $O(l^{-2(1-\theta_2)}) \sim l^{-0.85p}$ for $p = 2$. These must be compared with irrelevant perturbations of the homogeneous system, in the presence of the harmonic potential alone. In the limit $L \gg l$, these are $O(l^{-2\theta_2}) \sim l^{-0.45p}$, whereas, for $L \gtrsim l$, they are $O(L^{-\infty}) \sim L^{-0.78p}$. We conclude that the irrelevant perturbations provide the largest contribution to scaling corrections.

IV. CONCLUSIONS

We question the universality of the effective trap-size scaling theory first proposed in Ref. [13] by studying the critical behaviour of the trapped hard-core Bose-Hubbard model in 3D, Eq. (4) at vanishing and positive chemical potential $\mu$. The theory was so far only tested on the 2D Bose-Hubbard model, which belongs to the classical 2D XY universality class.

The standard TSS theory claims that the critical features of confined systems close to the centre of the trap $V(r) \sim r^p$ is determined by a trap exponent $\theta(p)$ that is shared among representatives of a common universality class. The finite-$T$ quantum critical behaviour of the trapped BH model can be mapped onto that of the classical XY model trapped by a potential $U \sim r^q$.

The effective TSS theory builds upon these results by showing that the trapped BH model at $\mu \neq 0$ corresponds to the XY model trapped by a potential with exponent $q = p$, while at $\mu = 0$ the correct mapping is $q = 2p$. The different behaviour at vanishing chemical potential is due to the shape of the superfluid lobe in the phase diagram of the model (see Fig. I), and in particular to the fact that

$$\frac{\partial T_c(\mu)}{\partial \mu} \bigg|_{\mu=0} = 0, \tag{29}$$

making the leading contributions of order $V^2 \sim r^{2p}$.

To validate the theory, we simulated the homogeneous hard-core 3D BH model at $\mu = 0$ to determine the transition temperature. Our finite-size scaling analysis results in $T_c^{\mu=0} = 1.00801(4)$, significantly improving the previous estimates. We then simulated the trapped model at $\mu = 0$ and $\mu = 2$ (for which the critical temperature was already known).

The data fully agree with the effective TSS theory. At $\mu = 0$, our TSS analysis clearly favours the exponent $\theta(2p)$ over $\theta(p)$, as predicted. At $\mu > 0$ the exponent $\theta(p)$ rules the critical properties of the system, although the data suffer from strong corrections to scaling. We detailed the sources of these corrections, and identified the dominant contributions with those due to irrelevant perturbations already present in the homogeneous system.

Notably, the effect of the trap on the system at positive $\mu$ is to locally push the gas towards the superfluid phase.
Sufficiently far from the centre of the trap, the system may locally reach \( \mu_{\text{eff}}(r) \leq -\mu \), thus crossing the phase boundary between the superfluid and normal fluid phases. When this happens, the two phases coexist inside the trap, leading to a break down of TSS.

We remark that, although we focussed on the hard-core limit of the Bose-Hubbard model, our results extend to soft-boson systems through universality arguments. In this sense, our work is relevant to experimental studies of cold bosonic gases in optical lattices, in which these conditions may be concretely realised. In these experiments, the momentum density distribution \( n(k) \) is often measured. This quantity is related to the two-point function by a Fourier transform,

\[
n(k) = \sum_{x,y} e^{i k \cdot (x-y)} G_0(x,y),
\]

and is experimentally accessed by the analysis of absorption images after a time-of-flight. Unfortunately, \( n(k) \) is not the ideal observable to probe the TSS critical behaviour. In fact, only the correlations within approximately a distance \( l^{-\theta} \) from the centre of the trap exhibit TSS scaling, whereas \( n(k) \) integrates over all pairs of positions \( (x,y) \) in the lattice, thus suppressing the critical features by approximately a factor of the total volume of the system.

Instead, a more promising observable is the density-density correlation function relative to the centre of the trap,\(^{12}\)

\[
G_n(0,r) = \langle n_0 n_r \rangle - \langle n_0 \rangle \langle n_r \rangle 
\approx l^{-2\theta(3-1/\nu)} G_0 (r l^{-\theta}).
\]

The latter is both accessible in experiments\(^{24–26}\) via \textit{in situ} imaging of the atomic cloud and exhibits TSS criticality. As already noticed at the end of Sec. II A, the fast depletion of the atomic cloud moving outwards from the centre of the trap requires that \( l \) be sufficiently large in order for the signal to noise ratio of the correlations to be significant. Furthermore, the trap size should be varied over a wide range of values in order to assess the critical scaling.

Despite the experimental challenges, any such measurement would constitute a significant leap from an approximate treatment of the confining potential to an exact probing of the influence of the trap on the critical behaviour of the system.

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Appendix A: Monte Carlo dynamics

The SSE with directed loops is a MC algorithm which acts on an extended \((d+1)\)-dimensional configuration space. The Hamiltonian of the system is written in terms of diagonal and off-diagonal bond operators. These operators, together with the identity operator, are inserted along the extra dimension of the configuration space\(^{17,19}\). A MCS is divided in three phases: (i) diagonal update (DU), in which diagonal and identity operators may be swapped; (ii) off-diagonal update (ODU), during which \( N_{\text{loop}} \) loops are built and diagonal and off-diagonal operators are exchanged with each other in the configuration; (iii) free-spin flipping (FSF), during which the sites of the \( d \)-dimensional lattice upon which no operator acts are flipped randomly.

\( N_{\text{loop}} \) is determined during equilibration and kept constant during the run. At fixed physical parameters, it may however vary slightly as the seed of the random number generator is changed. In our simulations, we coarsely round \( N_{\text{loop}} \) so that in all the runs at given physical parameters it takes the same value. From Fig. 7b we get an almost linear dependence of \( N_{\text{loop}} \) as \( L \) increases.

We estimate the scaling properties of the MC dynamics for the homogeneous system by looking at the integrated self-correlation time \( \tau_{\text{int}} \) of the critical observable \( \Upsilon \) at the critical temperature\(^{15}\). In general

\[
\tau_{\text{int}} \propto L^d L^z,
\]

where \( z \) is the dynamical exponent of the MC. From Fig. 7a we observe that, in units of MCS, \( \tau_{\text{int}} \) is almost constant as \( L \) increases.

However, it must be kept in mind that the MCS is not an elementary update, but is made of one DU, followed by \( N_{\text{loop}} \) loops and finally one FSF. At the critical temperature, the computational effort for all the elementary

![Figure 7: Bilogarithmic plots of the integrated self-correlation times \( \tau_{\text{int}}(L) \) (a) and of the loop number \( N_{\text{loop}} \) (b).](image-url)
updates (DU, loop, FSF) scales as the volume of the system. Moreover, the time needed for the DU and the FSF is negligible compared with the time of the ODU. According to Eq. and to the evidence of Fig. we conclude that the dynamical exponent is $z \approx 1$.

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