Trap-size scaling in confined particle systems at quantum transitions

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(Dated: January 11, 2010)

We develop a trap-size scaling theory for trapped particle systems at quantum transitions. As a theoretical laboratory, we consider a quantum XY chain in an external transverse field acting as a trap for the spinless fermions of its quadratic Hamiltonian representation. We discuss trap-size scaling at the Mott insulator to superfluid transition in the Bose-Hubbard model. We present exact and accurate numerical results for the XY chain and for the low-density Mott transition in the hard-core limit of the one-dimensional Bose-Hubbard model. Our results are relevant for systems of cold atomic gases in optical lattices.

PACS numbers: 05.70.Jk, 64.60.-i, 67.85.-d, 64.60.ae.

I. INTRODUCTION

The achievement of Bose-Einstein condensation in diluted atomic vapors of $^{87}$Rb and $^{23}$Na [1] and the impressive progress in the experimental manipulation of cold atoms in optical lattices (see, e.g., Ref. [2] and references therein) have provided a great opportunity to investigate the interplay between quantum and statistical behaviors in particle systems. In these systems, phase transitions are phenomena of great interest, see, e.g., Refs. [3–9].

Phase transitions related to the formation of the Bose-Einstein condensation in interacting Bose gases at a nonzero temperature, as the one reported in Ref. [3], are essentially driven by thermal fluctuations, giving rise to a classical critical behavior, see, e.g., Ref. [10]. Quantum fluctuations play a dominant role at $T = 0$ transitions, where the low-energy properties show a quantum critical behavior with a peculiar interplay between quantum and thermal fluctuations at low $T$, see, e.g., Ref. [11]. Quantum Mott insulator to superfluid transitions have been observed in experiments with ultracold atomic gases loaded in optical lattices [4–9].

A common feature of the above-mentioned experimental realizations is the presence of a trapping potential $V(r)$ coupled to the particle density. For example, atomic gases loaded in optical lattices are generally described by the Bose-Hubbard (BH) model [12]

$$H_{BH} = -J \sum_{\langle ij \rangle} (b_i^\dagger b_j + b_j^\dagger b_i) + \sum_i [(\mu + V(r_i)) n_i + Un_i(n_i - 1)],$$

where $\langle ij \rangle$ is the set of nearest-neighbor sites and $n_i \equiv b_i^\dagger b_i$ is the particle density operator. Far from the origin the potential $V(r)$ diverges, therefore $\langle n_i \rangle$ vanishes and the particles are trapped. The inhomogeneity due to the trapping potential strongly affects the phenomenology of quantum transitions in homogeneous systems. Correlation functions are not expected to develop a diverging length scale in the presence of a trap. Therefore, a theoretical description of how critical correlations develop in systems subjected to confining potentials is of great importance for experimental investigations.

We consider the trapping power-law potential

$$V(r) = v^p |r|^p \equiv (|\vec{r}|/l)^p,$$

where $v$ and $p$ are positive constants and $l = 1/v$ is the trap size, coupled to the particle number. Experiments are usually set up with a harmonic potential, i.e., $p = 2$.

Let us consider the case in which the system parameters are tuned to values corresponding to the critical regime of the unconfined system. In the presence of a confining potential, the critical behavior of the unconfined homogeneous system can be observed around the middle of the trap only in a window where the length scale $\xi$ of the critical modes is much smaller than the trap size, but sufficiently large to show the universal scaling behavior. If $\xi$ is large, but not much smaller than the trap size, the critical behavior gets somehow distorted by the trap, although it may still show universal effects controlled by the universality class of the phase transition of the unconfined system. In this paper we investigate this issue within quantum transitions.

In Ref. [13] we have shown that the critical behavior of trapped systems at classical continuous transitions can be cast in the form of a trap-size scaling (TSS), resembling the finite-size scaling theory for homogeneous systems [14, 15], but characterized by a further nontrivial trap critical exponent $\theta$, which describes how the length scale $\xi$ depends on...
the trap size at criticality, i.e., $\xi \sim l^\theta$, and which can be estimated using renormalization-group (RG) arguments. TSS was supported by numerical results for some lattice gas models.

In the present paper, we extend the study of the effects of trapping potentials to quantum critical behaviors at $T = 0$ transitions. We put forward a TSS scenario to describe how critical correlations develop in large traps, analogous to the one outlined in Ref. [13] for classical continuous transitions. We then check the validity of the TSS scenario within quantum transitions by determining the trap-size dependence in a few quantum models. As a theoretical laboratory, we consider a quantum XY chain in an external space-dependent transverse field, acting as a trap for the spinless fermions of its quadratic Hamiltonian representation. We present exact and very accurate numerical results which fully support TSS. Moreover, we discuss TSS at the Mott insulator to superfluid transitions, and present the RG arguments to derive the corresponding trap exponent $\theta$.

The paper is organized as follows. In Sec. II we outline the main ideas of the TSS theory. In Sec. III we study the XY chain in a space-dependent transverse field, which gives rise to an inhomogeneity analogous to the one arising from a trapping potential in particle systems. We show how TSS emerges by analytical and very accurate numerical results. In Sec. IV we consider the BH model (1) in a confining potential. We discuss the general features of the Mott insulator to superfluid transitions, and present the RG arguments to derive the corresponding trap exponent $\theta$.

Finally, in Sec. V we draw our conclusions.

II. TRAP-SIZE SCALING AT QUANTUM TRANSITIONS

Quantum phase transitions arise from a nonanalyticity of the ground-state energy, where the gap $\Delta = E_1 - E_0$ vanishes. In addition, continuous quantum transitions have a diverging length scale $\xi$, which gives rise to peculiar scaling properties, see, e.g., Ref. [11].

In a standard general scenario, a quantum $T = 0$ transition of a homogeneous $d$-dimensional system is generally characterized by one relevant parameter $\mu$, with critical value $\mu_c$ and RG dimension $y_\mu \equiv 1/\nu$, and a given dynamic critical exponent $z$. Interesting physical examples are the Mott insulator to superfluid transitions in BH models. The quantum critical behavior is characterized by a vanishing energy scale, for example the gap $\Delta$, and a diverging length scale $\xi$, behaving respectively as $\Delta \sim |\tilde{\mu}|^{z\nu}$ and $\xi \sim |\tilde{\mu}|^{-\nu}$, where $\tilde{\mu} = \mu - \mu_c$, thus $\Delta \sim \xi^{-\nu}$.

The confining potential gives rise to a space inhomogeneity, thus changing the scaling behavior of the homogeneous system, which could be only recovered in the limit of large trap size (keeping fixed the other parameters of the system). We want to describe how the critical correlations develop in a trap. Our starting point is a scaling Ansatz which extends the scaling laws of homogeneous systems at quantum transitions, to allow for the presence of a confining potential like (2). We write the scaling law of the singular part of the free energy density at the quantum transition as

$$F(\mu, T, v, x) = b^{-(d+z)} F(\tilde{\mu}^{y_v}, T^{b\nu}, vb^{y_v}, x/b),$$

where $b$ is any positive number, $y_v$ is the RG dimension of the trap parameter $v$, cf. Eq. (2), and $x$ is the distance from the middle of the trap. We are neglecting irrelevant scaling fields, because they do not affect the asymptotic behaviors. Then, fixing $vb^{y_v} = 1$ and introducing the trap size $l = v^{-1}$, we obtain the following trap-size scaling (TSS)

$$F = l^{-\theta(d+z)} F(\tilde{\mu}^{\theta/\nu}, T^{\theta z}, xl^{\theta})$$

where $\nu \equiv 1/y_v$ and $\theta \equiv 1/y_v$ is the trap exponent. $\theta$ depends on the universality class of the quantum transition. It can be computed by evaluating the RG dimensions of the corresponding perturbation. Analogously, one can derive the TSS of other observables. Any low-energy scale at $T = 0$, and in particular the gap, is expected to behave as

$$\Delta = l^{-\theta z} D(\tilde{\mu}^{\theta/\nu}),$$

with $D(y) \sim y^{z\nu}$ for $y \to 0$ to match the scaling $\Delta \sim |\tilde{\mu}|^{z\nu}$ in the absence of the trap. The correlation length $\xi$ around the middle of the trap, or any generic length scale associated with the critical modes, behaves as

$$\xi = l^{\theta} \xi'(\tilde{\mu}^{\theta/\nu}, Tl^{\theta z}),$$

with $\xi'(y) \sim y^{z}$.
where $X(y,0) \sim y^{-\nu}$ for $y \to 0$. This implies that at the $T=0$ quantum critical point the trap induces a finite length scale: $\xi \sim l^z$. In the case of a generic local operator $O(x)$, with RG dimension $y_o$, we expect that its expectation value and equal-time correlator behave as

$$
\langle O(x) \rangle = l^{-2y_o} \mathcal{O}(\tilde{\mu}^{\theta/\nu}, T^{\theta z}, x l^{-\theta}),
$$

(7)

$$
\langle O(x)O(0) \rangle_c = l^{-2y_o} \mathcal{G}_O(\tilde{\mu}^{\theta/\nu}, T^{\theta z}, x l^{-\theta}),
$$

(8)

where $x$ measures the distance from the origin, i.e., the middle of the trap. In the above scaling formulae we have neglected scaling corrections due to irrelevant perturbations, and possible analytic contributions.

When $p \to \infty$ the effect of the trapping potential is equivalent to confine a homogeneous system in a box of size $L = 2l$ with open boundary conditions, whose behavior can be described by a standard finite-size scaling [10, 14]. Therefore we must have that $\theta \to 1$ when $p \to \infty$.

The TSS theory outlined in this section provides an effective theoretical framework to describe quantum critical behaviors in confined systems. However, it is important to check the validity of its scaling Ansatz, because the quantum nature of the phenomenon may lead to subtle effects. For this purpose, in the following sections, we study the trap-size dependence at some specific quantum transitions of one-dimensional systems in the presence of a space-dependent confining potential.

### III. Trap-Size Scaling in the Quantum XY Chain

The quantum XY chain in a transverse field is a standard theoretical laboratory for issues related to quantum transitions, see, e.g., Ref. [11]. In this model, an inhomogeneity analogous to the one arising from a trapping potential in particle systems can be achieved by considering a space-dependent transverse field, i.e.,

$$
H_{\text{XY}} = -\sum_i \frac{1}{2} \left( (1 + \gamma) \sigma_i^x \sigma_{i+1}^x + (1 - \gamma) \sigma_i^y \sigma_{i+1}^y \right) - \mu \sigma_i^z - V(x_i) \sigma_i^z,
$$

(9)

where $\sigma^i$ are the Pauli matrices, $0 < \gamma \leq 1$ and $V(x) = v^p |x|^p \equiv (|x|/l)^p$, where $v$ and $p$ are positive constants and $l = v^{-1}$ is its length scale. This model can be mapped into a quadratic Hamiltonian of spinless fermions by a Jordan-Wigner transformation,

$$
H = \sum_i \left[ c_i^\dagger A_{ij} c_j + \frac{1}{2} (c_i^\dagger B_{ij} c_j + \text{H.c.}) \right],
$$

$$
A_{ij} = 2 \delta_{ij} - \delta_{i+1,j} - \delta_{i,j+1} + 2Q(x_i) \delta_{ij},
$$

$$
B_{ij} = -\gamma (\delta_{i,j} - \delta_{i,j+1}) + 2Q(x_i) \delta_{ij},
$$

$$
Q(x) = \tilde{\mu} + V(x), \quad \tilde{\mu} \equiv \mu - 1.
$$

In this picture $\mu$ plays the role of chemical potential for the $c$-particles, and the space-dependent field $V(x)$ acts as a trap for the $c$-particles, making their local density $\langle n_i \rangle \equiv \langle c_i^\dagger c_i \rangle$ vanish at large distance. In the following, $l \equiv v^{-1}$ will be considered the trap size.

In the absence of the trap, the model undergoes a quantum transition at $\tilde{\mu} = 0$ in the two-dimensional Ising universality class, separating a quantum paramagnetic phase for $\tilde{\mu} > 0$ from a quantum ferromagnetic phase for $\tilde{\mu} < 0$. Around $\tilde{\mu} = 0$, the quantum critical behavior shows a diverging length scale, $\xi \sim |\mu|^{-\nu}$, and a vanishing energy scale, $\Delta \sim \xi^{-z}$, where $z$ and $\nu$ are universal critical exponents: $z = 1$ and $\nu \equiv 1/y_\mu = 1$ ($y_\mu$ is the RG dimension of $\mu$).

In the presence of the confining potential, the critical behavior can be observed only in the limit of large trap size. The trap exponent $\theta$ controlling such limit can be determined by analyzing the RG properties of the corresponding perturbation at the critical point, which can be represented by $P_V = \int d^d x V(x) \phi(x)^2$, where $\phi(x)$ is the order-parameter field of the $\phi^4$ theory which describes the behavior of the critical modes [10, 13]. Since the RG dimensions of the potential $V(x)$ and the energy operator $\phi^2$, respectively $y_V = py_v - p$ and $y_{\phi^2} = d + z - y_\mu$, are related by $y_V + y_{\phi^2} = d + z$, we obtain $p y_v - p = y_\mu$, and therefore, since $z = 1$ and $y_\mu = 1$,

$$
\theta \equiv 1/y_v = p/(p + 1).
$$

(11)

Notice that $\theta \to 1$ when $p \to \infty$; this was to be expected, since when $p \to \infty$ the system becomes equivalent to a homogeneous chain with $-l \leq x \leq l$ and open boundary conditions.

We mention that some issues related to the presence of a space-dependent transverse field in the quantum XY chain model have been addressed in Refs. [16–19].
The Hamiltonian (10) can be solved by exact numerical diagonalization, even in the presence of the trapping potential, following, for example, Ref. [20]. We look for new canonical fermionic variables $\eta_k = g_k c_i^\dagger + h_k c_i$, which diagonalize the Hamiltonian, i.e., such that

$$H = \sum_k \omega_k \eta_k^\dagger \eta_k, \quad \omega_k \geq 0,$$

and the ground state satisfies $\eta_k|0\rangle = 0$ for any $k$. The diagonalization is achieved by introducing two sets of orthonormal vectors $\phi_k$ and $\psi_k$ with components $\phi_{ki} = g_{ki} + h_{ki}$ and $\psi_{ki} = g_{ki} - h_{ki}$ respectively, satisfying the equations

$$(A + B)\phi_k = \omega_k \psi_k, \quad (A - B)\psi_k = \omega_k \phi_k,$$

where the matrices $A$ and $B$ have been defined in Eq. (10). Thus, we have

$$(A - B)(A + B)\phi_k = \omega_k^2 \phi_k.$$

Once the vectors $\phi_k$ have been computed, one can easily determine $\psi_k$ and reconstruct the original $c$-operators as

$$c_i = \frac{1}{2} \sum_k (\phi_{ki} + \psi_{ki})\eta_k^\dagger + (\phi_{ki} - \psi_{ki})\eta_k^\dagger,$$

from which one can compute the correlation functions of the $c$-operators, by straightforward calculations.

In order to show how TSS emerges, we consider the continuum limit of Eq. (14). A similar approach was developed in Ref. [16] to study the critical behavior of the quantum XY chain in the presence of a gradient perturbation. By rewriting the discrete differences in terms of derivatives, near the critical point $\mu = 0$ and for sufficiently small values of $k$ (this is required by the smoothness hypothesis underlying the continuum limit), we obtain

$$[4Q(x)^2 + 4\gamma \partial_x Q(x) - 4\gamma^2 \partial_x^2 Q - 4Q(x)\partial_x^2 - 2\partial_x Q(x)\partial_x - 2\partial_x^2 Q(x) + \ldots] \phi_k(x) = \omega_k^2 \phi_k(x).$$

This equation has a nontrivial TSS limit: by rescaling

$$x = \gamma^{1/(1+p)} \rho/(1+p) X, \quad \mu = \gamma^{p/(1+p)} \rho/(1+p) \mu_r, \quad \omega_k = 2\gamma^{p/(1+p)} \rho/(1+p) \Omega_k,$$

and keeping only the leading terms in the large-$l$ limit (and for small $\omega_k$), we obtain

$$(\mu_r + X^p - \partial_X) (\mu_r + X^p + \partial_X) \phi_k(X) = \Omega_k^2 \phi_k(X).$$

Analogously, we obtain the equation for the function $\psi_k(x)$, i.e.,

$$(\mu_r + X^p - \partial_X) \psi_k(X) = \Omega_k \phi_k(X).$$

It is worth noting that the dependence on $\gamma$ in Eqs. (18) and (19) disappears, showing the universality of TSS with respect to changes of the values of $\gamma$ (of course, excluding the value $\gamma = 0$). One can easily check that the next-to-leading terms in the large-trap limit give rise to $O(l^{-\theta})$ scaling corrections. Corrections due to irrelevant perturbations already present in the homogeneous system are expected to be more suppressed: the exponent associated with the leading scaling corrections in generic systems belonging to the two-dimensional Ising universality class is $\omega = 2$ [10, 21], thus leading to $O(l^{-2\theta})$ corrections in TSS.

The solution of Eqs. (18) and (19) allows us to determine the critical correlations of the original $c$-operators, using Eq. (15). One can easily determine the large-distance behavior of the functions $\phi_k(x)$ and $\psi_k(x)$: they decay exponentially as $\sim \exp(-a|x|^{p+1})$ apart from prefactors. Their large-distance decay determines the large-distance behavior of the scaling correlation functions of the $c$ operators.

A natural question concerns the robustness of the TSS results with respect to variation of the trapping potential from a simple power law. For example, let us consider a potential given by

$$U(x) = (|x|/l)^p + b(|x|/l)^q, \quad q > p,$$

where $b > 0$ is a constant. A simple analysis based on the rescalings (17) shows that the TSS limit is determined by the smallest power law, while the higher power gives rise to $O(l^{-(q-p)/(1+p)})$ scaling corrections.
B. Trap-size scaling of observables

In the following we report results obtained by exact diagonalization at fixed trap size, and compare them with the TSS derived in Sec. II. The exact numerical diagonalization in the presence of the trap is done on a chain of length \( L \) with open boundary conditions, with \( L \) large enough to have negligible finite-size effects.

1. Trap-size scaling of low-energy scales

![Graph showing TSS of energy differences](image)

FIG. 1: (Color online) TSS of the energy differences \( \Delta_1 \equiv E_1 - E_0 \) and \( \Delta_2 \equiv E_2 - E_0 \) for \( p = 2 \) (above) and \( p = 4 \) (below) vs. \( \mu_r \equiv \gamma - \theta_l \mu \), for several values of \( \gamma \) and for \( l \geq 10 \). Numerical diagonalization results clearly approach universal TSS functions in the large-\( l \) limit (represented by full lines and obtained by extrapolations), with \( O(l^{-\theta}) \) scaling corrections (larger at small \( \gamma \) and for higher levels).

The universal TSS limit obtained after the rescalings (17) implies the following asymptotic behavior for any low-
energy scale:
\[ \Delta \approx \gamma^\theta l^{-\theta} D(\mu_r), \quad \mu_r \equiv \gamma^{-\theta} l^{\mu} \lim_{\mu \to \infty}, \]
which is approached with \( O(l^{-\theta}) \) scaling corrections. This proves the scaling behavior (5) obtained by RG arguments.

In Fig. 1 we plot the differences among the first few energy levels, \( \Delta_1 = E_1 - E_0 \) and \( \Delta_2 = E_2 - E_0 \), obtained by numerical diagonalization, for trapping potentials with \( p = 2 \) and \( p = 4 \) and for several values of \( \mu \) and \( \gamma \). The numerical results clearly approaches a universal TSS behavior in the large-\( l \) limit, as predicted by Eq. (21). The large-\( |\mu_r| \) behavior of the scaling functions \( D \), related to \( \Delta_1 \) are \( D_1 \sim 2\mu_r \) for \( \mu_r \to +\infty \), \( D_1 \to 0 \) for \( \mu_r \to -\infty \), and \( D_2 \sim 2|\mu_r| \) for \( \mu_r \to \pm\infty \); they are consistent with the behaviors of the corresponding quantities in the absence of the trap. The vanishing of \( D_1 \) for \( \mu_r \to -\infty \) is related to the degeneracy of the ground state in the quantum ferromagnetic phase.

2. Trap-size scaling of the particle density and its correlators

Other interesting quantities are the particle density and its correlation function. At the quantum critical point, the particle density is expected to behave analogously to the energy density in the standard Ising model [13], which presents leading analytic contributions arising from the analytic part of the free energy. At \( \bar{\mu} = 0 \) and in the middle of the trap, we expect
\[ \langle n_0 \rangle \equiv \langle c_0^\dagger c_0 \rangle = \rho_c(\gamma) + a_n \gamma^\theta/p l^{-\theta} + \ldots, \]
where we used the fact that the RG dimension of the particle density operator is \( y_n = d_z - y_\mu = 1 \), and the rescalings (17) to guess the dependence on \( \gamma \) of the amplitude of the scaling term. \( a_n \) is a constant that does not depend on \( \gamma \). \( \rho_c(\gamma) \) is the critical value of the homogeneous system without trap, for example \( \rho_c(1) = 0.1816901 \ldots \) [22]. Our numerical results for several values of \( \gamma \) support the scaling behavior (22). Scaling corrections are (consistent with) integer powers of \( l^{-\theta} \).

We have also studied the dependence on the distance from the middle of the trap, which must be an even analytic function of \( x \) at fixed trap size, but it may present a nontrivial scaling for large \( l \). Analogously to the scaling at the origin, we expect it to be given by a sum of an analytic behavior and a nonanalytic term in the trap size, such as
\[ \langle n_x - n_0 \rangle = \rho_{ns}(x/l) + a_n \gamma^\theta/p l^{-\theta} \mathcal{R}(x l^{-\theta}), \]
where \( \rho_{ns} \) is a nonsingular term which we expect to be a function of \( x/l \). Let us compare this Ansatz with the results from exact diagonalization. At small \( x \), the latter are consistent with the expansion
\[ \langle n_x - n_0 \rangle \approx b_2(l) x^2 + b_4(l) x^4 + \ldots, \]
with
\[ b_2(l) = b_{21} l^{-2} \ln l + b_{22} l^{-2} + \ldots, \quad b_4(l) = b_{41} l^{-10/3} + \ldots \]
for \( p = 2 \) (dots indicate terms that are more suppressed in the large-\( l \) limit by power laws), and
\[ b_2(l) = b_{21} l^{-12/5} + b_{22} l^{-16/5} + \ldots, \quad b_4(l) = b_{41} l^{-4} \ln l + b_{42} l^{-4} + \ldots \]
for \( p = 4 \). These results should be compared with the expansion of Eq. (23) in powers of \( x \). They are in substantial agreement; the only difference is given by the presence of logarithms. However, this should not be surprising, because logarithmic corrections to power laws are peculiar of the two-dimensional Ising universality class, see, e.g., the behavior of the specific heat, and arise [23] from integer resonances of the RG dimensions of different perturbations, see also Ref. [24]. Note that the logarithms appearing in the expansion (24) show up in the \( x^2 \) term for \( p = 2 \) and in the \( x^4 \) term for \( p = 4 \), while the trap-size power-law expansions of the two terms in Eq. (23) present an accidental degeneracy, just because \( 3\theta = 2 \) for \( p = 2 \) and \( 5\theta = 4 \) for \( p = 4 \). The large-distance behavior of the particle density turns out to be dominated by the nonuniversal analytic term, indeed at large distance we find
\[ \langle n_x \rangle \approx \gamma^2 \left( \frac{x}{7} \right)^{-2p}, \]
while the scaling nonanalytic part is expected to be exponentially suppressed, as suggested by the large-distance behavior of the solutions of Eq. (18).
The static particle-density correlator is not affected by analytic backgrounds; therefore, according to Eq. (8), we expect that at $\bar{\mu} = 0$ and for $x \neq 0$

$$G_n(x) \equiv \langle n_0 n_x \rangle - \langle n_0 \rangle \langle n_x \rangle \approx \gamma^{2 \theta/p l - \theta} G_n(X),$$

where $G_n(X)$ is a universal function. This is confirmed by the results of numerical diagonalization, as shown in Fig. 2 for $p = 2$ and $p = 4$. At small $X$, $G_n(X) \sim 1/X^2$, which is the behavior in the absence of trap, while at large $X$ it decays very rapidly.

In the limit $p \to \infty$ the system becomes equivalent to a homogeneous finite-size chain with $-l \leq x \leq l$ and open boundary conditions. Thus, in this limit we can exploit conformal field theory (CFT), by mapping the half-plane...
result for the two-dimensional Ising universality class [25] into the strip, obtaining the correlation function [26]

\[ G_n(x) = \frac{\pi^2}{4l^2\sin^2(\pi X/2)}, \quad X = x/l. \tag{29} \]

Since \( \theta \to 1 \) for \( p \to \infty \), this result agrees with TSS. Of course, the corresponding scaling function \( G_n(X) \equiv l^2G_n(x) \) is defined for \( |X| \leq 1 \), and vanishes for \( X = \pm 1 \). It is shown in Fig. 3.

3. Trap-size scaling of two-point correlation function

We have also computed the static correlation function of the spin operator \( \sigma^x \) at \( T = 0 \) and \( \mu_c \), following essentially the method of Ref. [27]. According to Eq. (8), \( G_s(x) \) behaves as

\[ G_s(x) \equiv \langle \sigma_0^x \sigma_x^x \rangle = a_s l^{-\theta}G_s(X), \tag{30} \]

where we used the fact that the RG dimension of the spin operator \( \sigma^x \) is \( \eta/2 \) with \( \eta = 1/4 \). The constant \( a_s \) is not universal, it is expected to depend on \( \gamma \). Our results from numerical diagonalization are perfectly consistent with Eq. (30): we find that, introducing a \( \gamma \)- (and \( p \)-) dependent normalization \( c \), determined phenomenologically, the combination \( cl^{\theta}G_s(x) \) plotted vs. \( X = \gamma^{-1/(1+p)}l^{-\theta}x \), for different values of \( x \) (not too small, e.g., \( x > 4 \)), \( l \) (large), and \( \gamma \), falls on a single curve; see Fig. 4. \( G_s(X) \) diverges as \( X^{-1/4} \) for \( X \to 0 \) (corresponding to the behavior in the absence of the trap) and decay rapidly at large \( X \), as \( \exp(-ax^{p+1}) \), in agreement with the large distance behavior of the solutions of Eq. (18).

One may also consider the susceptibility and second moment correlation length defined as

\[ \chi = \int dr G_s(r) \approx c\chi l^{(d-\eta)\theta} + B = a\chi l^{3\theta/4} + B, \tag{31} \]

\[ \xi^2 = \frac{1}{2\chi} \int dr r^2 G_s(r) \approx a\xi l^{2\theta}, \tag{32} \]

where \( B \) is a background constant term already present in the homogeneous system without trap [10]. Since the normalization of \( G_s(x) \) cancels out, \( \xi \) must scale as \( x \), i.e.,

\[ \xi = a\xi \gamma^{\theta/p}\theta[1 + O(l^{-\theta})], \tag{33} \]

with \( a_\xi \) dependent on \( p \) but not on \( \gamma \). The above scaling behaviors have been verified by numerical computations.
Finally, the $p = \infty$ limit of the correlation function (30) can be computed using CFT, analogously to the density-density correlation function (29), obtaining [26]

$$G_s(x) = \left[ \frac{\pi^2}{l^2 Y^2 \sin^2(\pi X/4)} \right]^{1/8} \frac{\sqrt{1+Y} - \sqrt{1-Y}}{\sqrt{2}},$$

$$Y = \sqrt{1 - \tan^2(\pi X/4)}, \quad X = x/l.$$  

(34)

The corresponding scaling curve $G_s(X) \equiv l^{1/4}G_s(x)$ is plotted in Fig. 5.

4. Trap-size scaling of quantum entanglement

We now discuss quantum entanglement in the presence of the confining potential.
FIG. 5: (Color online) The scaling function $G_s(X) \equiv t^p G_s(x)$ vs. $X \equiv x/l^\theta$ in the limit $p \to \infty$ where $\theta \to 1$, cf. Eq. (34).

We divide the chain in two parts of length $l_A$ and $L - l_A$. At $\bar{\mu} = 0$, in the absence of the trap and for open boundary conditions, the entanglement entropy is given by [28]

$$S(l_A; L) \approx \frac{c}{6} \ln \left[ L \sin(\pi l_A / L) \right] + E$$

(35)

where $c = 1/2$ is the central charge. The constant $E$ depends on $\gamma$:

$$E = \frac{a}{2} + \frac{1}{12} \ln(2\gamma/\pi)$$

(36)

where $a = 0.478558...$ [29].

In the presence of a trapping potential, and for sufficiently large lattice sizes $L$, we obtain

$$S(L/2; L) \approx \frac{c}{6} \ln \xi_e + E,$$

(37)

which defines an entanglement length $\xi_e$ at the critical point. Note that $E$ is the same constant appearing in Eq. (36). The ratio between $\xi_e$ and the correlation length $\xi$ defined from the correlation function of $\sigma^x$, cf. Eqs. (32) and (33), should be universal in the large-$l$ limit, thus independent of $\gamma$. This implies that at criticality $\xi_e$ has the asymptotic behavior

$$\xi_e = a_e \gamma^{p/2}[1 + O(l^{-\theta})],$$

(38)

with $a_e$ dependent on $p$ but not on $\gamma$.

The above scenario is fully supported by numerical computations, using the technique of Refs. [18, 30].

C. Trap-size dependence for $\mu < 1$

Finally, it is worth discussing the trap-size dependence at values of $\mu < 1$, i.e., $\bar{\mu} < 0$, within the quantum ordered phase. In this case the TSS theory outlined in Secs. II and IIIA does not apply, because the system is not critical in the middle of the trap. Around the middle of the trap we have a quantum ferromagnetic phase, up to the point $\bar{\mu} + V(x) = 0$, i.e., up to $|x_c| = (-\bar{\mu})^{1/p}$, around which critical fluctuations develop. Then, as before, at larger distances the system is in the quantum paramagnetic phase and the particle density vanishes for $|x| \to \infty$.

In Fig. 6 we plot the differences of the lowest energy levels, i.e., $\Delta_1 = E_1 - E_0$ and $\Delta_2 = E_2 - E_0$, for a few values of $\mu < 1$ for the harmonic potential, i.e., $p = 2$. $\Delta_1$ vanishes rapidly, apparently as $\Delta_1 \sim \exp(-\kappa l)$, where the constant

$\kappa$...
\(\kappa\) depends on \(\mu\). This behavior is clearly related to the degeneracy of the ground state in the quantum ferromagnetic phase in the absence of trapping potential.

It is interesting to note that also \(\Delta_2\) appears to vanish in the large-\(l\) limit, although at a much slower rate. Indeed, our data for \(\mu\) not too close to the critical value \(\mu = 1\) are consistent with the power-law behavior \(\Delta_2 \sim l^{-1/2}\). The vanishing of \(\Delta_2\) should be related to the developing of critical fluctuations at the points \(x_c = \pm(\mu - \bar{\mu})^{1/p}\) where the sum \(\mu + V(x)\) vanishes. Since around \(x_c\) the potential \(V(x) = |x|^p/L^p\) can be approximate by a linear potential, i.e.,

\[
V(x) \approx u(x - x_c), \quad u = p(\mu - \bar{\mu})^{1/p}/l,
\]

the exponent \(1/2\) should be related to the RG scaling dimensions of the parameter \(u\) of the linear potential. Using RG arguments analogous to those leading to Eq. (11), we obtain \(y_u = 2\), see also Ref. [16]. This explanation is further supported by the fact that the data for \(\Delta_2\) for different values of \(\mu < 1\) appear to merge to a unique curve as a function of \(u\) for sufficiently large trap size \(l\), as shown in Fig. 6 (\(\mu = 0.99\) clearly displays crossover effects because it is very close to the critical value \(\mu = 1\)).

**IV. TRAP-SIZE SCALING IN THE BOSE-HUBBARD MODEL**

A. General features

We now discuss TSS within the Bose-Hubbard (BH) model (1) at the Mott insulator to superfluid transitions. A review of results for the BH model can be found in Ref. [11]. In the homogeneous BH model without trap, the low-energy properties of the transitions driven by the chemical potential \(\mu\) are described by a nonrelativistic U(1)-symmetric bosonic field theory [31], whose partition function is given by

\[
Z = \int [D\phi] \exp \left( - \int_0^{1/T} dt d^2x \mathcal{L}_c \right),
\]

\[\mathcal{L}_c = \phi^* \partial_t \phi + \frac{1}{2m} |\nabla \phi|^2 + r |\phi|^2 + u |\phi|^4,\]

where \(r \sim \mu - \mu_c\). The upper critical dimension of this bosonic theory is \(d = 2\). Thus its critical behavior is mean field for \(d > 2\). For \(d = 2\) the field theory is essentially free (apart from logarithmic corrections), thus the dynamic critical exponent is \(z = 2\) and the RG dimension of the coupling \(\mu\) is \(y_\mu = 2\). In \(d = 1\) the theory turns out to be equivalent to a free field theory of nonrelativistic spinless fermions, from which one infers the RG exponents \(z = 2\) and \(y_\mu = 2\).

The special transitions at fixed integer density (i.e., fixed \(\mu\)) belong to a different universality class, described by a relativistic U(1)-symmetric bosonic field theory [31], whose Lagrangian is

\[
\mathcal{L}_c = |\partial_t \phi|^2 + v^2 |\nabla \phi|^2 + r |\phi|^2 + u |\phi|^4,
\]

for which \(z = 1\) and \(y_\mu = 1/\nu_{XY}\) where \(\nu_{XY}\) is the correlation length exponent of the \(D = d+1\) XY universality class. Thus \(\nu_{XY} = 1/2\) for \(d = 3\) (i.e., mean-field behavior apart from logarithms), \(\nu_{XY} = 0.6717(1)\) in the \(d = 2\) case [32], and formally \(\nu = \infty\) for the Kosterlitz-Thouless transition [33] at \(d = 1\).

In the presence of a confining potential, theoretical and experimental results have shown the coexistence of Mott insulator and superfluid regions when varying the total occupancy of the lattice, see, e.g., Refs. [8, 12, 34–37]. However, at fixed trap size, the system does not develop a critical behavior with diverging length scale [34, 35]. Criticality is recovered only in the limit of large trap size, where the critical behavior can be described in the framework of the TSS theory. The trap exponent \(\theta\) can be determined by an analysis of the corresponding RG perturbation, i.e.,

\[
\int d^2x dt V(x)|\phi(x)|^2,
\]

leading to the relation

\[
p y_v - p = d + z - y_\mu = y_\mu,\]

where \(y_\mu\) is the RG dimension of the coupling \(r\) of the quadratic term of Lagrangian (41) or (42). Therefore,

\[
\theta \equiv \frac{1}{y_v} = \frac{p}{p + y_\mu}.
\]

By replacing the corresponding value of \(y_\mu\), this relation yields the value of \(\theta\) for each specific transition.
FIG. 6: (Color online) Trap-size dependence at $\mu < 1$, i.e., in the quantum ferromagnetic phase, of the difference of the lowest energy levels for $\mu < 1$ and $p = 2$: $\Delta_1 \equiv E_1 - E_0$ vs. $l$ (above) and $\Delta_2 \equiv E_2 - E_0$ vs. $u^{1/2} \equiv 2^{1/2} (-\bar{\mu})^{1/4} l^{-1/2}$ (below).

B. TSS at the low-density Mott transition in the 1D hard-core Bose-Hubbard model

We now show how TSS emerges at the low-density Mott transition of the one-dimensional BH model, which is also of experimental relevance in optical lattices, see, e.g., Refs. [2, 5, 6, 9]. In particular, we consider its hard-core limit $U \to \infty$, which implies that the particle number is restricted to the values $n_i = 0, 1$. In this limit, analytical results can be obtained by exploiting exact mappings into the so-called XX chain model in the presence of a space-dependent external field,

$$H_{\text{XX}} = -\frac{1}{2} \sum_i \left( \sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y \right) - \mu \sum_i \sigma_i^z - \sum_i V(x_i) \sigma_i^z$$

(46)
(which is the Hamiltonian (9) with $\gamma = 0$). The Pauli spin matrices are related to the boson operators of the Bose-Hubbard Hamiltonian $H_{BH}$, cf. Eq. (1), by $\sigma^x_i = b_i^\dagger b_i$, $\sigma^y_i = i(b_i^\dagger - b_i)$, $\sigma^z_i = 1 - 2b_i^\dagger b_i$. Actually we have that $H_{XX} = 2H_{BH}(J = 1, U \to \infty)$. One can then map it into a model of free spinless fermions by a Jordan-Wigner transformation, given by Eq. (10) for $\gamma = 0$, see, e.g., Ref. [11].

In the absence of the trap, the 1D hard-core BH model has three phases: two Mott insulator phases, for $\mu > 1$ with $\langle n_i \rangle = 0$ and for $\mu < -1$ with $\langle n_i \rangle = 1$, separated by a gapless superfluid phase for $|\mu| < 1$. Therefore, there are two quantum transitions at $\mu = \pm 1$, with $z = 2$ and $y = 1/\nu = 2$. In the following we consider the low-density Mott transition at $\mu = 1$, for which we can analytically show the existence of the TSS limit, and compute the corresponding scaling functions. The results provide a further analytical check of the TSS theory in quantum transitions, in a case with dynamic exponent $z \neq 1$, whose quantum critical behavior is not described by a $d + 1$-dimensional conformal field theory.

The trap-size dependence, and corresponding TSS, turns out to be more subtle at the $\mu \leq 1$, for which we can analytically show the existence of the TSS limit, and compute the corresponding scaling functions. The results will be presented elsewhere.

In the fermion representation the Hamiltonian can be easily diagonalized: introducing new canonical fermionic variables $\varphi_k = \sum_i \varphi_{ki}c_i$, $k = 0, 1, \ldots$, where $\varphi_{ki}$ satisfies

$$A_{ij}\varphi_{kj} = \omega_k \varphi_{kj}$$

and $A_{ij}$ is the matrix defined in Eq. (10), we obtain

$$H = \sum_k \omega_k \varphi^\dagger_k \varphi_k.$$  \hspace{1cm} (48)

The ground state contains all $\eta$-fermions with $\omega_k < 0$, therefore the gap is

$$\Delta = \min_k |\omega_k|.$$  \hspace{1cm} (49)

A nontrivial TSS limit around $\bar{\mu} \equiv \mu - 1 = 0$, i.e., at the transition between a low-density superfluid and the empty vacuum state (named $\langle n_i \rangle = 0$ Mott phase above), is obtained (for small $|\omega_k|$) by rescaling

$$x = l^{p/(2 + p)}X, \quad \bar{\mu} = l^{-2p/(2 + p)}\mu_r, \quad \omega_k = l^{-2p/(2 + p)}\Omega_k.$$  \hspace{1cm} (50)

Indeed, neglecting terms which are suppressed in the large-$l$ limit, Eq. (47) becomes

$$(2X^p - \partial^2 X) \varphi_k(X) = (\Omega_k - 2\mu_r)\varphi_k(X).$$  \hspace{1cm} (51)

This shows that $\theta = p/(2 + p)$, in agreement with Eq. (45).

Moreover, this implies that any energy scale, and in particular the gap $\Delta = E_1 - E_0$, must behave as

$$\Delta \approx l^{-2\theta}D(\mu_r), \quad \mu_r = l^{2\theta}\bar{\mu},$$  \hspace{1cm} (52)

which agrees with the RG scaling equation (5), since $z = 2$ and $\nu = 1/2$. For $p = 2$, by solving Eq. (51), we obtain

$$D(\mu_r) = \min_k |2^{3/2}(k + 1/2) + 2\mu_r|, \quad k = 0, 1, \ldots;$$  \hspace{1cm} (53)

$D(\mu_r)$ is a triangle wave for $\mu_r \leq 0$ and it is linear for $\mu_r \geq -1/\sqrt{2}$.

The TSS of the particle density in the middle of the trap is obtained by computing

$$\langle n_0 \rangle = l^{-\theta} \sum_k |\varphi_k(0)|^2 (\varphi^\dagger_k \varphi_k),$$  \hspace{1cm} (54)

\[\text{---}

1 For $\mu < 1$, the ground state contains all the $\eta$-fermions diagonalizing the Hamiltonian with $\omega_k < 0$, cf. Eq. (48). In the presence of the trapping potential (2), level crossings of the lowest states occur in the $\mu$-$l$ plane separating the region with $N \equiv \sum_i (b_i^\dagger b_i) = n$ from $N = n + 1$. Since, in the absence of the trap potential and for $\mu < 1$, the ground state has a finite density $N/l > 0$, for fixed $\mu < 1$ the lowest states show an infinite number of level crossings as $l \to \infty$ (after $L \to \infty$) where the gap vanishes.
where \( \varphi_k(X) \) are the normalized eigenfunctions of Eq. (51); \( \langle \eta_k^\dagger \eta_k \rangle = 1 \) if \( \Omega_k < 0 \) and 0 otherwise; since \( \varphi_k(X) = (-1)^k \varphi_k(-X) \), only even \( k \)s contribute. For \( p = 2 \) we obtain the sum

\[
l^\theta \langle n_0 \rangle \equiv (2^{1/4}/\sqrt{\pi}) \sum [(2j - 1)!]^2/(2j)!
\]

over integer \( j \geq 0 \) satisfying \( 2^{1/2}(2j+1/2) + \mu_r < 0 \). Again, this result agrees with the TSS theory, taking into account that the RG dimension of the particle density is \( y_n = d + z - y_\mu = 1 \). Results from numerical diagonalization at \( p = 2 \) are shown in Fig. 7; they fully support the above TSS behaviors. Note the peculiar plateaux and the discontinuities in the particle density at negative values of the scaling variable \( \mu_r \equiv l^2 \delta \mu \). For \( \mu_r \to -\infty \), \( \langle n_0 \rangle \approx \sqrt{2\mu}/\pi \), which matches the critical behavior for \( \bar{\mu} < 0 \) in the absence of the trap [11].

Numerical results for higher power laws of the potential turn out to be in full agreement with the predictions of TSS and are qualitatively similar to the results for \( p = 2 \), including those for \( p \to \infty \) which effectively corresponds to the finite-size scaling of the homogeneous system without confining potential.

V. CONCLUSIONS

We have developed a trap-size scaling (TSS) theory for confined particle systems at quantum transitions. We propose an extension of the scaling laws of the homogeneous system to allow for the confining potential in the large trap-size limit. The quantum critical behavior of the confined system is cast in the form of a TSS, resembling finite-size scaling theory [10, 14, 15], with a nontrivial trap critical exponent \( \theta \), which describes how the length scale \( \xi \) of the system evolves with the trap size.
critical modes diverges with increasing trap size, i.e., $\xi \sim l^\theta$, at the quantum critical point. This provides a theoretical framework to describe the quantum critical behavior of confined systems.

We have shown by explicit analytical computation how TSS emerges in the quantum XY chain, where an inhomogeneity analogous to the one arising from a trapping potential in particle systems can be achieved by considering a space-dependent transverse field.

Moreover, we have discussed this issue within the Bose-Hubbard model with a confining potential, which is relevant for the description of cold atomic gases in optical lattices. In particular, we have presented some analytical results for the low-density Mott transition in the hard-core limit of the one-dimensional BH model. The results again support TSS, although the corresponding TSS functions show a peculiar behavior, like discontinuities in the scaling particle density, which are clearly related to the quantum nature of the transition.

Helpful discussions with P. Calabrese are gratefully acknowledged.

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