Quasi-long-range order in trapped systems

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We investigate the effects of a trapping space-dependent potential on the low-temperature quasi-long-range order phase of two-dimensional particle systems with a relevant U(1) symmetry, such as quantum atomic gases. We characterize the universal features of the trap-size dependence using scaling arguments. The resulting scenario is supported by numerical Monte Carlo simulations of a classical two-dimensional XY model with a space-dependent hopping parameter whose inhomogeneity is analogous to that arising from the trapping potential in experiments of atomic gases.

Statistical systems are generally nonhomogeneous in nature, while homogeneous systems are often an ideal limit of experimental conditions. Thus, in the study of critical phenomena, an important issue is how critical behaviors develop in nonhomogenous systems. Particularly interesting physical systems are interacting particles constrained within a limited region of space by an external potential. This is a common feature of the experimental realizations of the Bose-Einstein condensation (BEC) in diluted atomic vapors [1] and of optical lattices of cold atoms [2], which have provided a great opportunity to investigate the interplay between quantum and statistical behaviors in particle systems.

In the BEC scenario, a macroscopic number of bosonic atoms accumulate in a single quantum state and are described by a condensate wave function, which naturally provides the complex order parameter $\psi(x)$ of the phase transition and its relevant U(1) symmetry. These global features characterize the XY universality class which describes the universal critical behavior of a large class of systems, see, e.g., Ref. [3]. The critical behavior arising from the formation of the condensate in a trapped Bose gas has been investigated experimentally [4], observing an increasing correlation length compatible with the behavior expected at a continuous transition of homogeneous systems belonging the three-dimensional (3D) XY universality class. Two-dimensional (2D) homogeneous gases of bosonic particles do not show a real BEC with decreasing the temperature T. Nevertheless, they are expected to experience a finite-T Kosterlitz-Thouless (KT) transition [5] separating the high-T phase with short-ranged correlations from a low-T phase characterized by a quasi-long-range order (QLRO), where the one-body correlation function decays algebraically at large distance. Experimental evidences of such a transition in trapped Bose atomic gases have been provided in Refs. [6–8].

However, the inhomogeneity due to the trapping potential drastically changes the general features of the critical behavior at the transition separating the high-T and low-T phases, and, in the case of 2D systems, of the QLRO phase. For example, correlation functions of the critical modes do not develop a diverging length scale in a trap. The critical behavior of the unconfined homogeneous system could be observed around the middle of the trap only when the length scale ξ of the correlations is much smaller than the length scale ξ_t induced by the trap size, and one looks at small-distance correlations relatively to ξ_t. If ξ is large but not much smaller than the trap size, the critical behavior gets somehow distorted by the trap, although it gives rise to universal effects in the large trap-size limit, controlled by the universality class of the phase transition of the unconfined system [9, 10]. The understanding of the trap effects is necessary for an accurate determination of the critical parameters, see, e.g., Refs. [8, 11].

In this paper we consider 2D systems showing a low-T QLRO phase in their phase diagram, after a KT transition. We investigate how the presence of the trap changes the main features of the QLRO of the homogeneous system and, therefore, how one may get evidence of the QLRO phase from the behavior of the system in the presence of the trap. For this purpose, we resort to a scaling analysis which allows us to take into account the trap length scale when it becomes sufficiently large, exploiting the universality of the scaling behavior.

The above considerations also apply to other physically interesting models, such as the Bose-Hubbard (BH) model [12] at its finite-T superfluid transition, whose Hamiltonian in the presence of confining potential reads

$$\mathcal{H}_{\mathrm{BH}} = -\frac{J}{2}\sum_{\langle ij\rangle}(b_i^\dagger b_j + \mathrm{h.c.}) + \frac{U}{2}\sum_i n_i(n_i - 1)$$
$$+ \sum_i(\mu + v^2 r^2)n_i, \qquad (1)$$

where the sum runs over the bonds $\langle ij\rangle$ of a d-dimensional

lattice, b_i are bosonic operators, $n_i \equiv b_i^\dagger b_i$ is the particle density, r the distance from the center of the trap. The trap size is defined as $l \equiv J^{1/2}/v$, see, e.g., [14]. The BH model is of experimental relevance because it describes cold bosonic atoms trapped in a limited space region of optical lattices [13]. Other transitions in the XY universality class are the ^{4}He superfluid transition, insulator-superconductor transitions, like that of the attractive Hubbard model, etc....

In a standard scenario for a continuous transition, see, e.g., [3], the critical behavior of a d-dimensional system is characterized by two relevant parameters u_t and u_h, which may be associated with T, i.e., $u_t \sim T/T_c - 1$ and the external field h coupled to the order parameter, with renormalization-group (RG) dimension $y_t = 1/\nu$ and $y_h = (d + 2 - \eta)/2$. The presence of a trap of size l generally induces a further length scale ξ_t, which must be taken into account to describe the critical correlations. Within the trap-size scaling (TSS) framework [9, 10], the scaling law of the singular part of the free energy density around the center of the trap can be written as

$$F_{\rm sing} = l^{-\theta d}\mathcal{F}(u_t l^{\theta y_t}, u_h l^{\theta y_h}, x l^{-\theta}) \qquad (2)$$

where θ is the *trap exponent*. At the critical point ($u_t = 0$), the length scale induced by the trap behaves as $\xi_t \sim l^\theta$, and the correlation function of the order parameter as

$$G(x,y) \equiv \langle\bar\psi(x)\psi(y)\rangle_c = l^{-\theta\eta}\mathcal{G}(x l^{-\theta}, y l^{-\theta}). \qquad (3)$$

Finite size effects, due to a finite volume L^d, can be taken into account by adding a further dependence on $Ll^{-\theta}$ in the above scaling Ansatz [15].

The value of θ depends on the way the external confining field is coupled to the model variables. In the case relevant for the above-mentioned particle systems, the external trapping potential is coupled to the particle density. The corresponding perturbation can be inferred from the many-body Hamiltonian [16] in the presence of the external potential $V(x) = v^p x^p$, i.e., $P_V = \int d^d x\, V(x)|\psi(x)|^2$, where $\psi(x)$ is the complex order-parameter field. The computation of the RG dimensions of the trap parameter leads to [9] $\theta = p\nu/(1 + p\nu)$. In order to apply it to the KT transition of 2D U(1)-symmetric systems, we formally set $\nu = \infty$, corresponding to the KT exponential behavior of the correlation length $\xi \sim \exp(\tau^{-1/2})$ where $\tau \equiv T/T_c - 1 \to 0^+$, thus obtaining $\theta = 1$ for any power p of the potential. For comparison, we mention that $\theta = 0.57327(4)$ at the 3D BEC transition in a harmonic trap [9]. Moreover, in a Gaussian theory perturbed by P_V, since $\nu = 1/2$ we have $\theta = p/(2+p)$, for any spatial dimension. It is worth mentioning that analogous TSS behaviors [10], with the same trap exponents, apply to the quantum $T = 0$ superfluid-Mott transition of the BH model (1) at fixed integer density, which belongs to the $(d+1)$-dimensional XY universality class [12].

A standard representative model of the 2D XY universality class is the classical square-lattice XY model,

$$H = -J\sum_{\langle ij\rangle}{\rm Re}\,\bar\psi_i\psi_j, \quad \psi_i \equiv e^{i\varphi_i} \in {\rm U}(1), \qquad (4)$$

which presents the same universal features of 2D systems whose phase diagram shows a KT transition between high-T and low-T QLRO phases. We may further exploit universality to investigate the effects of an inhomogeneity analogous to that of 2D trapped particle systems, where the external confining potential is generally coupled to the particle density, which can be associated with an energy-density operator in a corresponding effective model. A 2D XY model with an external space-dependent field coupled to the energy density is obtained by considering a space-dependent hopping parameter U_{ij}, [17]

$$H_U = -J\sum_{\langle ij\rangle}{\rm Re}\,\bar\psi_i U_{ij}\psi_j, \qquad (5)$$

$$U_{ij} = 1 + V(r_{ij}), \quad V(r) = v^p r^p, \qquad (6)$$

where p is an even positive integer, r_{ij} is the distance from the origin of the midpoint of nearest-neighbor sites. We set $J = 1$. The inhomogeneity arising from the space dependence of U_{ij} is analogous to that arising from a trapping potential in particle systems, such as the BH model (1). Thus, $l \equiv 1/v$ may be considered as the analog of the trap size. At large distance, since $V(r) \to \infty$, the spin variables get effectively frozen. When $p \to \infty$ the effect of the external potential V is equivalent to confining a homogeneous system in a box of size $L = l = 1/v$, and the TSS becomes the standard finite-size scaling (FSS). At the critical KT temperature $T_c = 0.893(1)$ [18] of the homogeneous model (4), the TSS of the model (5) is expected to follow the scaling Ansatz (2) and (3), with $\eta = 1/4$ and $\theta = 1$ as computed above by RG arguments.

We now turn to the QLRO phase, which is the main issue of this paper. The homogeneous model is critical in the whole low-T region $T < T_c$, where the correlation function $\langle\bar\psi_x\psi_y\rangle$ decays as $1/|x-y|^{\eta(T)}$ with a T-dependent exponent $\eta(T)$: $\eta(T) = T/(2\pi) + O(T^2)$, increasing up to $\eta(T_c) = 1/4$ (some numerical estimates are reported in Refs. [19, 20]). This critical behavior is controlled by a line of Gaussian fixed points, essentially given by the spin-wave theory $H_{\rm sw} = \int d^2 x\,(\nabla\varphi)^2$, which is the leading nontrivial term for $T \to 0$. We may apply the same spin-wave approximation to infer the value of θ controlling the TSS in the QLRO phase. In the spin-wave limit we obtain

$$H_{\rm sw} = \int d^2 x\,\frac{1}{2}(1 + v^p r^p)(\nabla\varphi)^2. \qquad (7)$$

The trap exponent θ is related to the RG dimension y_v of parameter v, $\theta = 1/y_v$, which can be obtained from
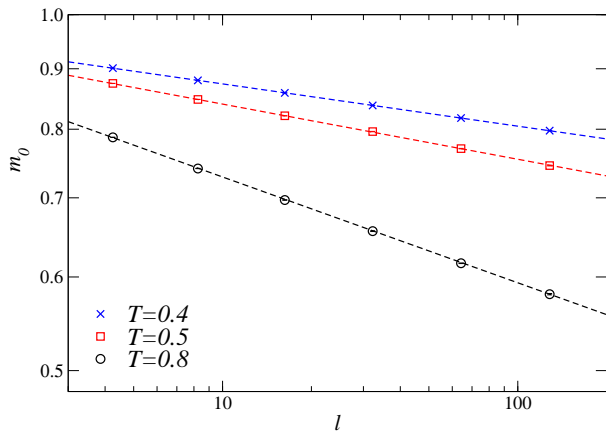
FIG. 1: Log-log plot of $m_0 \equiv \langle \psi_0 \rangle$ for the model (5), at $T = 0.4$, 0.5, 0.8, for $L/l \simeq 2$ [21]. Statistical errors are hardly visible. The lines show fits to $al^{-\zeta/2}$.
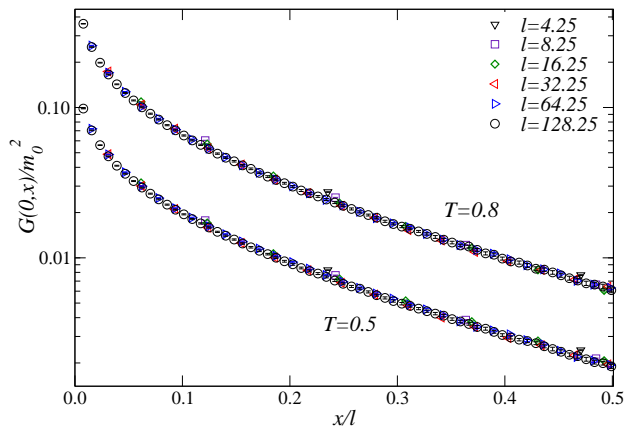

FIG. 2: $G(0,x)/m_0^2$ vs x/l for the model (5), at $T = 0.5$, 0.8, for several values of l, and $L/l \simeq 2$ [21]. The sets of data at fixed T are clearly converging to a nontrivial large-l limit

the relation $py_v - p + y_{(\partial_\mu \varphi)^2} = d$ taking also into account that $y_{(\partial_\mu \varphi)^2} = d$ in the spin-wave theory. We eventually obtain $\theta = 1$ independently of the power p.

Therefore, we have $\theta = 1$ at very low-T, where the spin-wave approximation holds, and at the KT transition at $T = T_c$. A natural scenario is that the TSS has universal features in the whole QLRO, with $\theta = 1$ for any $T \le T_c$. We shall provide numerical evidence of this scenario.

For this purpose, we present numerical results for the model (5) with $V(r) = (r/l)^2$, for $T < T_c \simeq 0.893$, obtained by Monte Carlo (MC) simulations. We center the trap in the middle of a square lattice $(2L+1) \times (2L+1)$. The parameter L and l are chosen so that the spin variables close to the boundaries are effectively frozen, making unnecessary the use of larger lattices. We use fixed boundary conditions $\psi_b = 1$. [21]

We consider the local magnetization at the origin and the two-point correlation function, defined as

$$m_0 \equiv \langle \psi_0 \rangle, \quad G(\vec{x}, \vec{y}) \equiv \langle \bar{\psi}_{\vec{x}} \psi_{\vec{y}} \rangle - \langle \bar{\psi}_{\vec{x}} \rangle \langle \psi_{\vec{y}} \rangle. \quad (8)$$

The boundary conditions $\phi_b = 1$ breaks the U(1) symmetry, thus allowing a nonzero local magnetization. According to the above scaling considerations, we expect that their asymptotic trap-size dependence is

$$m_0 \sim l^{-\eta(T)\theta/2}, \quad (9)$$
$$G(\vec{x}, \vec{y}) \approx l^{-\eta(T)\theta} \mathcal{G}(\vec{x}/l^\theta, \vec{y}/l^\theta), \quad (10)$$

where $\theta = 1$ and $\eta(T)$ is the T-dependent exponent of the homogeneous system. Since $\theta = 1$, a nontrivial simultaneous FSS and TSS limit can be achieved by keeping L/l fixed, where scaling behaviors analogous to Eqs. (9) and (10) apply. [22]

Fig. 1 shows data of m_0 for some values of $T < T_c$. A power-law trap-size dependence is clearly supported by the data. Fits to $al^{-\zeta/2}$, see Fig. 1, give $\zeta = 0.072(1)$, 0.093(1), 0.179(1) respectively for $T = 0.4$, 0.5, 0.8. Since according to Eq. (9) $\zeta = \eta\theta$ and $\theta = 1$, these results should be compared with the available estimates of $\eta(T)$ obtained in homogeneous systems, which are in good agreement [23].

Fig. 2 shows results for $G(0, \vec{x})$. In agreement with Eqs. (9) and (10), they show that $G(0, \vec{x})/m_0^2 = g(x/l)$ in the large-l limit. At small distance $x \ll l$, $g(y) \sim y^{-\eta(T)}$, to recover the behavior of the homogeneous system.

The spatial dependence of the local magnetization does not show a simple scaling behavior. The numerical results appear consistent with

$$\langle \psi_x \rangle \approx l^{-\eta(T_X)/2} f(X) \quad (11)$$

where $X \equiv x/l$ and $T_X \equiv T/(1 + X^2)$, which can be derived using arguments based on a local-temperature approximation, noting that T_X may be considered as an effective local (space-dependent) temperature.

We also consider a 2D XY model where the hopping parameter decreases moving far from the origin, i.e., replacing

$$U_{ij} = [1 + V(r_{ij})]^{-1}, \quad V(r) = v^2 r^2, \quad (12)$$

in Eq. (5). In this case the regions far from the origin are effectively in the high-T phase. The lattice system is set as before, but we use open boundary conditions which are compatible with a diverging hopping parameter at large distance. Thus, $\langle \psi_x \rangle = 0$ everywhere, including the origin. MC simulations show that the TSS is again characterized by the trap exponent $\theta = 1$. This is shown by Fig. 3, where we report $l^{\eta(T)} G(0, x)$ for several values of l, $L/l \approx 2$ [24], with $\eta(T)$ obtained from the data of Fig. 1. The sets of data for $T = 0.5$ and $T = 0.8$ are clearly converging to a nontrivial large-l limit, at least up to $X \equiv x/l$ corresponding to $T_X \simeq T/(1 + X^2) = T_c \approx 0.893$ ($X_c \approx 0.89$, 0.34 for $T = 0.5$, 0.8 respectively). [25]

In conclusion, we have characterized the trap-size dependence within the low-T QLRO phase and at the KT finite-T transition of 2D trapped systems. Using scaling
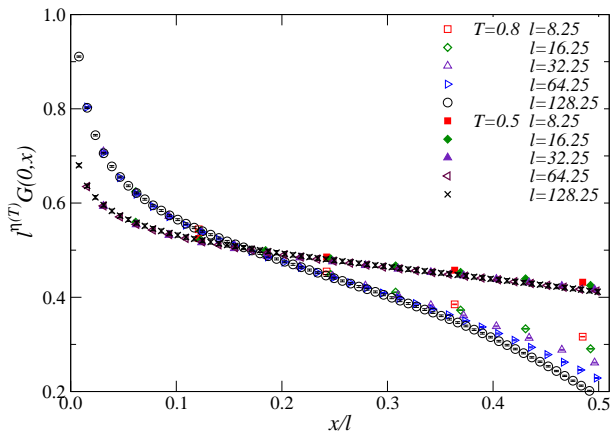
FIG. 3: $l^{\eta(T)}G(0,x)$ vs x/l, for the U_{ij} given in Eq. (12), at $T = 0.5$, 0.8, for several values of l, and $L/l \approx 2$.

arguments, we have argued that it is described by the TSS Ansatz (9) and (10) with the trap exponent $\theta = 1$ in the whole QLRO phase, up to the KT transition. This scenario has been supported by numerical results for classical 2D XY models with space-dependent hopping parameters, which give rise to inhomogeneities analogous to that of trapped atomic gases in actual experiments. These results should be useful to get evidence of QLRO in trapped systems, and also determine the critical parameters at the KT transition, such as T_c in model (5). For example, the KT critical point corresponds to a TSS with $\eta = 1/4$, while values $\eta < 1/4$ corresponds to the low-T QLRO phase.

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[21] In our simulations, we consider square lattices with $-L \le x_1, x_2 \le L$, and trap potential $V_L(\vec{x}) = c_v |x|^2/(L+1/2)^2$. At the boundaries $|x_1|, |x_2| = L + 1$ the spin variable is kept fixed: $\psi_b = 1$. The corresponding *trap* size is $l = (L+1/2)/\sqrt{c_v}$. We used a mixture of Metropolis and overrelation algoritms to update the spin variables [27]. We chose sufficiently large values of c_v to make finite-L effects negligible. The data shown in Figs. 1 and 2 were obtained using $c_v = 4$, corresponding to $L/l \approx 2$. We obtained analogous results for $c_v = 8$, i.e., $L/l \approx 2.8$.
[22] Scaling corrections are suppressed by powers of l. Since $\theta = 1$, they should be $O(l^{4-1/\eta(T)})$ as in the FSS of the homogeneous system [27].
[23] Estimates of η for the square-lattice nearest-neighbor XY model at $T = 0.4$, 0.5, 0.8 are respectively $\eta = 0.079(6)$, $0.098(7)$, $0.171(3)$ from Ref. [19], and $\eta = 0.074(6)$, $0.100(8)$, $0.19(2)$ from Ref. [20].
[24] Finite-L effects turn out to be stronger in this case. The data shown in Fig. 3 were obtained using $c_v = 4$ [21], corresponding to $L/l \approx 2$. We also performed MC simulations with $c_v = 16$, thus $L/l \simeq 4$, which showed a scaling behavior consistent with Eq. (10) as well.
[25] The behavior for $X > X_c$ is not completely clear. Our MC data, in particular for $L/l \approx 4$ up to $L = 256$ (not shown here), suggest a vanishing large-l limit for $X > X_c$.
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