Correlations at a quantum phase transition in interacting Bose systems

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Abstract

We have investigated the correlation functions of interacting bosons at the generic superfluid-insulator transition, a prototypical quantum phase transition, in two dimensions in the spherical limit. Unexpectedly the spatial correlation functions show non-power-law behavior consisting of two parts: short-range correlation due to the particle-hole pair excitations and long-range off-diagonal order due to the single-particle condensation. The temporal correlation functions, on the other hand, show power-law behavior.
Quantum phase transitions of interacting bosons have continuously drawn significant attention. They have been realized in many different systems, such as Josephson-junction arrays, thin film superconductors, \(^4\)He films and ultracold atoms in optical lattices. Typically the transition occurs between a superfluid and an insulator, and often serves as a prototype of the quantum phase transition because of its convenience in describing the transition in terms of the establishment of a macroscopic phase coherence.

Quantum phase transitions are frequently discussed in equivalent classical models which include fluctuations in the temporal direction. For the special case with the dynamical critical exponent \(z = 1\), the equivalence of the spatial and temporal directions directly confirms the validity of this mapping. In this scheme the properties of quantum phase transitions in \(d\) dimensions are readily derived from the classical models in \(d + 1\) dimensions. In general, however, asymmetry between the spatial and temporal directions in quantum phase transitions results in \(z \neq 1\). Even for this case, a simple extension of the above scheme into \(d + z\) dimensions is frequently assumed. Many scaling ansatz, such as hyperscaling relations, are constructed on the basis of this assumption. Similarly, correlation functions at the transition are assumed to have power-law behavior effectively in \(d + z\) dimensions. Some numerical works have used this assumed property to extract the value of \(z\) from correlation functions. However, it is quite plausible that the asymmetry of fluctuations in the spatial and the temporal directions, which brings non-unity of \(z\), would modify the correlation functions.

In this work, we investigate the scaling properties of the quantum rotor model, which is equivalent to the boson Hubbard model in large density limit, at the generic superfluid-insulator transition in two dimensions in the spherical limit. We find that the scaling behavior clearly supports hyperscaling in \(d + z\) dimensions with \(z = 2\), as predicted. However, the spatial correlation functions at the transition show, instead of power-law behavior, properties consisting of two parts: one is a short-range contribution from the particle-hole pair excitations and the other is the off-diagonal long-range order due to single-particle condensation. This implies that the macroscopic phase coherence is achieved through the single-particle condensation rather than the establishment of long-range correlation of fluctuations in a spatial direction, and we have the background particle-hole excitations as a normal fluid, instead of the single-particle excitations, even in the case with a charge-offset. The temporal correlation functions, on the other hand, show the power-law behavior as expected.
The universal features of quantum phase transitions in interacting Bose systems are divided into two universality classes depending on whether the transition is driven either by the phase fluctuations or by the density fluctuations of bosons. At a commensurate density the particle-hole symmetry is sustained across the transition, and the transition is driven by the phase fluctuations or, equivalently, by the particle-hole pair excitations. This transition belongs to the \((d+1)\)-dimensional classical XY spin model with \(z = 1\). In the presence of a charge-offset, however, either single particle or hole excitations are favored: the transition is marked by the disappearance of the energy gap for single particle or hole excitations. Therefore, the universality class of this transition, known as the generic superfluid-insulator transition, is characterized by the single-particle nature, carrying \(z = 2\) and the mean-field correlation length critical exponent \(\nu = 1/2\). It is interesting to investigate whether correlation functions could reveal directly the different nature of fluctuations in two universality classes.

The essential properties of strongly correlated interacting bosons can be captured by a boson Hubbard model

\[
H = \frac{U}{2} \sum_i n_i^2 - \mu \sum_i n_i - t \sum_{<ij>} (b_i^{\dagger} b_j + b_j^{\dagger} b_i),
\]

where \(b_j^{\dagger}\) is the boson annihilation operator at \(j\)-th site, and \(n_j\) is the number operator. \(U\) and \(t\) stand for the strength of on-site repulsion and nearest neighbor hopping respectively, and \(\mu\) is the chemical potential. It is convenient to put \(\mu/U \rightarrow n_0 + \mu/U\) with an integer \(n_0\) to make \(-1/2 < \mu/U < 1/2\). Here \(n_0\) is an integer representing the background number of bosons per site. We study the phase transition of this model on two-dimensional square lattices.

The phase transition of this model is characterized by establishment of the phase coherence of the order parameter. In the limit \(n_0 \gg 1\), the Hamiltonian is reduced to the quantum rotor model

\[
H = \frac{U}{2} \sum_i n_i^2 - \mu \sum_i n_i - 2J \sum_{<ij>} \cos(\theta_i - \theta_j),
\]

where \(\theta_j\) is the phase angle of the order parameter, \(n_j = -i \partial / \partial \theta_j\), and \(J = n_0t\).

Now we use the spherical approximation to investigate the quantum phase transition of the above model. The spherical approximation has been widely used in studies on phase
transitions, which is very powerful in handling models beyond the mean-field level. This
method treats phase transitions in a scheme which is exact in the limit that the number of order parameter components goes to infinity. It has been used to study quantum phase transitions in Bose systems\[13\]. Previously this method was used\[14\] to study the superfluid-insulator quantum transition at a commensurate density in two dimensions, yielding $\nu = 1$ and $z = 1$, as expected.

Through a path integral mapping, we can construct the corresponding classical action

$$S_0[\psi] = -\int_0^\beta d\tau [K \sum_i \psi_i^*(\tau) (\partial_\tau - \mu)^2 \psi_i(\tau) - \sum_{i,j} (\delta_{ij} \sigma - J_{ij}) \psi_i^*(\tau) \psi_j(\tau)],$$

where $K = 1/(2U)$, $\beta$ denotes the inverse temperature, $J_{ij}$ denotes the nearest neighbor hopping matrix elements, and $\psi_j = e^{-i\theta_j}$. The trace in the partition function should be taken with the constraint $|\psi_j| = 1$ for every $j$. But we introduce a Lagrange multiplier $\sigma$ to replace the constraint by a less strict self-consistent condition $1 = \langle \psi_j(\tau) \psi_j^*(\tau) \rangle_0$, where $\langle ... \rangle_0$ represents the average over $S_0$, which is called the spherical approximation.

In this work we focus on the case with a charge-offset ($\bar{n} = \mu/U \neq 0$). Scaling theories predicted that the dynamical critical exponent $z = 2$\[2\]. To confirm this through the hyperscaling hypothesis in $d + z$ dimensions, we investigate the finite-size scaling behavior of the superfluid stiffness

$$\rho_s = L^{-(d+z-2)} X_\rho(L^{1/\nu}(K - K_c), \bar{\beta}/L^z),$$

where $X_\rho$ is a scaling function. By diagonalizing the equation $\sum_{j} (\sigma \delta_{ij} - J_{ij}) \phi^q_j = \epsilon^q \phi^q_i$ to have $\phi^q_i = (1/\sqrt{L^2}) e^{i\vec{q} \cdot \vec{R}_i}$ and $\epsilon^q = \sigma - 2J(\cos q_x + \cos q_y)$, where $\vec{R}_j$ is the position vector of $j$-th site and $\vec{q} = (2\pi/L)(n_x, n_y)$ is the wave vector with integer $n_x$ and $n_y$, we can easily derive the formula

$$\rho_s = \frac{1}{L^2} \sum_{\vec{q}} \left\{ \frac{J}{2\sqrt{K \epsilon^q}} (\cos q_x - \frac{J \sin^2 q_x}{\epsilon^q}) \left[ \coth \frac{\bar{\beta}}{2} (\sqrt{\epsilon^q/K - \mu}) + \coth \frac{\bar{\beta}}{2} (\sqrt{\epsilon^q/K + \mu}) \right] 
- \frac{J^2 \bar{\beta} \sin^2 q_x}{4\epsilon^q K} \left[ \frac{1}{\sinh^2 \frac{\bar{\beta}}{2} (\sqrt{\epsilon^q/K - \mu})} + \frac{1}{\sinh^2 \frac{\bar{\beta}}{2} (\sqrt{\epsilon^q/K + \mu})} \right] \right\}. \quad (5)$$

Here we set the lattice constant to be 1, and take the energy unit $J = 1$.

Figure\[1\] shows the finite-size scaling behavior of $\rho_s$ for $\bar{n} = 0.1$. With $z = 2$, curves for different sizes $L = 60, 80, 100, ..., 200$ cross at a point $K_c = 0.09513(2)$. Here we fix the aspect ratio to have $\bar{\beta}/L^z = 0.02$, and obtain the correlation critical exponent $\nu = 0.5$, as
FIG. 1: The finite-size scaling behavior of the superfluid stiffness, $\rho_s$, for $\bar{n} = 0.1$. High quality crossing behavior at $K_c = 0.09513(2)$ with $z = 2$ for $L = 60, 80, 100, \ldots, 200$ is obtained without suffering from any statistical errors. We set $\bar{\beta}/L^z = 0.02$. Inset: The data collapse onto a single curve as a function of the scaling variable $L^{1/\nu}(K - K_c)$ with $\nu = 0.5$.

shown in the inset. The high quality crossing behavior implies that $\rho_s L^{d+z-2}$ is indeed a universal quantity in the vicinity of the critical point, strongly supporting the hyperscaling hypothesis in $d + z$ dimensions.

Now we turn our attention to the correlation functions. The correlation function between $\vec{R}_i$ and $\vec{R}_j$ with distance $\tau$ in time is given by

$$G(|\vec{R}_i - \vec{R}_j|, \tau) = \frac{1}{L^2} \sum_q e^{i\vec{q} \cdot (\vec{R}_i - \vec{R}_j)} \left[ e^{-\beta(\sqrt{e^q/K} + \mu)} + \frac{e^{-\tau(\sqrt{e^q/K - \mu})}}{1 - e^{-\beta(\sqrt{e^q/K - \mu})}} \right],$$

for $0 < \tau < \bar{\beta}$. It was assumed $^{2, 10}$ that at the critical point the correlation functions show long-range power-law behavior in $d + z$ dimensions so that $G(|\vec{R}_i - \vec{R}_j|, \tau) \sim 1/(|\vec{R}_i - \vec{R}_j|^2 + \tau^{2\eta})^{y/2}$, where $y = d + z - 2 + \eta$ ($\eta$ is the anomalous critical exponent). Based on this assumption, estimation of the value of $z$ has been made $^{10, 11, 15}$ by comparing the asymptotic behavior of the spatial and temporal correlation functions.

Figure 2 shows the spatial correlation functions along a spatial direction at the critical point. Surprisingly they do not show the power-law behavior; instead, the correlation functions have forms

$$G(x, 0) = A(x^{-1}e^{-x/\lambda} + (L - x)^{-1}e^{-(L-x)/\lambda}) + C$$

(7)
FIG. 2: Log-log plot of the correlation functions along a spatial axis at the critical point $K_c = 0.095132$ for $\bar{n} = 0.1$. They do not show the power-law behavior. The curves are fitted perfectly onto the form $G(x,0) = A(x^{-1}e^{-x/\lambda} + (L-x)^{-1}e^{-(L-x)/\lambda}) + C$.

for $1 \ll x \ll L$, where $\lambda$ is a finite number, insensitive to the size of the system, $C$ is a constant depending on the size, and $A$ is a fitting parameter. For example, for the curve in Fig. 2 with $L = 200$, $A = 0.26$, $\lambda = 6.11$, and $C = 1.17 \times 10^{-4}$. Similar features found in Monte Carlo calculations were discussed as a result of finite-size effect\[15\]. Here we use the same value of the aspect ratio $\bar{\beta}/L^z = 0.02$, previously used in Fig. 1. For significantly wide range of $\bar{\beta}/L^z$, the same behavior is found. Very small aspect ratios, however, change the behavior, possibly due to finite-temperature effects, but still no power-law behavior occurs.

We can easily identify the meaning of the constant $C$. The spatial correlation function is actually flat for $x \approx L/2$. In other words, $C = G(L/2,0) = |\langle \psi \rangle|^2$, where $|\langle \psi \rangle|$ is the off-diagonal long-range order parameter. Note that the constant $C$ is absent for the case $\bar{n} = 0$ in which the correlation functions show pure power-law behavior $G(x,0) \sim x^{-1}$\[14, 16\]. Figure 3 shows the scaling behavior of $|\langle \psi \rangle|$. We obtain the mean-field critical exponents $\nu = 0.5$ and $\beta/\nu = 1$, where $\beta$ is the critical exponent characterizing the scaling properties of the order parameter.

The long-range off-diagonal order is coming from the single-particle condensation. We can find this clearly by observing the momentum distribution, $n_q$, in Figure 4. Here we plot the momentum distribution as a function of $\bar{q} = (2\pi/L)(m,m)$. The density of the
FIG. 3: The finite-size scaling behavior of the off-diagonal long-range order parameter for $L = 100, 120, ..., 200$, providing the mean-field critical exponents $\nu = 0.5$ and $\beta/\nu = 1$.

FIG. 4: Momentum distribution of the quantum rotor model near the superfluid-insulator transition. The density of condensate at $\vec{q} = 0$ rises sharply as the superfluid onset transition is tuned. The momentum distribution consists of the single-particle condensate at $\vec{q} = 0$ and background normal fluid, bringing the macroscopic phase coherence and contributing to short-range correlations, respectively. It is quite interesting to note that the normal fluid of interacting bosons is not the single-particle excitations but the particle-hole pair excita-
FIG. 5: The range of the correlation due to the particle-hole excitations as a function of the charge-offset $\bar{n}$. It diverges like $\lambda \sim 0.61/\bar{n}$ as $\bar{n} \to 0$.

ions which contribute to the asymptotic correlation $G(x,0) \sim x^{-y}e^{-x/\lambda}$ with $y = 1$ rather than $y = 2$. The correlation range of the particle-hole pair fluctuations at the transition diverges like $\lambda \sim 0.61/\bar{n}$ as $\bar{n} \to 0$, as shown in Figure 5, ultimately yielding the power-law correlations at $\bar{n} = 0$.

The temporal correlation functions, however, show the power-law behavior $G(0,\tau) \sim 1/\tau^{(z+\eta)/z}$ with $(z+\eta)/z = 1.0$, implying $\eta \approx 0.0$. This exponent and other exponents obtained above confirm the hyperscaling relation $2\beta = \nu(d + z - 2 + \eta)$. But it is not possible to determine the value of $z$ directly from the correlation functions if they do not show the power-law behavior.

In this work, we have studied the generic superfluid-insulator transition in interacting Bose systems via the spherical approximation. Scaling properties of physical quantities, such as the superfluid stiffness and the off-diagonal order, confirm the hyperscaling relations in $d + z$ dimensions, providing the critical exponent $z = 2$, $\nu = 1/2$, and $\beta = 1/2$. These values of the critical exponents, supporting the mean-field nature of the transition, are consistent with theoretical predictions and other calculations. However, the spatial correlation functions at the transition do not show the power-law behavior. Instead they indicate that the correlations consist of two parts: short-range correlations due to the normal fluid of the particle-hole pair excitations and macroscopic long-range off-diagonal order due to the
FIG. 6: The temporal correlation functions at $K = 0.095132$ for $\bar{n} = 0.1$. They show the power-law behavior $G(0, \tau) \sim 1/\tau^{(z+\eta)/z}$ with $(z+\eta)/z = 1.0$. It implies that $\eta \approx 0.0$, but the determination of $z$ is not possible.

single-particle condensations. The temporal correlation function, on the other hand, show the power-law behavior even though direct determination of $z$ is not possible.

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