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Universal properties of the Higgs resonance in (2+1)-dimensional $U(1)$ critical systems

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We present spectral functions for the magnitude squared of the order parameter in the scaling limit of the two-dimensional superfluid to Mott insulator quantum phase transition at constant density, which has emergent particle-hole symmetry and Lorentz invariance. The universal functions for the superfluid, Mott insulator, and normal liquid phases reveal a low-frequency resonance which is relatively sharp and is followed by a damped oscillation (in the first two phases only) before saturating to the quantum critical plateau. The counter-intuitive resonance feature in the insulating and normal phases calls for deeper understanding of collective modes in the strongly coupled (2+1) relativistic field theory. Our results are derived from analytically continued correlation functions obtained from path-integral Monte Carlo simulations of the Bose-Hubbard model.

Field theories of a complex scalar order parameter, Ψ, can have two types of collective excitations. The first one originates from fluctuations of the phase of Ψ and describes a Bogoliubov sound mode. The second one, if present, describes amplitude fluctuations and is associated with a Higgs mode. In superfluids, sound excitations are gapless while the Higgs mode, if present, is gaped but the gap may go to zero under special circumstances such as an emergent particle-hole symmetry and Lorentz invariance. This is what happens in the vicinity of the superfluid (SF) to Mott insulator (MI) quantum critical point (QCP) of the Bose-Hubbard model when the phase transition is crossed at constant density.

Mean-field theory predicts a stable Higgs particle. In (3+1) dimensions, where the QCP is a Gaussian fixed point (with logarithmic UV corrections), there is compelling experimental evidence for the existence of a Higgs mode, most beautifully illustrated for the TlCuCl$_3$ compound [1] (see Ref. [2] for the latest results with cold gases). In (2+1) dimensions, where scaling theory is expected to apply, the massive Higgs particle is strongly coupled to sound modes and it was argued for a long time, on the basis of a $1/N$-expansion to leading order ($N = 2$ corresponds to our case), that it cannot survive near criticality [3–6]. Moreover, since the longitudinal susceptibility diagram has an IR divergence going as ω^{-1}, it may well dominate any possible Higgs peak. However, it was recently emphasized that the type of the probe is important [7–9]: for scalar susceptibility (i.e., the correlation function of $|\psi|^2$) the spectral function $S(\omega)$ vanishes as ω^3 at low-frequencies [3, 7], and this offers better conditions for revealing the Higgs peak. In the scaling limit the theory predicts that $S(\omega)$ in the SF phase takes the form

$$S_{\mathrm{SF}}(\omega) \propto \Delta^{3-2/\nu}\Phi_{\mathrm{SF}}(\frac{\omega}{\Delta}) , \qquad (1)$$

where Δ is the MI gap for the same amount of detuning from the QCP, and $\nu = 0.6717$ is the correlation length exponent for the $U(1) \equiv O(2)$ universality in $(2 + 1)$ dimensions [10, 11]. The universal function $\Phi_{\mathrm{SF}}(x)$ starts as $\Phi_{\mathrm{SF}}(x \to 0) \propto x^3$ and saturates to a quasi plateau $\Phi_{\mathrm{SF}}(x \gg 1) \propto x^{3-2/\nu} \approx x^{0.0225}$. The Higgs resonance (at $x \sim 1$) can be seen right before the incoherent quantum critical continuum with weak ω-dependence.

We are not aware of solid state studies of the Higgs mode in two-dimensional (2D) superfluids near the QCP. Recently, the cold atom experiment [12], where a 2D Bose-Hubbard system was gently 'shaken' by modulating the lattice laser intensity and probed by in-situ single site density measurements, saw a broad spectral response whose onset softened on approach to the QCP, in line with the scaling law (1), and no Higgs resonance. This outcome can be explained by tight confinement, finite temperature, and detuning from the QCP, as shown by Quantum Monte Carlo (MC) simulations [14] performed for the experimental setup 'as is' in the spirit of the quantum simulation paradigm [13]. On the other hand, simulations for the homogeneous Bose-Hubbard model (below J, U, and μ stand for the tunneling amplitude, on-site interaction, and chemical potential, respectively; in what follows energy and frequency are measured in units of J)

$$H = -J \sum_{<ij>} b_i^\dagger b_j + \frac{U}{2} \sum_i n_i(n_i - 1) - \mu \sum_i n_i , \quad (2)$$

in the vicinity of the SF-MI point featuring emergent particle-hole symmetry and Lorentz-invariance [15] unambiguously revealed a well-defined Higgs resonance which becomes more pronounced on approach to the QCP [14]. However, its universal properties, *i.e.*, the precise structure of $\Phi_{\mathrm{SF}}(x)$, were not answered in Ref. [14].

The Higgs mode is not discussed in the MI phase since

the order parameter is zero in the thermodynamic limit. Likewise, no resonance is expected in the normal quantum critical liquid (NL), *i.e.*, at finite temperature for critical parameters $(U, \mu) = (U_c, \mu_c)$. However, simulations reveal a resonance in the MI phase right after the gap threshold [14] suggesting that finite-energy probes are primarily sensitive to local correlations at length scales where MI and SF are indistinguishable. The universality of the MI response was likewise never clarified.

In their most recent calculation, Sachdev and Podolsky [16] found that including next-order corrections in a $1/N$ expansion in the scaling limit radically changes previous conclusions in that $S(\omega)$ does contain an oscillatory component, in line with MC simulations. However, the precise shape of the $\Phi_{\mathrm{SF}}(x)$ function could not be established within the approximations used.

In this Letter, we aim to determine the universal scaling spectral functions when approaching the QCP from the SF, MI, and NL phases. We rely on the worm algorithm [18–20] in the path integral representation to perform the required large-scale simulations. By collapsing spectral functions evaluated along the trajectories specified by the dashed lines in Fig 1, we extract universal features for all three phases. They are summarized in Fig. 2, which is our main result. Surprisingly, all of them include a universal resonance peak (relatively sharp in SF and MI phases), followed by a broad secondary peak (in SF and MI phases only) before merging with the incoherent critical quasi-plateau (the plateau value is the same in all cases, as expected). Our results are in agreement with scaling theory, and firmly establish that the damped resonance is present in all three phases. [The integrated spectral weight of the ω^3-law at low frequencies is too small to be resolved reliably by analytical continuation methods [14].]

The phase diagram of the 2D Bose-Hubbard model, shown in Fig. 1, is known with high accuracy [21–23] both at zero and finite temperature. The QCP is located at $U_c = 16.7424(1)$, $\mu_c = 6.21(2)$. When the system is slightly detuned from the QCP, either by changing the chemical potential or the interaction strength, we define the corresponding characteristic energy scale Δ using the energy gap in the MI phase, $E_{\mathrm{gap}}(g)$, by the rule illustrated in Fig. 1: For positive $g = (U - U_c)/J$ it is half the gap, $\Delta(g > 0) = E_{\mathrm{gap}}(g)/2$, where $E_{\mathrm{gap}} = \mu_c^{(+)} - \mu_c^{(-)}$ is deduced from the upper and lower critical chemical potentials for a given g. For $g < 0$ along the trajectory i in the SF phase it is $\Delta(g < 0) = E_{\mathrm{gap}}(-g)/2$. For $U = U_c$ and negative $g_\mu = (\mu - \mu_c)/J$ along the trajectory ii in the SF phase we first find g such that $\mu_c^{(-)}(g) = \mu$ and then define $\Delta(g_\mu) = C E_{\mathrm{gap}}(g)/2$ where the constant $C = 1.2$ (see below) is fixed by demanding that the universal function is the same along both SF trajectories. Note that $E_{\mathrm{gap}}(g)$ in the thermodynamic limit can be determined accurately from the imaginary time Green
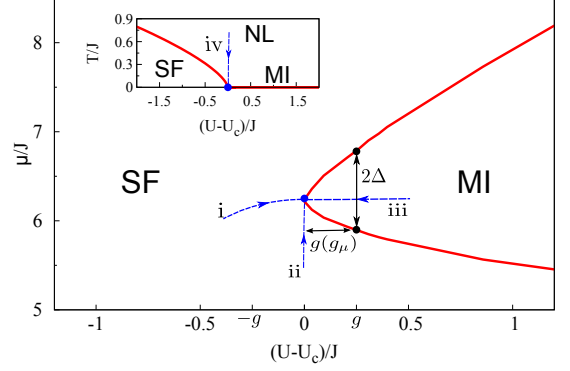

FIG. 1. (Color online) Ground state phase diagram of the Bose-Hubbard model in the vicinity of the QCP marked by a large (blue) dot (based on Ref. [22] data). The (blue) dashed curves specify trajectories in parameter space used to detune the system away from the QCP (trajectories i and iii correspond to unity filling factor $n = 1$, trajectory ii has constant interaction strength). The (black) lines with arrows explain how the characteristic energy scale Δ is obtained for these parameters (see text). The inset shows the phase diagram at finite temperature, and the trajectory taken in the NL phase.

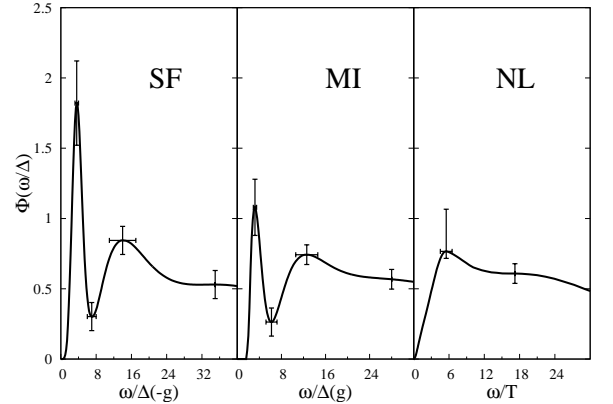function data [22] and finite-size scaling analysis.

FIG. 2. Universal spectral functions for scalar response in the superfluid, Mott insulator, and normal liquid phases. For SF, the Higgs peak is at $\omega_H/\Delta = 3.3(8)$; for MI, $\omega_H/\Delta = 3.2(8)$; and for NL, $\omega_H/T = 6(1)$. There is a secondary peak around $\omega/\Delta \approx 15$ in the SF and MI phases, and all responses reach a quasi-plateau at the same height 0.6(1) at higher frequencies. The error bars on $\Phi_{\mathrm{SF,MI}}$ come from the spread of collapsed curves, while the ones on Φ_{NL} are based on the variance of the analytical continuation results [14].

To study the scalar response, we can imagine adding a small uniform modulation term to the Hamiltonian

$$\delta H(t) = -\delta J \cos(\omega t) \sum_{<ij>} b_i^\dagger b_j \equiv \frac{\delta J}{J} K(t), \quad (3)$$

where $\delta J/J \ll 1$. The imaginary time correlation function for kinetic energy, $\chi(\tau) = \langle K(\tau) K(0) \rangle - \langle K \rangle^2$, is

related to $S(\omega)$ through the spectral integral with the finite-temperature kernel, $N(\tau, \omega) = e^{-\omega\tau} + e^{-\omega(1/T - \tau)}$:

$$\chi(\tau) = \int_0^{+\infty} N(\tau, \omega) S(\omega) . \qquad (4)$$

We employ the same protocol of collecting and analyzing data as in Ref. [14]. More specifically, in the MC simulation we collect statistics for the correlation function at Matsubara frequencies $\omega_n = 2\pi T n$ with integer n

$$\chi(i\omega_n) = \langle K(\tau)K(0)\rangle_{i\omega_n} + \langle K \rangle \qquad (5)$$

which is related to $\chi(\tau)$ by a Fourier transform. In the path integral representation, $\chi(i\omega_n)$ has a direct unbiased estimator, $|\sum_k e^{i\omega_n \tau_k}|^2$, where the sum runs over all hopping transitions in a given configuration, i.e. there is no need to add terms (3) to the Hamiltonian explicitly. Once $\chi(\tau)$ is recovered from $\chi(i\omega_n)$, the analytical continuation methods described in Ref. [14] are applied to extract the spectral function $S(\omega)$. A discussion on the reproducibility of the analytically continued results for this type of problems can also be found in Ref. [14].

We consider system sizes significantly larger than the correlation length by a factor of at least four to ensure that our results are effectively in the thermodynamic limit. Furthermore, for the SF and MI phases, we set the temperature $T = 1/\beta$ to be much smaller than the characteristic Higgs energy, so that no details in the relevant energy part of spectral function are missed.

We consider two paths in the SF phase to approach the QCP: by increasing the interaction $U \to U_c$ at unity filling factor $n = 1$ (trajectory i perpendicular to the phase boundary in Fig 1), and by increasing $\mu \to \mu_c$ while keeping $U = U_c$ constant (trajectory ii tangential to the phase boundary in Fig 1). We start with trajectory i by considering three parameter sets for $(|g|, L, \beta)$: $(0.2424, 20, 10)$, $(0.0924, 40, 20$, and $(0.0462, 80, 40)$. The prime data in imaginary time domain are shown in Fig. 3 using scaled variables to demonstrate collapse of $\chi(\tau)$ curves at large times. Analytically continued results are shown in the inset of Fig. 4. After rescaling results according to Eq. (1) we observe data collapse shown in the main panel of Fig.4. This defines the universal spectral function in the superfluid phase, Φ_{SF}.

When approaching the QCP along trajectory ii, with $(|g_\mu|, L, \beta) = (0.40, 25, 15)$, $(0.30, 30, 15)$, and $(0.20, 40, 20)$ we observe a similar data collapse and arrive at the same universal function Φ_{SF}, see Fig. 5. The final match is possible only when the characteristic energy scale $\Delta(g_\mu) = C\Delta(g(g_\mu))$ involves a factor of $C = 1.2$.

The universal spectral function Φ_{SF} has three distinct features: a) A pronounced peak at $\omega_H/\Delta \approx 3.3$, which is associated with the Higgs resonance. Since the peak's width $\gamma/\Delta \approx 1$ is comparable to its energy, the Higgs mode is strongly damped. It behaves as a well-defined particle only in a moving reference frame; b) A minimum and another broad maximum between $\omega/\Delta \in [5, 25]$
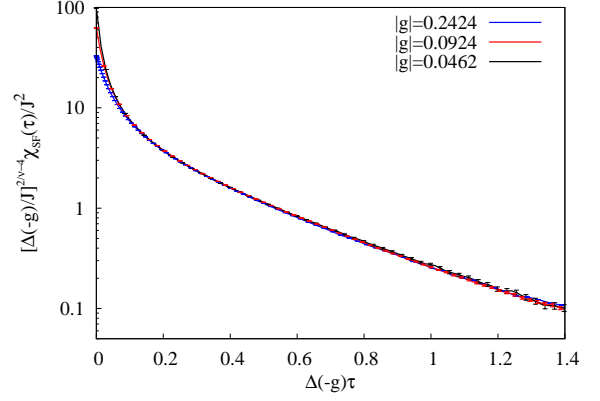

FIG. 3. (Color online) Collapse of correlation functions in imaginary time domain for different values of U along trajectory i in the SF phase, labeled by the detuning $g = (U - U_c)/J$.
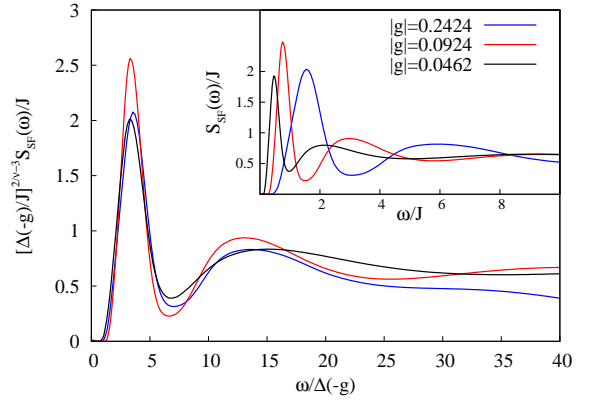

FIG. 4. (Color online) Collapse of spectral functions for different values of U along trajectory i in the SF phase, labeled by the detuning $g = (U - U_c)/J$. Inset: original data for $S_{SF}(\omega)$.

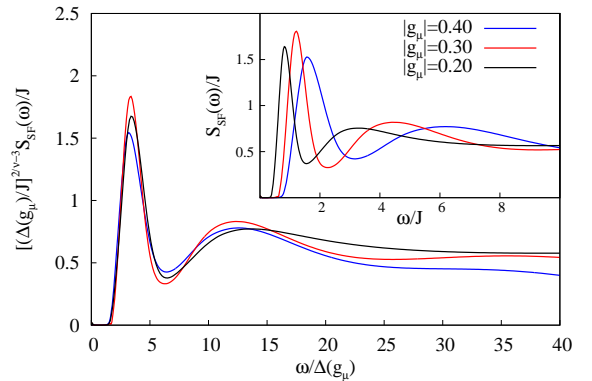FIG. 5. (Color online) Collapse of spectral functions for different μ along trajectory ii in the SF phase, labeled by the detuning $g_\mu = (\mu - \mu_c)/J$. Inset: original data for $S_{SF}(\omega)$.

which may originate from multi-Higgs excitations [14]; c) The onset of the quantum critical quasi-plateau, in agreement with the scaling hypothesis (1), starting at $\omega/\Delta \approx 25$. These features are captured by an approximate analytic expression with normalized $\chi^2 \sim 1$,

$$\Phi_{\text{SF}}(x) = \frac{0.65x^3}{35 + x^{2/\nu}}\left[1 + \frac{7\sin(0.55x)}{1 + 0.02x^3}\right] \quad (6)$$

We only claim that a plateau is consistent with our imaginary time data and emerges from the analytic continuation procedure which seeks smooth spectral functions; *i.e.,* other analytic continuation methods may produce an oscillating behavior in the same frequency range within the error bar in Fig. 2

In the MI phase we approach the QCP along trajectory iii in Fig 1. The scaling hypothesis for the spectral function has a similar structure to the one in Eq. (1),

$$S_{\text{MI}}(\omega) \propto \Delta^{3-2/\nu}\Phi_{\text{MI}}(\frac{\omega}{\Delta}) \ . \quad (7)$$

The low-energy behavior of Φ_{MI} starts with the threshold singularity at the particle-hole gap value, $\Phi_{\text{MI}}(x) \approx 1/\log^2(4/(x-2))\theta(x-2)$, see Ref. [16]. At high frequencies $\Phi_{\text{MI}}(x \gg 1)$ has to approach the universal quantum critical quasi-plateau (same as in the SF phase). Our results for the spectral functions at $g = 0.2576$ (with $L = 20, \beta = 10$) and $g = 0.1276$ (with $L = 40, \beta = 20$) are presented in Fig.6. The universal scaling spectral function shows an energy gap (this is also fully pronounced in the imaginary time data). The left side of the first peak is much steeper than in the SF phase, in agreement with the theoretical prediction for the threshold singularity.
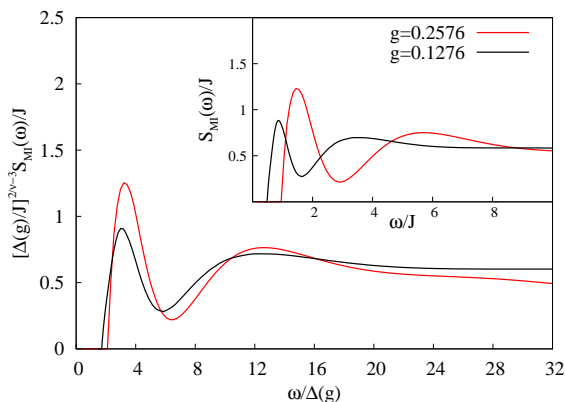

FIG. 6. (Color online) Collapse of the spectral functions for different U along trajectory iii in the MI phase, labeled by the detuning $g = (U - U_c)/J$. Inset: original data for $S_{\text{MI}}(\omega)$.

The universal spectral function in the MI is remarkably similar to its SF counterpart featuring a sharp resonance peak. [since MI and SF are separated by a critical line

their scaling functions Φ_{MI} and Φ_{SF} remain fundamentally different at energies smaller than ω_H]. This observation is rather counter-intuitive given that the superfluid order parameter is zero and raises a number of theoretical questions regarding the nature and properties of collective excitations in the MI phase at finite energies. In particular, can it be linked to the established picture of renormalized free-energy functional for the order parameter field [17] at distances under the correlation length?

If finite energy excitations probe system correlations predominantly in a finite space-time volume, one would expect that some resonant feature may survive even in the NL phase at sufficiently low, but finite temperature $T < J$ (at $g = g_\mu = 0$, the superfluid transition temperature is zero) In this quantum critical region, temperature determines the characteristic energy scale, thus $S_{\text{NL}}(\omega) \propto T^{3-2/\nu}\Phi_{\text{NL}}(\omega/T)$, and all excitations are strongly damped. Simulations performed at $T/J = 0.5$ on the trajectory iv in the inset of Fig. 1 indeed find a peak at low energies before the critical quasi-plateau, see Fig. 2, but it is much less pronounced and the oscillatory component (second peak) is lost. Unfortunately, numerical complexity does not allow us to verify the scaling law directly by collapsing simulations at lower temperatures and bigger system sizes. Our case for universality of $\Phi_{\text{NL}}(x)$ is thus much weaker and rests solely on the theoretical consideration that the plateau (at the same value as in the SF and MI phases) separates universal physics from model specific behavior.

In conclusion, we have constructed the universal spectral functions Φ for the kinetic energy correlation function for all three phases in the vicinity of the interaction driven QCP of the 2D Bose-Hubbard Model. Although the nature of excitations in these phases is fundamentally different at low temperature, their Φ-functions all feature a resonance peak which in the SF and MI phases is followed by a broad second peak and evolve then to a quasi-platform at higher energy in agreement with scaling predictions. In the SF phase, the first peak is interpreted as a damped Higgs mode. In the MI and NL phase, the existence of a resonance is unexpected and requires further theoretical understanding of amplitude oscillations at mesoscopic length scales. Experimental verification with cold gases requires flatter traps and lower temperatures and is accessible within current technology. It would signify a new hallmark, going beyond the previous studies of criticality near Gaussian fixed points.

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