Order-Parameter Correlation Functions in Quantum Critical Phenomena

Min-Chul Cha\(^1\) and Gerardo Ortiz\(^2\)

\(^1\)Department of Applied Physics, Hanyang University, Ansan, Kyunggi-do 426-791, Korea
\(^2\)Department of Physics, Indiana University, Bloomington, IN 47405, USA

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We investigate the functional form of the order-parameter (two-point) correlation function in quantum critical phenomena. Contrary to the common lore, when there is no particle-hole symmetry we find that the equal-time correlation function at criticality does not display a diverging correlation length. We illustrate our conclusions by Monte Carlo calculations of the quantum rotor model in \(d = 2\) space dimensions.

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To probe the dynamical response of an interacting quantum many-body system one typically investigates its response to an externally applied time-dependent force that perturbs the system slightly away from equilibrium. The two-point time-dependent correlation function (TPCF) is the quantity which encodes the physical response of the system to that perturbation in linear response theory\(^1\). In this way, the TPCF contains information about the nature of the excitations of the unperturbed system. If the system is close to a continuous (thermodynamic or quantum) phase transition, under certain assumptions (e.g. long-distances), the order-parameter TPCF may acquire a universal form independent of the microscopic details of the interactions. This is the beauty and power of the general theory of critical phenomena. Establishing this universal functional form, and determining the exponents involved, is a common theme in classical and quantum critical phenomena\(^2\).

Quantum Critical Phenomena has been introduced as an straightforward extension of Classical Critical Phenomena\(^3\). The motivation is clear and can be traced back to the formal functional-integral mapping between a quantum problem in \(d\) space dimensions and a classical statistical mechanics problem in \(d + 1\), where the extra dimension corresponds to the (imaginary) time axis \(\tau\) (see, for example, \(^4\)). Space and time coordinates do not necessarily satisfy Lorentz symmetry. A measure of the asymmetry is quantified by the dynamic critical exponent \(z\) which is equal to unity when Lorentz invariance is present. Common wisdom dictates that at the critical point \(g_c\), continuous phase transitions display a correlation length \(\xi\) diverging as \(\xi \sim |g - g_c|^{-\nu}\) with critical exponent \(\nu > 0\), and control parameter \(g\) (temperature in the case of thermodynamic phase transitions). Similarly, the correlation time diverges as \(\tau_c \sim \xi^z\). This fact reflects the scale invariance of the system at criticality. It is then emphasized that consequently the equal-time (order-parameter) TPCF \(G(\mathbf{r}, \tau - \tau' = 0)\) should decay algebraically with the distance \(r = |\mathbf{r}|\), \(G(\mathbf{r}, 0) \sim 1/r^{d+2+2\eta}\), thus defining a characteristic exponent \(\eta\) (anomalous dimension). Different relations or laws are satisfied by the various exponents as a result of scaling hypotheses (e.g. in the free energy\(^5\)).

The purpose of this paper is to note that the common lore depicted above is not always mathematically justified in quantum critical phenomena and, most importantly, inadequate in certain cases of physical relevance. The root of the discrepancy lies in the lack of particle-hole symmetry in the case of non-vanishing chemical potential \(\mu\), which leads to a non-divergent length at criticality and short-range equal-time correlations as determined from \(G(\mathbf{r}, 0)\). This in turn implies that when \(\mu \neq 0\) there is no power law scaling ansatz in \(G(\mathbf{r}, 0)\) at the critical point. On the other hand, the zero-frequency order-parameter correlation function, \(G(\mathbf{r}, \omega = 0)\), does display long-range power law behavior at criticality with a divergent correlation length \(\xi\) for arbitrary \(\mu\). This illustrates the fundamental physical distinction between equal-time and zero-frequency correlations. We will present both a theoretical proof of these statements within the Ginzburg-Landau-Wilson (GLW) paradigm of quantum phase transitions, with an analytic calculation for the quantum spherical model, and a numerical confirmation in the quantum rotor model. Our conclusions rigorously apply as long as the dynamics of the order parameter of a given microscopic quantum model is faithfully described by this kind of GLW effective field theory. This holds regardless of the nature of the original degrees of freedom, i.e whether bosonic or fermionic. Moreover, similar derivations can be performed with multicomponent order parameters.

Our starting quantum model is of the familiar phenomenological GLW form

\[
S[\psi, \psi^*] = \frac{1}{2} \int_0^1 d\tau \int_V d^d r \left\{ - \psi^*(\mathbf{r}, \tau) [(\partial_\tau - \mu)^2 + \nabla^2_{\mathbf{r}}] \psi(\mathbf{r}, \tau) + r_0 |\psi(\mathbf{r}, \tau)|^2 + \frac{\mu_0}{2} |\psi(\mathbf{r}, \tau)|^4 \right\}, \tag{1}
\]
where $\psi(r, \tau)$ is the space and (Euclidean) time-dependent complex order parameter field, $r_0$ and $u_0$ are physical parameters, $V = L^d$ is the volume, and $T$ is the temperature. The partition function is given by $Z = \int D[\psi]D[\psi^*] \exp(-S[\psi, \psi^*])$. This (Euclidean) action $S$ is symmetric under the transformation $\psi(r, \tau) \rightarrow -\psi(r, \tau)$, but it is not particle-hole symmetric because $\mu$ is, in general, not zero. This GLW functional represents an analytic expansion (in the vicinity of the critical point) in $\psi(r, \tau)$ with interaction terms respecting the group of symmetries $G$ of the disordered phase.

Under the assumption of (bosonic) periodic boundary conditions along the time axis, one can Fourier transform with Matsubara frequencies $\omega = 2\pi T n$ ($n = 0, \pm 1, \pm 2, \cdots$), and discrete momenta $k_\alpha = 2\pi p_\alpha / L$ ($p_\alpha = 0, \pm 1, \pm 2, \cdots$) with $\alpha = 1, \cdots, d$. Then,

$$S = \frac{1}{2} \sum_{k, \omega} [(\omega - i\mu)^2 + k^2 + r_0]|\hat{\psi}(k, \omega)|^2 + \frac{u_0}{4} \int_0^{1/T} d\tau \int_V d^d r |\psi(r, \tau)|^4.$$

Introducing an auxiliary scalar field $\phi(r, \tau)$, we decouple the last term by the Hubbard-Stratonovich identity

$$e^{-}\frac{u_0}{4} \int d^d r f d^d r |\psi(r, \tau)|^4 = \text{const.} \times \int D[\phi] e^{-\int d^d r f d^d r |\phi(r, \tau)|^2 + \frac{1}{4u_0} \phi^2(r, \tau)}$$

with the result for the modified action $\tilde{S}[\psi, \psi^*, \phi]$

$$\tilde{S} = \frac{1}{2} \sum_{k, \omega} [(\omega - i\mu)^2 + k^2 + r_0]|\hat{\psi}(k, \omega)|^2 + \frac{1}{2} \int_0^{1/T} d\tau \int_V d^d r \left[ \frac{1}{2u_0} \phi^2(r, \tau) + i\phi(r, \tau) \right]^2. $$

In order to investigate the order-parameter TPCF explicitly, we will adopt a saddle-point approximation to evaluate the integral over $\phi$. The resulting (quantum spherical model) action is

$$\tilde{S} = \frac{1}{2} \sum_{k, \omega} [(\omega - i\mu)^2 + k^2 + \bar{r}_0]|\hat{\psi}(k, \omega)|^2,$$

where $\bar{r}_0 = r_0 + i\bar{\phi}$. For the sake of clarity, in the following we will concentrate in the $T = 0$ and infinite volume case.

The resulting self-consistent equation is

$$i\bar{\phi} = u_0 \int_0^\infty d\omega \int \frac{d^d k}{(2\pi)^d} \frac{1}{[(\omega - i\mu)^2 + k^2 + \bar{r}_0]}.$$

Equivalently, we can define a correlation length $\xi$

$$\xi^{-2} = r_0 - \mu^2 + u_0 \int \frac{d^d k}{(2\pi)^d} \frac{1}{2\sqrt{k^2 + \mu^2 + \xi^{-2}}}$$

where $\xi^{-2} \equiv r_0 + i\bar{\phi} - \mu^2$. Clearly, this integral displays an ultraviolet divergence that needs to be regularized. To avoid this divergence, here we adopt a lattice regularization by replacing $k^2 \rightarrow \sum_\alpha 2(1 - \cos k_\alpha)$ and $\int \frac{d^d k}{(2\pi)^d} \rightarrow (1/V) \sum_k$, which correctly takes into account the long-wavelength contributions while providing an intrinsic cutoff due to the lattice constant.

Figure 1 shows the behavior of $\xi$ in two and three dimensions, where, without loss of generality, we set $u_0 = 1$ and use $r_0$ as the control parameter to signal the quantum phase transitions for $\mu = 0$ and $\mu \neq 0$. We see that $\xi$ diverges as one approaches the quantum critical point. Below we show that $\xi$ is actually the correlation length, which gives the diverging (or singular) behavior at criticality, but it is not the length characterizing the TPCF.

With this correlation length $\xi$, the order-parameter (connected) TPCF is given by

$$G(r, \tau) = \langle \psi(r, \tau) \psi^*(0, 0) \rangle - \langle \psi(r, \tau) \rangle \langle \psi^*(0, 0) \rangle = \int \frac{d^d k d\omega}{(2\pi)^{d+1}} \frac{\exp\left(i\mu r - \omega \tau + i\phi(r, \tau) \right)}{\sqrt{2\pi \lambda (d-1)/2} K_{d-1/2}(\rho)}$$

for $d \geq 1$, where $\lambda^{-2} \equiv \mu^2 + \xi^{-2}$, $\rho = (r^2 + \tau^2)^{1/2}/\lambda$, and $K_n(\rho)$ is the modified spherical Bessel function of

![FIG. 1: (color online) The correlation length, $\xi$, determined by the self-consistent Eq. (7), diverges as one approaches the transition point by tuning $r_0$. Here we consider the three- and two-dimensional cases. ($u_0 = 1$)](image)
the third kind whose asymptotic form is

\[ K_n(\rho) \sim \begin{cases} (\frac{\pi}{2})^{1/2} e^{-\rho/2} & \rho \gg 1; \\ \frac{\Gamma(n)}{2} \rho^{-n} & \rho \ll 1, \end{cases} \]

where \( \Gamma(n) \) is the Gamma function. Therefore, for \( \mu \neq 0 \), the long-range behavior of the TPCF near the critical point \( (\xi^{-2} \to 0) \) reduces to

\[ G(\mathbf{r}, \tau) \sim \frac{e^{-\mu(\sqrt{r^2 + \tau^2} - \tau)}}{(\tau^2 + \tau^2)^{d/4}}, \]

while, for \( \mu = 0 \), \( G(\mathbf{r}, \tau) \sim 1/(r^2 + \tau^2)^{(d-1)/2} \). We note that, for \( \mu \neq 0 \), the equal-time spatial correlation shows a short-range behavior characterized by a length \( \lambda \sim 1/\mu \), not by the diverging \( \xi \), while the temporal correlation does display long-range behavior.

The long-range correlation associated with the divergence of \( \xi \), however, leads to the susceptibility thermodynamic sum rule \( \Sigma = 0 \) so that \( G(\mathbf{k}, \omega) = 1/[(\omega - i\mu)^2 + k^2 + \mu^2 + \xi^{-2}] \to \infty \) as \( \xi \to \infty \) in the long-wavelength \( (k \to 0) \) and low-frequency \( (\omega \to 0) \) limit. Therefore, the range of the zero-frequency correlation function is characterized by \( \xi \) in the form

\[ G(\mathbf{r}, \omega = 0) \sim \begin{cases} \exp(-r/\xi)/r^{(d-1)/2} & r/\xi \gg 1; \\ 1/r^{d-2} & r/\xi \ll 1, \end{cases} \]

which, at criticality, is often compactly represented as \( G(\mathbf{r}, \omega = 0) \sim \exp(-r/\xi)/r^{d-2} \). Note that this form is the same as that of the \( d \)-dimensional classical criticality. We may view that the long-range spatial correlation at zero-frequency is brought by the long-range temporal correlation, even though the equal-time correlations are short ranged.

We see that in the model a non-vanishing \( \mu \) brings in an imaginary term linearly coupled to \( \omega \) in the action. Without this term, the quantum fluctuations along the temporal and spatial directions are isotropic, yielding a dynamical critical exponent \( z = 1 \), and the mapping of the \( d \)-dimensional quantum phase transition to the \( (d + z) \)-dimensional classical phase transition is well justified. For \( \mu \neq 0 \), the term breaking the particle-hole symmetry causes an asymmetry in the temporal direction leading to \( z = 2 \) (i.e. there is no Lorentz invariance). This asymmetry property should not change at higher orders in \( u_0 \). The formal solution, including the effect of \( u_0 \), is

\[ G(\mathbf{k}, \omega) = \frac{1}{(\omega - i\mu)^2 + k^2 + r_0 - \Sigma(r_0, u_0, \mu; k, \omega)}, \]

where the self-energy \( \Sigma(r_0, u_0, \mu; k, \omega) \to 0 \) as \( u_0 \to 0 \) and \( \Sigma(r_0c, u_0, \mu; 0, 0) = r_0c - \mu^2 \) at the critical point \( r_0 = r_0c \). Therefore, we expect that the self-energy term does not alter the nature of the broken particle-hole symmetry caused by a non-zero \( \mu \), although it may introduce an anomalous exponent \( \eta \neq 0 \).

Our analytic results are now confirmed by a Monte Carlo calculation of the quantum rotor model

\[ H = \frac{U}{2} \sum_{\mathbf{r}} \frac{1}{i} \frac{\partial}{\partial \theta_\mathbf{r}} - \bar{n})^2 - 2J \sum_{(\mathbf{r}, \mathbf{r}')} \cos(\theta_\mathbf{r} - \theta_{\mathbf{r}'}, \]

where \( U \) represents the rotational energy scale of a rotor at site \( \mathbf{r} \), \( J \) denotes the coupling strength between nearest-neighbor sites \( (\mathbf{r}, \mathbf{r}') \), and a non-zero \( \bar{n} \) \( (\bar{n} \equiv \mu/U) \) breaks the particle-hole symmetry. In the following, we will show that the correlations of this model near criticality are correctly captured by the effective (GLW) model of Eq. (1).

We performed Monte Carlo calculations of the total TPCF \( G_t(\mathbf{r}, \tau) = \langle \psi(\mathbf{r}, \tau) \psi^*(0, 0) \rangle = e^{i[\theta(\mathbf{r}, \tau) - \theta(0, 0)]} \) in a square lattice of size \( L \times L \times L \), with periodic boundary conditions, where \( L \) is the size in a spatial direction and \( L_\tau \) in the temporal direction. For Monte Carlo calculations, we represent the quantum rotor model in the form of a classical \( (d + 1) \)-dimensional action \[ S[J] = \frac{1}{2K} \sum_{(\mathbf{r}, \tau)} \{ J^2 \}

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\] where \( K \sim \sqrt{2J/U} \) is the tuning parameter controlling the quantum fluctuations, \( J_n \)'s are integers, and \( \nabla \cdot \mathbf{J} = 0 \) represents the current conservation condition at each site. We use a recently developed worm algorithm \[ 7 \] to update the current configurations in Eq. (14) and measure the correlation functions.

Figure 2 shows the TPCF as a function of \( x \), a distance along a spatial axis, in a lattice of size \( 40 \times 40 \times 400 \) in the vicinity of the critical point \( K_c = 0.2978 \), which is determined by finite-size scaling of the superfluid stiffness, for \( \mu/U = 0.20 \). Inspired by Eq. (10), we use the fitting function

\[ G_t(x, \tau = 0) = C + A \left( e^{-x/\ell} + e^{-(L-x)/\ell} \right), \]

for \( 1 \ll x \ll L \) and obtain \( \ell \approx 1.4 - 1.9 \) for different \( K \)'s and sizes, while \( C = |\langle \psi \rangle|^2 \) depends sensitively on \( K \). This result strongly supports the fact that the equal-time TPCF has a short-range behavior, characterized by a finite rather than a diverging correlation length.

To understand the nature of \( \ell \), we measure it as a function of \( \mu \) at the critical point in Fig. 3. Our results clearly show that \( 1/\ell \) is proportional to \( \mu \), and \( \ell \) remains finite except at integer fillings \( (\mu = 0) \) where the particle-hole symmetry is restored.

The long-range nature of one-particle correlations can be observed in \( G(\mathbf{r}, \omega = 0) \). In Fig. 4 the zero-frequency total correlation function, defined by \( G_t(x, \omega = 0) = \sum_{\tau=1}^{L_\tau} G_t(x, \tau) \), displays long-range behavior near the critical point. We can easily see that, by subtracting out the constant part to obtain \( G(\mathbf{r}, \omega = 0) \), the correlation range is still beyond the size of the system.
In summary, we have shown that, when particle-hole symmetry is broken, the physical quantity that displays a diverging length at criticality is the zero-frequency and not the equal-time correlation function. The latter is short-ranged and within our paradigm of quantum phase transitions it is not Lorentz invariant. We have not only proved this statement analytically but also illustrated its correctness by studying the planar quantum rotor model. This model shares the same critical properties as the Bose-Hubbard model assuming that only phase fluctuations are responsible for its critical behavior. This observation is quite relevant given the current interest in the experimental simulation of quantum phase transitions in optical lattices of ultracold atomic gases.

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