Phase Fluctuations in High Temperature Superconductors

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(Dated: September 24, 2008)

Within the phase fluctuation picture for the pseudogap state of a high-$T_c$ superconductor, we incorporate the phase fluctuations generated by the classical XY model with the Bogoliubov-de Gennes formalism utilizing a field-theoretical method. This picture delineates the inhomogeneous characteristics of local order parameters observed in high-$T_c$ superconductors above $T_c$. We also compute the local density of states near a non-magnetic impurity with a strong scattering potential. The resonance peak smoothly evolves as temperature increases through $T_c$, without showing any sudden broadening, which is consistent with recent experimental findings.

PACS numbers: 74.25.Jb, 74.40.+k, 74.50.+r

One of the most defining features of high-$T_c$ superconductors, the pseudogap state, has drawn very intense attention in recent years$^{[1]}$. Various theoretical models have attempted to explain this state; they generally fall into two categories. One is the pre-formed pair category, where the superfluid stiffness is zero. A second category is the competing gap scenario, where, for example, a density-wave gap coexists with the superconducting gap$^{[2, 3, 4, 5, 6, 7]}$. In this picture, the Cooper pairs continue to exist above $T_c$, in the pseudogap state below $T^*$ without phase coherence, where the superfluid stiffness is zero. A second category is the competing gap scenario, where, for example, a density-wave gap coexists with the superconducting gap$^{[2, 3, 4, 5, 6, 7]}$. This distinction can be fairly subtle, and the nature of this phase continues to attract growing interest. Angle-resolved photoemission spectroscopy experiments$^{[8]}$ have supported the phase fluctuation scenario since the pseudogap seems to evolve into the superconducting gap as the temperature changes through $T_c$. Further support can be found in the Nernst experiments$^{[9, 10]}$, where a large Nernst signal induced by vortex motions is observed above $T_c$ in hole-doped cuprates. This result has been interpreted as evidence for phase fluctuations. In the pseudogap state, from the viewpoint of the phase fluctuation scenario, one can conceive a spatially dependent order parameter $\Delta(\mathbf{r}) = |\Delta| e^{i\theta(\mathbf{r})}$ at a location $\mathbf{r}$. In fact, an intrinsic inhomogeneity$^{[11, 12]}$ of local order parameters has been observed even at a low temperature. In a two-dimensional theory$^{[3, 4, 5, 6, 7]}$, the transition into the superconducting state at $T_c$ is not BCS-like. Instead, it is the Kosterlitz-Thouless (KT) transition$^{[13]}$. Consequently, we identify $T_{KT} = T_c$, which depends on the superfluid stiffness. Denoting $T_{MF}$ as the temperature when Cooper pairs preform, we also define $T_{MF} = T^*$, which is determined by the strength of the pairing potential.

Recently, spatial variations of the order parameter were visualized in topographic images$^{[14, 15]}$. Gomes et al.$^{[16, 17]}$ have examined statistically the evolution of the order parameter in atomic scale of Bi$_2$Sr$_2$CaCu$_2$O$_{8+x}$ for various doping cases with increasing $T$ from a low $T$ through $T_c$ to a high $T$. They illustrated the distribution $D$ as well as the probability $P$ of local order parameters. The distribution $D(\Delta)$ is an ordered list of local order parameters, which describes how many sites have the order parameter less than $\Delta$. Thus $D(\Delta + \epsilon) - D(\Delta)$ gives the number of sites with the order parameter between $\Delta + \epsilon$ and $\Delta$. Since $P(\Delta)$ is the probability to find a local order parameter of $\Delta$, $P(\Delta) \propto \partial_\Delta D(\Delta)$. On the other hand, Chatterjee et al.$^{[19]}$ observed that the impurity resonance survives for $T > T_c$ in the study of the scanning tunneling microscopy (STM) for Bi$_{2-x}$Pb$_x$Sr$_2$CaCu$_2$O$_{8+x}$. The STM study$^{[20]}$ for high-$T_c$ superconductors is performed usually at a low $T \ll T_c$. Since $T_c$ of this compound is 15K, they carried out the $T$ dependence of the impurity resonance through $T_c$. In this paper, we wish to demonstrate that these recent findings$^{[15, 20]}$ are understandable, at least qualitatively, within the framework of the phase fluctuation scenario.

In the theoretical formulation, we separate the order parameter into the mean-field value and the phase fluctuation part using the field-theoretical approach. The mean-field value is determined by the Bogoliubov-de Gennes(BdG) formalism while phase fluctuations will be incorporated the phase fluctuations generated by the classical XY model with the Bogoliubov-de Gennes(BdG) formalism. Using a set of impurity sites $\mathbf{I}$, one can write $U_i$ as $\sum_{l \in \mathbf{I}} U_l \delta_{l,i}$. For the nearest neighbor pairing, $V_{i,j} = \delta_{i,j}$.
We set the lattice constant to be unity and use units such that $\hbar = k_B = 1$. The partition function of $\mathcal{H}$ in the path integral is $Z = \int D\psi D\bar{\psi} e^{-S[\psi,\bar{\psi}]}$ where $S[\psi,\bar{\psi}] = \int d\tau \left[ \sum_{i,j} \frac{1}{V_{i,j}} |\phi_{ij}|^2 - \sum_{<i,j>} t_{ij} \bar{\psi}_i \tilde{\tau}_j \psi_j + \sum_i (U_i - \mu) \bar{\psi}_i \tilde{\tau}_i \psi_i - \sum_{i,j} \left( \phi_{ij} \bar{\psi}_i \tilde{\tau}_j \psi_j + \phi_{ij}^\dagger \bar{\psi}_j \tilde{\tau}_i \psi_i \right) \right]$. The range for the integral over imaginary time $\tau$ in the action $S$ is from 0 to $\beta = 1/T$.

$$S[\phi, \phi^\dagger, \psi, \psi^\dagger] = \int d\tau \left[ \sum_{i,j} \frac{1}{V_{i,j}} |\phi_{ij}|^2 - \sum_{<i,j>} t_{ij} \bar{\psi}_i \tilde{\tau}_j \psi_j + \sum_i (U_i - \mu) \bar{\psi}_i \tilde{\tau}_i \psi_i - \sum_{i,j} \left( \phi_{ij} \bar{\psi}_i \tilde{\tau}_j \psi_j + \phi_{ij}^\dagger \bar{\psi}_j \tilde{\tau}_i \psi_i \right) \right].$$

In the saddle point approximation, $\delta S[\phi, \phi^\dagger, \psi, \psi^\dagger]/\delta \phi^\dagger = 0$, the auxiliary field can be identified as the order parameter; namely, $\phi_{ij} = V_{i,j} \bar{\psi}_j \tilde{\tau}_i - \Delta_{ij}$. Now $\delta[\Delta, \Delta^\dagger, \psi, \psi^\dagger] = \sum_{i,j} \frac{\beta}{V_{i,j}} |\Delta_{ij}|^2 + \beta \mathcal{H}_{BdG}[\psi, \psi^\dagger]$, where the BdG Hamiltonian is

$$\mathcal{H}_{BdG}[\psi, \psi^\dagger] = -\sum_{<i,j>} t_{ij} \bar{\psi}_i \tilde{\tau}_j \psi_j + \sum_i (U_i - \mu) \bar{\psi}_i \tilde{\tau}_i \psi_i - \sum_{i,j} \left( \Delta_{ij} \bar{\psi}_i \tilde{\tau}_j \psi_j + \bar{\psi}_j \tilde{\tau}_i \psi_i + h.c. \right).$$

The effective partition function can be written as

$$Z = \int D\Delta D\Delta^\dagger \exp \left[ -\sum_{i,j} \frac{\beta}{V_{i,j}} |\Delta_{ij}|^2 \right] Z_{BdG}$$

where $Z_{BdG} = \text{Tr} \left[ e^{-\beta \mathcal{H}_{BdG}} \right]$ is the partition function corresponding to the BdG Hamiltonian. Note that $Z_{BdG}$ depends on $\Delta_{ij} = |\Delta_{ij}| e^{i\theta_{ij}}$, where $\theta_{ij}$ represents phase fluctuations (see below). However, as a mean field approximation, the BdG formalism does not consider phase fluctuations. To incorporate the fluctuations into the framework, we utilize the two-dimensional XY model [22] with $\mathcal{H}_{XY} = -J_{XY} \sum_{<i,j>} \cos(\theta_i - \theta_j)$, where $J_{XY}$ is the coupling strength (or the superfluid stiffness) and $\theta_i$ is the angle made by a classical spin at a site $i$. Following Ref. [22], we perform simulations using the Monte Carlo method with the Metropolis algorithm. The lattice size in our calculations is $24 \times 24$ with periodic boundary conditions. The minimum length of phase fluctuations is set to be 2. Starting from a random configuration, the XY model system is cooled down to a working $T$. It is known that $T_{FK} \approx 0.9 J_{XY}$ in numerical simulations. To benchmark our simulations, we also compute the specific heat to be 2. Starting from a random configuration, the XY model is obtained self-consistently by solving the BdG equation:

$$\sum_j \left( \mathcal{H}_{ij,\sigma} - \mathcal{H}_{ij,\sigma}^* \right) \left( \begin{array}{c} u_{ij,\sigma} \\ v_{ij,\sigma} \end{array} \right) = \begin{array}{c} E_n \\ v_{ij,\sigma} \end{array} \left( \begin{array}{c} u_{ij,\sigma} \\ v_{ij,\sigma} \end{array} \right)$$

Introducing the Hubbard-Stratonovich transformation with auxiliary field $\phi_{ij}$ as a field-theoretical method to deal with phase fluctuations, we obtain the partition function as follows: $Z = \int D\phi D\phi^\dagger D\psi D\psi^\dagger e^{-S[\phi, \phi^\dagger, \psi, \psi^\dagger]}$, where, for the static case: $\partial_t \bar{\psi}_i = 0$.

$$\mathcal{H}_{ij,\sigma} = -t_{ij} + (U_i - \mu) \delta_{ij}.$$ The bonding order parameter is evaluated as

$$\Delta_{ij} = (V/4) \sum_n \left[ u_{ij}^n v_{ij}^n + v_{ij}^n u_{ij}^n \right] \tanh(E_n/2T).$$

The local d-wave order parameter at a site $i$ is given by

$$\Delta_i^\sigma = \frac{1}{2} \sum_j \Delta_{ij} \left[ \theta_{ij} \delta_{i+j,0} + \delta_{i,j-1} + \theta_{ij} \delta_{i,j+1} - \delta_{i-1,j} - \delta_{i+1,j} \right].$$

Rigorously speaking, $\Delta_{ij} = \Delta_{ij} e^{i\theta_{ij}}$, where $\Delta_{ij} = |\Delta_{ij}| e^{i\theta_{ij}}$. Consequently, $\Delta_{ij} = |\Delta_{ij}| e^{i\theta_{ij}}$. The phase $\theta_{ij}$ associated with the mean-field value is determined within the BdG calculations. On the other hand, $\theta_{ij}$ is generated based on the XY model as mentioned. Assuming the effective phase of the local d-wave order parameter varies slowly over a distance of the coherence length $\xi$, it is reasonable to define $\theta_{ij} = [\theta_i + \theta_j] / 2$, which corresponds to the phase of the center of mass of a Cooper pair in the continuum limit.

Let us now calculate the average of $\langle \Delta_{ij} \rangle$ over phase fluctuations. It is straightforward to show that $\langle \Delta_{ij} \rangle = \Delta_{ij} e^{i\theta_{ij}}$, where

$$\langle e^{i\theta_{ij}} \rangle = \frac{\int D\theta \ e^{i\theta_{ij}} Z_{BdG}[\Delta, \theta]}{\int D\theta \ Z_{BdG}[\Delta, \theta]}$$

with $Z_{BdG} = \prod_n (1 + e^{-\beta E_n})$. As in Refs. [4, 7], $\langle e^{i\theta_{ij}} \rangle$ is numerically evaluated using the Monte Carlo method. Generating a phase configuration $\{\theta_{ij}\}$ at $T$ and diagonalizing the BdG Hamiltonian with $\Delta_{ij}$, we obtain $E_n$ corresponding to the given configuration. In the averaging process, the total number of phase configurations of an ensemble at $T$ is about $10^6$. The local d-wave order parameter now is evaluated as $\langle \Delta_{ij} \rangle = \frac{1}{2} \sum_j \langle \Delta_{ij} \rangle \left[ \theta_{ij} \delta_{i+j,0} + \delta_{i,j-1} + \theta_{ij} \delta_{i,j+1} - \delta_{i-1,j} - \delta_{i+1,j} \right]$. Following this procedure yields a statistical distribution $D$ of local order parameters $\Delta \equiv |\Delta_{ij}|$. As explained earlier, the probability $P(\Delta)$ is given by $\partial_\Delta D(\omega) / \Delta$. In Fig. 1 we plot $P(\Delta)$ (in an arbitrary unit) at various $T$ in the units of the hopping amplitude. Other parameters used are $V = 2.05$, $\mu = 0$, and $J_{XY} = 0.11$ and impurities are not considered. At low $T$, $P(\Delta)$ shows a sharp peak at $\Delta = 0.25$, which is the mean-field value at $T = 0$, because phase fluctuations are not significant. Even near
\( T_c \simeq \frac{1}{4} T_{MF} \), \( P(\Delta) \) is confined within \( \Delta \simeq 0.21 \sim 0.24 \). As \( T \) increases above \( T_c \), the probability spreads; however, it sharpens back when \( T \to T_{MF} \) because the mean-field gap diminishes rapidly. Since the median of \( P(\Delta) \) moves towards zero, the spatial average of the local order parameters decreases. The inset of Fig. 1 demonstrates such a behavior compared with its mean-field counterpart. In particular, the spatial average does not change much until \( T > 1.5T_c \). This is consistent with a variation of the density of states computed in Ref. [4]. We also performed the same calculations choosing \( V = 0.92 \) for which \( T_c \simeq \frac{2}{6} T_{MF} \) and obtained qualitatively similar results. Gomes et al. [19] measured local \( d \)-wave order parameters of \( Bi_2Sr_2CaCu_2O_{8+x} \) to show the order parameter distribution. They also presented the probability for the overdoped \( Bi_2Sr_2CaCu_2O_{8+x} \) in a histogram with an interval of \( 2meV \), which is equivalent to \( \epsilon \) in our definitions. The histogram illustrates the probability spreads as \( T \) increases while it becomes a sharp peak at a high \( T \). It is also indicated that the median of the probability moves towards zero with increasing \( T \). The detailed behavior of the probability in Ref. [19] is not completely identical to that shown in Fig. 1. Nonetheless, important characteristics of the histogram are congruent with Fig. 1.

Another interesting experimental observation using the STM has been recently reported by Chatterjee et al. [20]. They observed the evolution of the impurity resonance as \( T \) increases from low \( T \) to high \( T(> T_c) \) and found that the resonance survives above \( T_c \). Moreover, the resonance evolves smoothly with increasing \( T \) and does not show any sudden broadening near \( T_c \). In fact, it was argued that such a sudden broadening near \( T_c \) would occur in the phase fluctuation scenario [23]. This led Chatterjee et al. to conclude that the phase fluctuation scenario is not consistent with their findings. However, in Ref. [23], the phase of the local order parameters is assumed to vary on the length scale of the London penetration depth so that the quasiclassical approximation is applicable. Within our framework, such an assumption corresponds to weak phase fluctuations and, thus, \( T_c \) would not be much less than \( T^* \). The only assumption we made following Refs. [3, 4] is that the phase varies slowly over the coherence length without any larger length scale employed, and the BdG formalism is applied. Consequently, the phase varies at any length scale greater than the lattice constant, and any degree of fluctuations can be considered.

The local differential conductance is described by the local density of states (LDOS) in the theoretical calculations. We apply the supercell technique to compute the LDOS as in Refs. [24, 25]. If the lattice size is \( N_x \times N_y \) as a unit cell and the number of unit cells is \( M_x \times M_y \), then the total size becomes \( N_xM_x \times N_yM_y \). We also introduce the quasimomenta \( \phi(y) = \frac{2\pi n_y}{N_yM_y} \), where \( n_y = 0, 1, \cdots , M_y - 1 \). It is obvious that \( Z_{gdc} \), now, depends on \( p_x(y) \). In the presence of phase fluctuations, one can think of two different supercell techniques depending on how to associate the fluctuations with \( p_x(y) \). One way is to start with the same random configuration of phases regardless of \( p_x(y) \) while the other would be to use different random configurations for different values of \( p_x(y) \). Nonetheless between the two methods we found no practical difference in the LDOS averaged over the ensemble. In particular, for \( T \geq T_c \) we obtain identical results. We obtain the averaged LDOS as follows: the LDOS is calculated for a given phase configuration and its average is computed over the ensemble. For a single impurity, we choose a strong impurity potential \( U = 100 \), which is close to the unitary limit [26]. Other parameters are \( V = 1.1, \mu = 0, \) and \( J_{XY} = 0.033 \). For the lattice size, \( N_x = N_y = 24 \) and \( M_x = M_y = 10 \). In Fig. 2, we plot the LDOS at the nearest neighbor site to the impurity (solid curves) as well as at a site far away from the impurity (dashed curves) for \( T = 0.01, 0.02, 0.03 \) and \( 0.04 \). Note that the impurity resonances survive above \( T_c \approx 0.03 \). Moreover, the resonance does not change much with increasing \( T \) near \( T_c \). The displayed behavior is consistent with the experimental findings [20]. It is illustrated further in Fig. 3 for \( V = 1.1 \) and for a weaker pairing potential \( V = 0.6 \) at \( T = 0.02, 0.03, \) and \( 0.04 \). This indicates that the impurity resonance above \( T_c \) does not strongly depend on parameters. From the theoretical point of view, it is originated from the fact that for these cases phase fluctuations (\( \theta_{ij} \)) cannot dis-
turb significantly the phase difference of the mean-field value $\pi = \bar{\theta}_{i,x+i,y} - \bar{\theta}_{i,x+i,y}$. In conclusion, considering recent experiments on the imaging of the inhomogeneous local order parameters above $T_c$ as well as the impurity resonance peak in high-$T_c$ superconductors, we calculated a distribution of the local order parameters and the local density of states near an impurity based on the phase fluctuation scenario. The order parameter distribution is qualitatively agreed with experimental observations. Randomly distributed impurities may be necessary for more realistic model calculations. A smooth evolution of the impurity resonance peak, through $T_c$, seen in the STM measurement also supports this picture. The resonance peak computed within our framework does not show any sudden broadening near $T_c$ and consistent with the experimental results.

We acknowledge N.P. Ong for useful discussions. This work was supported by the Robert A. Welch Foundation and the Texas Center for Superconductivity at the University of Houston through the State of Texas, the Ministry of Science and Technology of China (973 project No: 2009CB929200), NSFC Grant No. 10874032, and the Program for Professor of Special Appointment (Eastern Scholar) at Shanghai Institutions of Higher Learning.

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