Quantum Phase Fluctuations Responsible for Pseudogap

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The effect of ordering field phase fluctuations on the normal and superconducting properties of a simple 2D model with a local four-fermion attraction is studied.Neglecting the coupling between the spin and charge degrees of freedom an analytical expression has been obtained for the fermion spectral function as a single integral over a simple function. From this we show that, as the temperature increases through the 2D critical temperature and a nontrivial damping for a phase correlator develops, quantum fluctuations fill the gap in the quasiparticle spectrum. Simultaneously the quasiparticle peaks broaden significantly above the critical temperature, resembling the observed pseudogap behavior in high-$T_c$ superconductors.

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The pseudogap, or depletion of the single particle spectral weight around the Fermi level,\textsuperscript{1} is the most striking demonstration that cuprate superconductors are not described by the BCS scenario of superconductivity. The pseudogap opens in the normal state as the temperature is lowered below a crossover temperature $T^*$ and extends over a wide range of temperatures in the underdoped cuprates. ARPES\textsuperscript{2,3} and the scanning tunneling spectroscopy (STS) (see Refs. in \textsuperscript{1}) provide particularly complete information about the pseudogap behavior and show a smooth crossover from the pseudo- to superconducting (SC) gap. The transition from SC to normal behavior appears to be driven by phase fluctuations\textsuperscript{4} and is well described by the Berezinskii-Kosterlitz-Thouless (BKT) theory of vortex-pair unbinding.

There are currently many possible explanations for the unusual behavior of HTSC. One of these is based on the nearly antiferromagnetic Fermi liquid model\textsuperscript{5}. Another explanation, proposed by Anderson, relies on the separation of the spin and charge degrees of freedom.\textsuperscript{6} The third approach, which we follow in this paper, relates the observed anomalies to precursor SC fluctuations, and in particular fluctuations in the phase of the complex ordering field, as originally suggested by Emery and Kivelson\textsuperscript{7}. The phase diagram for a simple microscopic 2D model (see (\ref{eq:1}) below) which formalizes the scenario of\textsuperscript{7} has been studied in.\textsuperscript{8} The Green’s function (GF) for this model was derived in\textsuperscript{9} using the correlator $\langle \exp(i\theta(x)/2)\exp(-i\theta(0)/2) \rangle$ for the phase fluctuations in the classical (static) approximation and neglecting the coupling between the spin and charge degrees of freedom.

The associated spectral function (SF) $A(\omega,k) = -(1/\pi)\text{Im}G(\omega+i0,k)$ has also been derived analytically in\textsuperscript{9}. Being proportional to the intensity of ARPES\textsuperscript{2}, the SF encodes information about the quasiparticles and pseudogap. The result of\textsuperscript{9} showed that, while the temperature behavior of the quasiparticle peaks is in correspondence with experiment\textsuperscript{2}, the gap in the spectrum remains unfilled.\textsuperscript{9} In an earlier paper\textsuperscript{1} filling of the gap has been achieved as a result of a Doppler shift in the quasiparticle excitation spectrum. This Doppler shift originated from the semiclassical coupling of the mean field $d$-wave quasiparticles to the supercurrents induced by classically fluctuating unbound vortex-antivortex pairs. It was shown in\textsuperscript{1} that the shift can be identified with the coupling of the spin and charge degrees of freedom.

The purpose of the present paper is to show analytically that filling of the gap can also result from the quantum (dynamical) phase fluctuations, even when the coupling between charge and spin degrees of freedom is entirely neglected. As pointed out in\textsuperscript{13} the mechanism of the gap filling has to be understood yet even for the simplest attractive Hubbard model. Thus we contribute into the discussion\textsuperscript{13} as to which mechanism or mechanisms lead to pseudogap filling but within the scenario based on phase fluctuations, by studying the mechanism proposed in\textsuperscript{14}. The advantage of our calculation is that the SF is obtained as a single integral with an analytical integrand, no numerical analytical continuation was necessary resulting in far greater accuracy. Let us consider the continuum version of the 2D attractive Hubbard model defined by the Hamiltonian density:

$$
\mathcal{H} = -\psi_\sigma^\dagger(x) \left( \frac{\nabla^2}{2m} + \mu \right) \psi_\sigma(x) - V\psi_\sigma^\dagger(x)\psi_\uparrow(x)\psi_\downarrow(x)\psi_\uparrow(x),
$$

(1)

where $x = r, \tau$ denotes the space and imaginary time variables, $\psi_\sigma(x)$ is a fermion field with spin $\sigma = \uparrow, \downarrow$, $m$ is the effective fermion mass, $\mu$ is the chemical potential, and $V$ is an effective local attraction constant; we take $\hbar = k_B = 1$. Clearly the Hamiltonian (1) is too simple to be adequate for systems as complex as cuprate HTSC. However, it has proved itself as a very convenient model...
for both numerical, in particular Monte Carlo simulations, and analytical approaches which does exhibit gap-like behavior above $T_c$ (see also Refs. in the review [13]). Moreover one may use the model to obtain a fully analytic treatment of the pseudogap properties, and apply such results to obtain a better understanding of more complex and less tractable models.

The calculation of the GF is performed in Nambu variables and the fermions are treated as composite objects, comprising both spin and charge parts:

$$\Psi^\dagger(x) = \left( \psi_\uparrow^\dagger(x) \quad \psi_\downarrow(x) \right) = \mathcal{Y}^\dagger(x) \exp[-i\tau_3 \theta(x)/2],$$  \hspace{1cm} (2)

where $\mathcal{Y}^\dagger(x)$ is the Nambu spinor of neutral fermions. Substituting (2) into the standard definition of the GF $G(x) = \langle \Psi(x) \Psi^\dagger(0) \rangle$ one obtains the GF of the charged (observed) fermions

$$G_{\alpha\beta}(x) = \sum_{\alpha',\beta'} G_{\alpha'\beta'}(x) \langle \{e^{i\tau_3 \frac{\theta(x)}{2}}\}_{\alpha\alpha'} \{e^{-i\tau_3 \frac{\theta(0)}{2}}\}_{\beta\beta'} \rangle,$$  \hspace{1cm} (3)

as the product of the GF for the neutral fermions $G_{\alpha\beta}(x) = \langle Y_{\alpha}(x) Y^\dagger_{\beta}(0) \rangle$ and the phase correlator $\langle \exp(i\tau_3 \theta(x)/2) \exp(-i\tau_3 \theta(0)/2) \rangle$. For the frequency-momentum representation of Eq. (3) one has

$$D_{\alpha\beta}(\omega_n,i\mathbf{p}) = \frac{1}{\omega_n + \xi^2(\mathbf{p}) + \mu^2} \frac{\mathcal{P}}{2m} \frac{\mathcal{P}}{\omega_n},$$  \hspace{1cm} (4)

where $\mathcal{P} = \frac{1}{2}(\mathbf{I} \pm \tau_3)$ are the projectors; $\mathbf{I}$ and $\tau_3$ are unit and Pauli matrices; $D_{\alpha\beta}(i\Omega_n,i\mathbf{q})$ is the Fourier transformation of the phase correlator $D_{\alpha\beta}(x) = \langle \exp(ia\theta(x)/2) \exp(-ia\theta(0)/2) \rangle$; $\omega_n = (2n + 1)\pi T$ and $\Omega_n = 2\pi n T$ are respectively odd and even Matsubara frequencies. The GF of neutral fermions is taken in the mean-field approximation (see [11]).

$$G(\omega_n,i\mathbf{p}) = \frac{-\omega_n \mathbf{I} + \tau_3 \xi(\mathbf{p})}{\omega_n^2 + \xi^2(\mathbf{p}) + \mu^2},$$  \hspace{1cm} (5)

with $\mathbf{p}$ being a 2D vector and $\rho \equiv \langle \rho(x) \rangle$, where $\rho(x)$ is the modulus of a complex ordering field $\Phi(x) = \rho(x) \exp[i\theta(x)]$. Note that $\langle \Phi(x) \rangle = 0$ for $T \neq 0$ as it should be in 2D in accordance with the Coleman-Mermin-Wagner-Hohenberg theorem, while the value of $\rho$ is allowed to be nonzero. Note also that the GF (4) does not contain the symmetry violating term $\sim \tau_1$ which could originate from the terms $P_\pm G(\omega_n,i\mathbf{p})$ since the correlators $D_{+} = D_{-} = 0 \hspace{1cm} (6)$.

The representations (4), (5) for the fermion GF with decoupled spin and charged degrees of freedom are appropriate when one can neglect the fluctuations of the modulus $\rho(x)$ and when the energy of the phase distortions is smaller than the energy gain due to nontrivial $\rho$. For the present s-wave model this means that the condition $\rho \gg T$ should be satisfied, so that the modulus-phase representation (6) should be useful even for $T$ close to $T_{\text{BKT}}$ and allows one to study the evolution of the SC gap to the pseudogap. The region of temperatures $T$ where the condition $\rho \gg T$ is satisfied depends crucially on the relative size of the pseudogap region $(T^* - T_{\text{BKT}})/T^*$ which may be reasonably large in 2D for intermediate coupling [13]. The pseudogap in the current work is the result of the low dimensionality of the system and does not need the existence of preformed local pairs. The nonzero value of $\rho$ is due to average local density of Cooper pairs which do not have coherence above $T_{\text{BKT}}$.

The representation (4) shows (see the explanation after Eq. (4)) that the GF for the charged fermions is defined by the correlator $D(x) = D_{++}(x) = D_--(x)$. The asymptotic form of the correlator at large distances, describing also the temporal decay of correlations, is given by the form [14] \[ D(t, r) = \exp(-\gamma t)(r/r_0)^{-T/8\pi J}(r/\xi_+(T)). \] (6)

Here $t$ is the real time, $\gamma$ is a decay constant, $r_0 \equiv (2T)/(J/\hbar K)^{1/2}$ is the scale for the algebraic decay of correlations in the SC BKT phase ($T < T_{\text{BKT}}$, where $T_{\text{BKT}}$ is the temperature of the BKT transition), $\xi_+(T)$ is the phase coherence length for $T = T_{\text{BKT}}$, $\xi_+(T \to T_{\text{BKT}}^+) \to \infty$. The constants $J$ and $K$ are the bare (mean-field) superfluid stiffness and compressibility, respectively which have been calculated in [1] and [2].

Previously, using the representation (3), only the classical (static $\Omega_n = \gamma = 0$) fluctuations have been considered analytically [4]. The Fourier transform of (3) for this case is

$$D(\Omega_n,i\mathbf{q}) \approx \delta_{n,0} C[\mathbf{q}^2 + (1/\xi_+)^2]^{-\alpha}/T,$$  \hspace{1cm} (7)

where $C \equiv 4\pi(\Gamma(\alpha)/\Gamma(1-\alpha))(2r_0/\hbar K)^{2\alpha-2}$ and $\alpha \equiv 1 - T/\pi J$. For $T \sim T_{\text{BKT}}$ the value of $\alpha \approx 1 - T/32\pi J$. The presence of $\alpha \neq 1$ in (7) is related to the preexponent factor $(r_0/\hbar K)^{-T/8\pi J}$ in (6). This factor was not included in the analysis of [11,12], but the treatment of [14] includes this factor.

One can now extend the analysis to the case of quantum (dynamical) phase fluctuations. We propose the following generalization of (7):

$$D(\Omega_n,i\mathbf{q}) = \frac{C(v^2)^\alpha}{[w^2 - (v/\xi_+)^2 + \Omega_n^2 + 2\gamma|\Omega_n|^2]^\alpha},$$  \hspace{1cm} (8)

where $v$ is the velocity of the Bogolyubov excitations. Recall that in 2D $v = v_F/\sqrt{2}$, where $v_F$ is the Fermi velocity. The asymptotic form of the retarded GF corresponding to the GF (4) is

$$D^R(t, \mathbf{q}) \sim \begin{cases} t^{\alpha-1}e^{-\gamma t} & v^2 q^2 \gg \gamma^2 - v^2 \xi_+^2 \\ t^{\alpha-1}e^{-t\gamma - v^2 q^2 / \gamma^2} & v^2 q^2 < \gamma^2 - v^2 \xi_+^2 \\ t \to +\infty. \end{cases}$$  \hspace{1cm} (9)
Eq. (3) can be regarded as a convenient (for analytical studies) generalization of the phenomenological dependence \( \gamma(T) \) which for nonzero \( \gamma \) includes the decay of the phase correlations due to the presence of free vortices above \( T_{BKT} \). One can see that for \( v^2 q^2 < \gamma^2 - v^2 \xi_+^2 \) the decay rate is less than \( \gamma \) and it is minimal for \( q = 0 \). This means that, for large distances, phase fluctuations do not feel the pair vortices which have smaller size.

In the present work both \( \gamma \) and \( \xi_+ \) are phenomenological parameters which can be derived from the theory of the BKT transition. Since in the SC BKT phase the vortices are confined, one can state \( 21 \) that there is a critical slowing down of the phase fluctuations when the temperature approaches \( T_{BKT} \), i.e. \( \gamma(T \to T_{BKT}) = 0 \).

In fact the detailed theory of BKT transition predicts that \( \gamma(T) \sim \xi_+^{-1}(T) \), where \( z \) is the dynamical exponent and \( \xi_+^{-1}(T) = \xi_0^{-1} \exp(-b/\sqrt{T - T_{BKT}}) \), where \( b \) is a positive constant. In what follows we just restrict ourselves by comparing two cases: \( \gamma \neq 0 \) above \( T_{BKT} \) and \( \gamma = 0 \) for \( T < T_{BKT} \).

We note that there is now experimental evidence \( 4 \) for the vortex-pair unbinding (BKT) nature of the SC transition in the Bi-cuprates. We stress also that, despite the rather simple form of the GF, it takes into account the presence of vortices while the self-consistent T-matrix approximation (see e.g. \( 23,24,25 \)) cannot describe them.

The SF associated with GF (8) can readily be expressed in terms of the corresponding SF for the GF (9) and (8) as

\[
A(\omega, k) = -\frac{1}{\pi} \text{Im} G_{11}(\omega + i0, k) = \int_{-\infty}^{\infty} d\omega' \left[ \frac{1}{1 + e^{\omega'/T}} - \frac{1}{1 - e^{(\omega' - \omega)/T}} \right] \int \frac{d^2 p}{(2\pi)^2} a_{F}(\omega', p) a_{B}(\omega - \omega', k - p). \tag{10}
\]

where these SF are

\[
a_{F}(\omega, p) = (\omega + \xi(p)) \delta(\omega^2 - \xi^2(p) - \rho^2) \text{sgn}\omega, \tag{11}
a_{B}(\Omega, q) = -\frac{1}{\pi} \text{Im} D^{R}(\Omega, q). \tag{11}
\]

The \( \delta \)-function in \( a_{F} \) allows one to perform the angular integration in (10). Finally integrating over momentum the SF can be expressed as a single integral:

\[
A(\omega, k) = -\frac{1}{2\pi^2 T} \frac{\Gamma(\alpha)}{\Gamma(1 - \alpha)} \left( \frac{2}{m v_0^2} \right)^{\alpha - 1} \int_{-\infty}^{\infty} d\omega' \text{sgn}(\omega' + \omega) \times \left[ \frac{1}{1 - e^{\omega'/T}} - \frac{1}{1 + e^{(\omega' + \omega)/T}} \right] \frac{\theta(\omega' + \omega^2 - \rho^2)}{\sqrt{(\omega' + \omega)^2 - \rho^2}} \times \left[ I(\omega, k, \omega') \left( \omega' + \omega + \sqrt{(\omega' + \omega)^2 - \rho^2} \right) \times \theta(\mu + \sqrt{(\omega' + \omega)^2 - \rho^2}) + \sqrt{(\omega' + \omega)^2 - \rho^2} \rightarrow -\sqrt{(\omega' + \omega)^2 - \rho^2} \right], \tag{12}
\]

where we have introduced a function \( I(\omega, k, \omega') \):

\[
I(\omega, k, \omega') = \pi \text{Im} \left[ (x_+ - a - ib)^{-\alpha} F \left( x_+ - a - ib - x_-, x_+ - a + ib - x_- \right) \right],
\]

\[
a = \frac{1}{2m} \left( \frac{\omega'}{\mu^2} - \xi_+^2 \right), \quad b = \frac{\gamma \omega'}{mv_0^2},
\]

\[
x_\pm = \sqrt{\frac{k^2}{2m} \pm \sqrt{\mu + \sqrt{(\omega' + \omega)^2 - \rho^2}^2}}. \tag{13}
\]

For \( \gamma = 0 \) the expression (12) can be rewritten in the following form

\[
A(\omega, k) = -\frac{1}{2\pi^2 T} \frac{\Gamma(\alpha)}{\Gamma(1 - \alpha)} \left( \frac{2}{m v_0^2} \right)^{\alpha - 1} \int_{-\infty}^{\infty} d\omega' \text{sgn}\omega' \times \text{sgn}(\omega' + \omega) \left[ \frac{1}{1 + e^{\omega'/T}} - \frac{1}{1 + e^{(\omega' + \omega)/T}} \right] \times \theta((\omega' + \omega)^2 - \rho^2) \theta(\omega^2 - \rho^2) \times \left\{ \left( \pi(x_+ - a -\omega)^{-\alpha} F \left( \frac{1}{2}; 1; 1; \frac{x_+ - a - \omega}{x_+ - a - \omega} \right) \theta(a - x_+) + (x_+ - a - \omega)^{-1/2} (a - x_+ - \omega)^{1/2 - \alpha} B \left( \frac{1}{2}, 1 - \alpha \right) \times \left( \omega' + \omega + \sqrt{(\omega' + \omega)^2 - \rho^2} \right) \theta(\mu + \sqrt{(\omega' + \omega)^2 - \rho^2}) + \sqrt{(\omega' + \omega)^2 - \rho^2} \rightarrow -\sqrt{(\omega' + \omega)^2 - \rho^2} \right\} \right. \tag{14}
\]

which describes the case of the non-damped dynamical phase fluctuations. While Eq. (14) appears to be more complicated than the more general Eq. (12), it proves useful for making a general statement about the gap filling.

Expressions (12) and (14) present the main result of the paper for the SF in the case of quantum phase fluctuations. Before proceeding to the discussion of their numerical integration, we recap briefly the case of classical phase fluctuations. The static SF, obtained in \( 9 \), is reproduced from (14) after changing the variable \( \omega' \rightarrow \omega' \) and taking formally the limit \( v \rightarrow 0 \). It was discussed in detail in \( 9 \) and we would like to stress here only two main points. The first is that the SF is identically zero inside the gap \( A_{cl}(\omega, k) = 0 \) for \( |\omega| < \rho \). The second is that in addition to the usual quasiparticle peaks it reveals extra peaks at \( \omega = \pm \rho \).

Let us now return to the discussion of the results of numerical integration based on Eqs. (12) and (14) which are shown in Fig. 1.

a) For \( T < T_{BKT} \) there are two highly pronounced quasiparticle peaks at \( \omega = \pm E(k) \equiv \pm \sqrt{\xi_+^2(k) + \rho^2} \). Since below \( T_{BKT} \) both \( \xi_+^{-1} \) and \( \gamma \) are zero, the width of the peaks
is almost entirely controlled by $\alpha$ whose deviation from 1 gives the non-Fermi liquid behavior of the GF \cite{1}. Since the value of $\alpha$ is very close to 1 this non-Fermi liquid behavior is hardly distinguishable from ordinary widening of the quasiparticle peaks due to damping. Furthermore, because $\alpha \to 1$ as $T \to 0$ the width of the peaks is temperature dependent so that the peaks become sharper as $T$ decreases resembling the data of ARPES for the anti-node direction. \cite{2}

We note also that $k \neq k_F$ in Fig. 1 so that the quasiparticle peaks are not equal to each other in contrast to the case of symmetrized ARPES data \cite{1}. The reason for choosing $k \neq k_F$ in Fig. 1 was to prove that the extra peaks present in the SF calculated for the classical phase fluctuations \cite{3,4} are now absent.

The gap in the SF remains almost unfilled and has "U"-like shape. We stress, however, that in contrast to the static case \cite{3} the SF \cite{2} is nonzero even for $|\omega| < \rho$ and this is evidently related to the presence of the quantum (dynamical) phase fluctuations, i.e. the terms with $\Omega_n \neq 0$. In particular, using Eq. (14) one can check analytically that even for $\gamma = 0$ due to these terms $A(\omega = 0, k = k_F) \neq 0$. We estimated the temperature $T_{cl}$ of the quantum to classical crossover in the way similar to that of \cite{23}. For the lower carrier densities this gives $T_{cl} \sim T_{BKT}$, while for the higher carrier densities, where the pseudogap phase shrinks \cite{6} we obtain $T_{cl} \sim \rho(T = 0) \sim T^\ast$. Thus, the crossover temperature is always too large (in the absence of dissipation) for classical fluctuations to play a significant role at low $T$.

d) Due to the smooth dependence of $\xi_+^{-1}$ and $\gamma$ on $T$ as the temperature passes through $T_{BKT}$ there is no sharp transition at $T_{BKT}$ in agreement with experiment \cite{1,3}. A similar filling of the gap was obtained in \cite{14} for $\gamma = 0.5\mu$ where the correlator \cite{1} was used for the numerical computation of the self-energy of the fermions and the subsequent extraction of the SF from the fermion GF. A recent Monte Carlo simulation \cite{14} also shows similar behavior for the quasiparticle peaks and the filling of the gap. However it is the analytical character of the present work, which relies on the explicit introduction of the charge and spin degrees of freedom \cite{2} for the Nambu spinors, that enables us to unambiguously state the correspondence between the parameters of the model and the observed features of the SF \cite{2}.

In spite of some similarities between the results observed and those just obtained, the latter are only illustrative since we have considered a model with non-retarded s-wave attraction. However, it is likely that for d-wave pairing, the properties obtained can be used for the description of the systems in the anti-node direction on the Fermi surface. It is however essential to consider fluctuations in the modulus of the order parameter to extend the analysis to the nodal directions on the Fermi surface. The value of $\gamma = 0.5\mu$ which results in a filled gap appears to be too large to be due to the vortex-vortex interaction. This leads one to the conclusion that the mechanism considered here for gap filling may not be the only possible mechanism and that other interactions which lead to the filling of the gap above $T_c$, see \cite{1,2,13}, are also important.

In summary we studied the effect of the fluctuations in the phase of the complex ordering field on the properties of a 2D system with four-fermion attraction. The fermion SF has been given as a single integral over a function known in closed form. Through the use of analytical techniques, we have been able to demonstrate that the quantum phase fluctuations in the presence of dissipation lead to the filling of the pseudogap even if one ignores the spin-charge coupling.

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It is practically impossible to make such a statement relying on numerical results. For example, using our own result for the GF from [4] calculated on the imaginary axis to ten digits of precision, we tried to recover the known static SF using the method of numerical analytic continuation, H.J. Vidberg and J.W. Serene, J. Low Temp. Phys. 29 (1977) 179. Even for over 100 Matsubara frequencies the gap remained filled numerically.

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FIG. 1. The spectral function \(A(\omega, k)\) as a function of \(\omega\) in units of the zero temperature SC gap \(\Delta\) for \(k > k_F\) taken at two different temperatures, \(T_1 < T_{BKT} < T_2\).