Cooperon propagator description of high temperature superconductivity

C. Berthod and B. Giovannini *

DPMC, Université de Genève, 24 Quai Ernest-Ansermet, 1211 Genève 4, Switzerland

Abstract

A phenomenological description of the high-\(T_c\) superconductors based on the Cooperon propagator is presented. This model allows one to study the effects of local pairing correlations and long-range phase fluctuations on the same footing, both above and below \(T_c\). Based on numerical calculations, it is shown that the two types of correlations contribute to the gap/pseudogap in the single-particle excitation spectra. The concourse of these two effects can induce low energy states, which should be observable in underdoped materials at very low temperature.

Key words: Superconductivity, Cuprates, Pseudo-gap

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The nature of the pseudogap phase in the high-\(T_c\) cuprate superconductors (HTS) is still the subject of lively debate and its elucidation may be one of the keys to the understanding of these materials. At present we may perhaps, from the experimental point of view, state the following: (1) The pseudogap — defined as a depletion of the single particle density of states (DOS) around the Fermi energy, which appears gradually at a temperature \(T^*\) — goes smoothly into the superconducting gap at \(T_c\), as seen in STM[1] and ARPES[2] measurements. (2) The STM measurements of vortices below \(T_c\) show that the DOS in the center of the vortex core resembles strongly the DOS observed above \(T_c\) in the pseudogap regime[3,4]. (3) The fluctuations above \(T_c\) (and outside the 3D critical regime near \(T_c\)) seem to correspond to a phase fluctuation regime, quantitatively well described by the Kosterlitz-Thouless (KT) theory above \(T_{KT}[5,6]\). (4) This phase fluctuation regime seems to disappear at a characteristic temperature well below \(T^*[5,6]\). One is therefore in need of a theoretical framework which (i) is able to show a smooth transition of the DOS across \(T_c\), (ii) connects the phase fluctuation regime with the properties of the KT theory, and (iii) relates the properties within a vortex core to the properties of the

* Corresponding author. Fax: +41-22-7026869
Email address: bernard.giovannini@physics.unige.ch (B. Giovannini).
pseudo-gapped phase. Such a theoretical framework has been developed 40 years ago by Kadanoff and Martin (KM)[7], who presented a theory of superconductivity entirely based on the pair correlation function (Cooperon propagator). In a recent paper[8], we applied this framework for the \( s \)-wave symmetry. The purpose of this communication is to extend these results to the \( d \)-wave symmetry case.

In the KM formalism, the relation between the two-body Cooperon propagator \( L(\mathbf{r}, \mathbf{r}'; \mathbf{s}', \mathbf{s}; \tau) = \langle \psi_\uparrow(\mathbf{r}, \tau)\psi_\downarrow(\mathbf{r}', \tau)\psi_\downarrow^\dagger(\mathbf{s}, 0)\psi_\uparrow^\dagger(\mathbf{s}', 0) \rangle \) and the self-energy is

\[
\Sigma(\mathbf{r}, \mathbf{s}, \tau) = -\int d\mathbf{r}' d\mathbf{s}' V(\mathbf{r}, \mathbf{r}')L(\mathbf{r}, \mathbf{r}'; \mathbf{s}', \mathbf{s}; \tau)V(\mathbf{s}', \mathbf{s})G_0(\mathbf{s}', \mathbf{r}', -\tau), \tag{1}
\]

where \( G_0 \) is the free Green’s function and \( V(\mathbf{r}, \mathbf{r}') \) is the effective interaction between the electrons. In a translationally invariant system with a short-ranged interaction, we may approximate the product \( VLV \) in Eq. (1) by the form \( \varphi(\mathbf{r} - \mathbf{r}')\varphi(\mathbf{s}' - \mathbf{s})\Lambda(\mathbf{r}' - \mathbf{s}', \tau) \), where \( \varphi(\mathbf{r}) \) reflects the symmetry of the short-range correlations and \( \Lambda(\mathbf{r}, \tau) \) describes their strength and long-range properties. Thus Eq. (1) can be rewritten in Fourier-Matsubara representation as:

\[
\Sigma(\mathbf{k}, \omega_n) = k_B T \sum_m \int \frac{d\mathbf{q}}{(2\pi)^2} \frac{\varphi^2(\mathbf{k})\Lambda(\mathbf{k} + \mathbf{q}, \omega_n + \omega_m)}{-i\omega_m + \varepsilon(\mathbf{q})}, \tag{2}
\]

where \( \varepsilon(\mathbf{k}) \) is the free dispersion. The self-energy recovers the BCS form when \( \Lambda \) is independent of distance and time, i.e. \( \Lambda \propto \delta(\mathbf{k} + \mathbf{q}) \delta(\omega_n - \omega_m) \) in Eq. (2). In this formalism, the superconducting order is therefore related to the long-range properties of the function \( L \), rather than to the strength of the superconducting correlations.

Along the lines of Ref. [8], we use the following phenomenological model for \( \Lambda \):

\[
\Lambda(\mathbf{r}, \tau) = \Delta_0^2 e^{-r/\varrho_0} + \Delta_1^2 e^{-r/\xi(T)}, \tag{3}
\]

where static (\( \tau \)-independent) correlations are assumed for simplicity. The first term corresponds to the local correlations of range \( \varrho_0 \) and the second term describes the phase fluctuations regime above \( T_c \) — \( \xi(T) \) is the correlation length of the KT theory — and the phase coherence below \( T_c \). Both types of correlations are supposed to have the same symmetry. With this model, the self-energy on the real-frequency axis becomes \( \Sigma(\mathbf{k}, \omega) = \varphi^2(\mathbf{k})\int \frac{d\mathbf{q}}{(2\pi)^2} \Lambda(\mathbf{k} + \mathbf{q}) \left[\omega + i0^+ + \varepsilon(\mathbf{q})\right] \). In the following, we consider \( \Delta_0 \) and \( \Delta_1 \) as temperature independent parameters, and we calculate numerically the spectral function \( A(\mathbf{k}, \omega) = -\frac{1}{\pi} \text{Im} \left[\omega + i0^+ - \varepsilon(\mathbf{k}) - \Sigma(\mathbf{k}, \omega)\right]^{-1} \) for a uniform two-dimensional square lattice, a \( d \)-wave factor \( \varphi(\mathbf{k}) = \frac{1}{2}(\cos k_x - \cos k_y) \), and a dispersion \( \varepsilon(\mathbf{k}) \) representative of the \( \text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+x} \) (\( \text{Bi}2212 \)) band structure[9].

The resulting \( A(\mathbf{k}, \omega) \) at the antinodal point of the Fermi surface is shown in Fig. 1 (upper panels) for several temperatures above \( T_c \). One can see marked differences
between the strong ($\Delta_0 > \Delta_1$) and weak ($\Delta_0 < \Delta_1$) pseudogap cases. In the former case, the spectral function is dominated by the contribution of the local correlations and remains basically temperature independent. In the latter case, the quasiparticle peak broadens with increasing temperature, and moves toward the Fermi energy. It is worth noting, in this connection, that the gap in the spectral function does not relate solely to the strength of the correlations — or to the amplitude of the superconducting order parameter — but also to the range of these very correlations; this is particularly clear in the right part of Fig. 1, since $\Delta_1$ is the same for all curves. Therefore, the spectral function alone does not provide a reliable measure of the amplitude of the fluctuating order parameter above $T_c$.

In order to compare our results with the experimental data, we must take into account the angular ($\delta \theta \approx 5^\circ$) and energy ($\delta \omega \approx 15$ meV) resolutions of the ARPES measurements. We thus estimate the ARPES intensity $I(k, \omega)$ as a convolution of the calculated $A(k, \omega)$ and $f(\omega)$, $f$ the Fermi function, with a Gaussian of appropriate width in $k$ and $\omega$. The calculated $I(k, \omega)$ is shown in the lower panels of Fig. 1.
Fig. 2. Upper panels: Density of states from $T_c$ to room temperature in the strong (left) and weak (right) pseudogap cases. Lower panels: Calculated tunneling conductance from $T = 10$ to 300 K. The model parameters are the same as in Fig. 1. The curves are offset vertically by equal amounts. The thick curves correspond to $T = T_c$.

Because of the $k$-dependence of the spectral function, the effect of a finite angular resolution is mainly to add a background in the ARPES signal. In the strong pseudogap case, we find that the peak position is more or less temperature independent, in agreement with the experimental results in underdoped Bi2212[2]. In the weak pseudogap case, however, the peak approaches the Fermi level as observed in overdoped Bi2212[2]. The ARPES lineshapes in Fig. 1 do not show a sudden disappearance of the quasiparticle peak at $T_c$[10]. This might be due to our assumption of static correlations in Eq. (3). Short time correlations above $T_c$ can be expected to decrease the quasiparticle lifetime and eventually to induce a redistribution of the spectral weight over a large energy window.

In Fig. 2 (upper panels), we plot the calculated density of states (DOS) $N(\omega) = \int dK A(k, \omega)$ for temperatures above $T_c$ (the DOS below $T_c$ is equal to the DOS at $T_c$ in the present model). The lower panels show the tunneling conductance across $T_c$, calculated as $dI/dV \propto \int d\varepsilon f'(\varepsilon - eV) \int dK |T_k|^2 A(k, \varepsilon)$ with a uniform matrix element $T_k \equiv T_0$. The behavior of the DOS as a function of temperature parallels the behavior of the spectral function in Fig. 1. In the strong pseudogap case, the effect
of the local correlations is to broaden the DOS, resulting in smaller coherence peaks and in a large zero-bias conductance. In addition, we find characteristic shoulders near the Fermi energy, reminiscent of the low-energy states observed in Bi2212 vortex cores[3,4]. As Fig. 2 shows, these states disappear above $T_c$, leading to a more U-shaped spectrum. Moreover, we have verified that these structures are absent if $q_0 \gtrsim 20a$, and that they do not appear if $\Delta_0 = 0$ or $\Delta_1 = 0$. These findings indicate that the low energy states result from the interplay of the short-range and long-range correlations. This is confirmed by our numerical results in the weak pseudogap case. Indeed, subgap structures can be seen in the DOS for $T > 100 \text{K}$, i.e. a temperature range where $\xi(T)$ is smaller than $q_0$.

In the tunneling spectra shown in Fig. 2 (lower panels), the superconducting gap evolves smoothly across $T_c$ into a pseudogap, but the coherence peaks and the gap structure is suppressed more rapidly in the weak pseudogap case as the temperature is raised. Also, the width of the pseudogap appears to be almost temperature independent in both strong and weak pseudogap cases. These trends are consistent with the experimental observations in under- and overdoped Bi2212[1], respectively.

In summary, based on a phenomenological theory of HTS connected to the properties of the Cooperon propagator, we have investigated the effect of local pairing correlations and long-range phase fluctuations on the spectral properties of a 2-dimensional $d$-wave superconductor. The energy and temperature dependence of the spectral functions was shown to vary with the relative strength $\Delta_0/\Delta_1$ and the relative range $q_0/\xi(T)$ of both types of correlations. In particular, low energy states were found to appear in the DOS in two distinct regions of the parameter space: $\Delta_0/\Delta_1 > 1$, $q_0/\xi(T) \ll 1$ (strong pseudogap case at low temperature) and $\Delta_0/\Delta_1 < 1$, $q_0/\xi(T) > 1$ (weak pseudogap case at high temperature), i.e. when one type of correlation is stronger in strength and weaker in range with respect to the other type of correlation.

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