Unconventional temperature dependence of the cuprate excitation spectrum

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Abstract. Key properties of the cuprates, such as the pseudogap observed above the critical temperature $T_c$, remain highly debated. Given their importance, we recently proposed a novel mechanism based on the Bose-like condensation of mutually interacting Cooper pairs [W. Sacks, A. Mauger, Y. Noat, Supercond. Sci. Technol. 28, 105014 (2015)]. In this work, we calculate the temperature dependent DOS using this model for different doping levels from underdoped to overdoped. In all situations, due to the presence of excited pairs, a pseudogap is found above $T_c$ while the normal DOS is recovered at $T^*$, the pair formation temperature. A similar behavior is found as a function of magnetic field, crossing a vortex, where a pseudogap exists in the vortex core. We show that the precise DOS shape depends on combined pair (boson) and quasiparticle (fermion) excitations, allowing for a deeper understanding of the SC to the PG transition.

1 Introduction

As is well known, the superconducting (SC) state of cuprates is characterized by a dome-shaped critical temperature $T_c$, versus carrier density and an unconventional pseudogap (PG) state above $T_c$ (see Ref. [1] for a review). In addition, these compounds exhibit a spatially inhomogeneous [2,3] and unconventional quasiparticle (QP) dispersion (see Refs. [4–6] and references therein), the “peak-dip-hump” structure, with a characteristic gap $\Delta_p$ typically larger than the critical temperature energy scale $\sim k_B T_c$ in the underdoped regime.

Many of these properties remain highly debated, in particular the Cooper pair formation mechanism and the origin of the pseudogap state, which appears below the higher temperature $T^*$. The spectral gap is of the same order of magnitude at $T_c$ as in the vortex core [7], indicating that the PG characterizes the loss of SC coherence [8]. In agreement with Renner et al. [9], recent experiments by Sekine et al. [10] on quasiparticle excitation spectra up to $T^*$ are particularly intriguing. The spectral gap indeed starts to disappear and vanishes only at the higher temperature $T^*$.

To summarize, a solution of the high-$T_c$ problem must account for:

(i) multiple energy scales ($T_c$, $T^*$) and large gap $\Delta_p$;
(ii) large $T_c$, however with $k_B T_c \ll \Delta_p$;
(iii) the dome-shape of the $T-p$ phase diagram;
(iv) the unconventional SC to PG transition;
(v) the unusual QP dispersion (“peak-dip-hump”).

With these questions in mind, we have recently proposed a model [11,12], based on the mutual interaction between pre-formed pairs, able to take into account both phases of the system. It describes cogently the shape of the low-temperature excitation spectrum in cuprates and links the superconducting and pseudogap phases.

In an early approach, Franz and Millis [13] addressed the temperature dependence of the QP excitation spectrum based on the effects of classical phase fluctuations. Unfortunately, their model does not match the precise shape of the STS data, especially the important dip present at low temperature, a clear signature of HTc superconductivity.

More recently, Pieri et al. [14] considered pair fluctuations in the t-matrix framework, but again no dip in the zero temperature spectra was clearly demonstrated. In a related paper involving pair fluctuations [15], a repulsive pair-pair interaction was inferred, like in our model, but an explicit calculation of the density of states was not reported. To the contrary, our model gives for the first time the low-temperature peak-dip-hump feature and the full temperature dependence of the QP spectra up to $T^*$.

At the heart of the model, an incoherent state consists of preformed pairs [16] with an energy distribution $P_0(\Delta_i)$...
The superconducting gap, $\Delta$, is determined by the self-consistent equation \[ \beta \Delta = \Delta_0 + \Delta_p \cos(2\theta). \] (1)

where $\Delta_0$ and $\sigma_0$ are respectively the average gap and the width of the distribution. Alternatively, $P_0(\Delta_1)$ can be considered as the density of pair states.

Pairs in the PG state have a random energy distribution, making long range order impossible. Interactions between pairs, with characteristic coupling energy $\beta_0$, makes the superconducting gap $\Delta$ determined by the self-consistent equation \[ \Delta_0(E_k) = \Delta_{0,k} - 2 \beta_0 P_0(E_k) \] (2)

with $E_k = \sqrt{\epsilon_k^2 + \Delta_0^2}$, the quasiparticle dispersion. The self-consistent solution of this equation at $\epsilon_k = 0$ gives the condensation level $\Delta_k = \Delta_0 \cos(2\theta)$. In the antinodal direction ($\theta = 0$), the condensation energy is thus $\epsilon_+ = \Delta_0 - \Delta_p = 2\beta_0 P_0(\Delta_p)$.

The interaction term $\beta_0 P_0(\Delta_k)$ with the quasiparticle energy $E_k$ expresses the interaction of a quasiparticle with pair excited states (see the diagram, Fig. 1).

The coefficient $\beta_0 \propto \beta_0 N_{oc}(T)$ is proportional to the number of pairs in the condensate $N_{oc}(T)$ and plays the role of an order parameter vanishing at $T_c$. The zero-temperature gap is related to the fundamental parameters and energy scales of the material (Debye frequency, electron-phonon coupling, DOS at the Fermi energy). Proportional to the critical temperature, it has a universal value: $\Delta(T = 0) \approx 1.7k_B T_c$.

The tunneling density of states (DOS) is a direct consequence of the QP dispersion:

\[ N_S(E) = N_{oc}(E_F) \frac{|E|}{\sqrt{E^2 - \Delta^2}} \Theta(|E| - \Delta) \] (3)

where $N_{oc}(E_F)$ is the normal DOS at the Fermi energy and $\Theta(z)$ is the heaviside function.

2 Quasiparticle excitation spectrum

2.1 Case of conventional superconductors

The excitations of the system are important for all thermodynamic and transport properties. In the BCS theory [17], at finite temperature, the presence of condensed Cooper pairs below $T_c$ is accompanied by quasiparticle excitations having the dispersion $E_k = \sqrt{\epsilon_k^2 + \Delta_0^2}$ where $\epsilon_k$ is the kinetic energy relative to the Fermi energy and $\Delta(T)$ is the SC gap. The latter decreases as a function of temperature as a result of QP excitations governed by Fermi-Dirac statistics $f(E, T) = (e^{(E - \mu)/k_B T} + 1)^{-1}$ and eventually vanishes at the critical temperature $T_c$.

The tunneling density of states (DOS) is a direct consequence of the QP dispersion:

\[ N_S(E) = N_{oc}(E_F) \frac{|E|}{\sqrt{E^2 - \Delta^2}} \Theta(|E| - \Delta) \] (4)

where $N_{oc}(E_F)$ is the normal DOS at the Fermi energy and $\Theta(z)$ is the heaviside function.

![Fig. 1. Left panel: distribution of excited pair states. Right panel: energy diagram to illustrate the coupling between quasiparticles and excited pair states.](image)
At low temperatures, it reveals a sharp energy gap at the Fermi-level – first measured by Giaever using planar junctions \cite{18} – delimited by high symmetric peaks. The DOS has since been measured many times with a high precision by tunneling spectroscopy using planar junctions or STM geometries \cite{19} and later on using Angle Resolved Photon Emission Spectroscopy (ARPES) in cuprates \cite{20,21}.

2.2 Unconventional superconductors

In our model, the situation is radically different from the BCS situation. In this case, the gap does not vanish at $T_c$ but at $T^*$, the pair formation onset temperature. On the other hand, the condensation energy $\epsilon_c \propto \beta_0 N_{oc}(T)$ vanishes at $T_c$, which is much smaller than $T^*$. Thus, for the temperature dependent DOS, two additional contributions arise, absent in the BCS case: first the contribution of excited pairs increasing with temperature up to $T_c$, and second the dissociation of pairs increasing up to $T^*$.

The DOS as a function of temperature for optimal doping is reported in Figure 2, left panel. At zero temperature, it exhibits the characteristic shape of the excitation spectrum of the cuprates, with the characteristic “peak-dip” features. As the temperature rises, the quasiparticle peak heights decrease while the gap width remains roughly constant, contrary to the BCS case. At $T_c$, there is a clear pseudogap with attenuated QP peaks. For higher temperature ($T > T_c$), one notes the filling of states inside the gap while the QP peaks are further smoothed. The gap eventually disappears completely at $T^*$.

Note that other theories have been proposed for the “peak-dip-hump” structure in the DOS measured by STM/ARPES. The most popular approach is the coupling to a spin collective mode (see Refs. \cite{22,23} and references therein). It appears that the fit to the experimental spectra is rendered difficult in this framework due to the necessarily retarded interaction. Furthermore, to our knowledge, its extension to finite temperature has not been done.

To the contrary, the pair-pair interaction model accurately reproduces the DOS measured by STM/STS in BiSr$_2$Ca$_2$Cu$_2$O$_{8+\delta}$ \cite{9} or TlBa$_2$Ca$_2$Cu$_3$O$_{8.5+\delta}$ \cite{10}. As observed in experiments \cite{7,24,25}, we find a similar situation as function of the magnetic field, crossing a vortex (see Fig. 2, right panel). Here we assume that the effect of magnetic field is to reduce the coherence energy $\beta$, quite analogous to the effect found in case of a disorder potential \cite{3,26}. The coherence peaks decrease when approaching the vortex center where finally a peakless pseudogap is found in the vortex core. In a general way, the loss of coherence of the SC to PG transition is driven by the vanishing of $\beta$, the pair-pair interaction.

3 DOS in the pair-pair interaction model

Contrary to standard models, we express the quasiparticle DOS as a sum of three terms:

$$N(E, T) = N_{\text{cond}}(E, T) + N_{\text{ex}}(E, T) + N_{\text{diss}}(E, T)$$

where the distinct contributions are:

(i) the condensate, $N_{\text{cond}}(E, T)$;

(ii) the excited pairs, $N_{\text{ex}}(E, T)$;

(iii) the dissociated pairs, $N_{\text{diss}}(E, T)$.

3.1 Condensate

The contribution of the condensate $N_{\text{cond}}(E, T)$ is proportional to the number of pairs in the condensate at temperature $T$:

$$N_{\text{cond}}(E, T) = N_{oc}(T) \times N_{SC}^0(E, T)$$

where $N_{SC}^0(E, T)$ is the zero-temperature superconducting DOS, found when all pairs belong to the condensate, i.e. when $N_{oc}(T = 0) = n_0$. 

Fig. 2. Left panel: temperature evolution of the QP-DOS from zero temperature through $T_c$ (SC to PG transition) up to $T^*$ (normal state). Right panel: expected evolution of the QP-DOS crossing a vortex core. The coherence peaks disappear leaving a peakless PG spectrum. Note that the additional thermal broadening ($\sim 3.5 k_B T_c$) due to the tunneling process is not included throughout this work.
As shown in references [12,27], neglecting any QP lifetime broadening, the condensate DOS along the \( \theta \) direction is:

\[
N_{\text{SC}}(E, \theta) = \frac{N_n(E_F)}{2\pi} \int_0^\infty dk \delta(E_k - E) = \frac{N_n(E_F)}{2\pi} \left( \frac{\partial \epsilon_k}{\partial E_k} \right)_{E_k = E}
\]

with

\[
\frac{\partial \epsilon_k}{\partial E_k} = \epsilon_k + \frac{\Delta_k(\epsilon_k, \theta) \cos(2\theta)}{\sqrt{E_k^2 - \Delta_k(E_k)^2}}
\]

where \( N_n(E_F) \) is the normal DOS at the Fermi energy.

The superconducting DOS is thus inversely proportional to the slope of \( E_k(\epsilon_k) \), depending explicitly on the gap function (2). Therefore, the fine structure in the DOS, the “peak-dip-hump” features, originates from the interaction term, \( 2\hbar B_0 F_0(E_k) \), of the gap equation. While these features have been studied at \( T = 0 \) [12,27], in the following we address the question of their temperature dependence.

### 3.2 Excited pairs

As soon as the temperature increases, excited pairs start to contribute (see Fig. 3) to the DOS. This leads to the term:

\[
N_{\text{ex}}(E, T) = A(T) \sum_{\epsilon_i > \delta \cos(2\theta)} f_B(\epsilon_i, T) N_i(E, \Delta_i)
\]

where \( \epsilon_i = \Delta_i - \Delta_p \cos(2\theta) \) is the excitation energy and \( f_B(E, T) \) is the Bose distribution. \( N_i(E, \Delta_i) \) is the DOS associated with each pair \( \Delta_i \). In the standard \( d \)-wave form, assuming that excited pairs are not interacting, we have:

\[
N_i(E, \Delta_i) = \frac{N_n(E_F)}{2\pi} \int_0^{2\pi} d\theta \frac{|E|}{\sqrt{E^2 - (\Delta_i \cos(2\theta))^2}}.
\]

### 3.3 Dissociated pairs

The bosons in our model are composite fermions but, distinct from the BCS case, as the temperature rises an increasing fraction of the pairs dissociate at the Fermi energy. This appears as some of the \( \Delta_i \) vanish, i.e. when \( \Delta_p(T) \) starts to decrease. This gives rise to the third term:

\[
N_{\text{diss}}(E, T) = N_n(E_F) \times N_{\text{diss}}(T).
\]

Here \( N_{\text{diss}}(T) \) is the number of dissociated pairs at the temperature \( T \) (see Fig. 3). It increases up to \( T^* \), where finally \( N_{\text{diss}}(T^*) = n_0 \).

### 4 Discussion

#### 4.1 Pair densities

The number of pairs (including dissociated pairs) must follow a sum rule:

\[
N_{\text{oc}}(T) + N_{\text{ex}}(T) + N_{\text{diss}}(T) = n_0.
\]

This rule involving the number of pairs guarantees the conservation of states in the DOS at any temperature \( T \):

\[
\int_{-\infty}^{\infty} dE N(E, T) = C
\]

where \( C \) is a constant. In addition, we assume that the total number of pairs (i.e. condensed plus excited pairs) must follow

\[
N_{\text{tot}}(T) = N_{\text{oc}}(T) + N_{\text{ex}}(T) + N_{\text{diss}}(T) \sim \Delta_p(T)^2
\]

which vanishes as \( \sim |T - T^*| \) near \( T^* \). Note that the precise shape of \( N_{\text{tot}}(T) \) has never been investigated. Our assumption on its particular temperature dependence does not influence the basic conclusions of the paper.

As previously noted, at \( T = 0 \), all pairs belong to the condensate: \( N_{\text{oc}}(T = 0) = n_0 \). As the temperature increases, pairs are progressively excited from the condensate, i.e. \( N_{\text{ex}}(T) \) increases with temperature in opposition to \( N_{\text{oc}}(T) \), as in Figure 3. Only low-lying excited states dominate owing to the boson occupation \( f_B(E, T) \) in equation (3). With temperature, the condensate empties while the number of excited pairs increase. Finally, at the critical temperature, there is no longer a condensate:

\[
N_{\text{oc}}(T_c) = 0.
\]
Fig. 4. Comparison of the $T$-dependent DOS for three different doping levels: underdoped (left panel), optimal (middle panel), overdoped (right panel). The corresponding temperatures ($T_c, T^*$) are indicated. The upper figures show the temperature range of the boson and fermion excitations. It is important to note the striking difference between the onset of quasiparticle and pair dissociation, for the overdoped and underdoped cases.

In the underdoped regime, where $T_c \ll T^*$ (the case of Fig. 3), the number of dissociated pairs is negligible, so that all pairs are excited at $T_c$:

$$N_{ex}(T_c) \approx n_0.$$  

In the more general case, to be discussed below, some pairs are already dissociated at the critical temperature and one has:

$$N_{diss}(T_c) = n_0 - N_{ex}(T_c) > 0.$$  

The effect of pair dissociation is highly sensitive to the $(T^* - T_c)$ difference, in practice to the doping value. An in-depth work of Gomes et al. [28–30] investigated the zero bias conductance in the SC and PG states. While it is quite uniform in the superconducting state, it showed significant variations above $T_c$. This result can be directly explained by the presence of dissociated pairs, giving rise to the third term in equation (5).

It is important to stress that the progressive broadening of the QP peaks from SC to PG state is not due to a finite quasiparticle lifetime ($\Gamma_{Dynes}$ broadening [31]). Instead, it results from the second term in equation (5) due to excited pairs existing at finite temperature. The calculation leads to a larger PG in the vortex core (see Fig. 2, right panel), where it directly stems from the distribution of preformed pairs $P_0(\Delta_i)$, rather than at $T_c$ where it also involves the Bose statistics $f_B(E, T)$. Such a filling of the DOS is a direct consequence of the statistical occupation of pair excitations inherent to the model.

4.2 Changes of the DOS with doping

Using the previous relations, we have calculated the temperature evolution of the DOS for three different doping levels corresponding to the underdoped regime (Fig. 4a), optimally doped (Fig. 4b) and overdoped regime (Fig. 4c). At low temperature, the excitation spectrum exhibits the characteristic $d$-wave shape of HTc cuprates (see Ref. [6] for a review) and the “peak-dip” features. Note that it is more pronounced in the underdoped case, while it is slightly attenuated in the overdoped case.

The coherence peaks broaden as the temperature rises, as a consequence of the increasing contribution of incoherent excited pairs, and eventually vanish at $T_c$, where all bosons have left the condensate. The contribution
of $N_{c\sigma}(T)$ gives rise to a clear pseudogap at $T_c^*$ for the three different doping values.

The remarkable difference between underdoped and overdoped samples emerges as the limit at which quasiparticle QP* and normal electrons appear (it is defined as the temperature at which the total number of pairs $N_{tot}(T)$ decreases significantly, i.e. when it reaches $0.9 n_0$). They originate respectively from excited pairs $\Delta_i^*$, which give rise to quasiparticles $E_i^* = \sqrt{\epsilon_i^2 + \Delta_i^2}$, and from dissociated pairs (with energy $\sim 2\epsilon_i$). The presence of normal electrons implies that some states are present inside the gap, leading to a finite value in the DOS at $E = 0$. As a rule of thumb, pair excitations attenuate the QP peaks while the normal states fill in the gap.

The situation is quite extreme in the underdoped case, wherein $T_c$ is much smaller than $T^*$ (Fig. 4a, upper panel). Consequently quasiparticles QP* and normal electrons arise well above $T_c$. In this case, the SC to PG transition is dominated by boson excitations, the fermion contribution being negligible. This quasi-Bose transition is characterized by the vanishing of the condensate (B) at $T_c$ leaving only pair excitations (B*) just above $T_c$. The opposite scenario is found in the overdoped regime where quasiparticles and normal electrons coexist below $T_c$. Finally, in the optimally doped regime, with the highest $T_c$, it is remarkable that the onset of quasiparticle and normal excitations (QP*+N, in Fig. 4b) coincides with the critical temperature.

Given their importance, further experiments should be done to verify the density profiles with the predictions of the model.

5 Conclusion

In summary, we proposed a comprehensive model for HTc superconductors based on an underlying disordered state of preformed pairs. Coherence is achieved by means of the pair-pair interactions leading to a Bose-type condensation. Contrary to the standard BCS theory, several contributions to the DOS at finite temperature: (i) the condensate; (ii) the presence of excited pairs; (iii) normal electrons arising from pair dissociation.

As a direct consequence of our model, the first contribution decreases with temperature, while the two other contributions, preformed pairs and normal electrons, coexist at finite temperature. The low temperature DOS exhibits the well-known “peak-dip” structure – directly related to the pair-pair interaction – which characterizes superconducting coherence. Due to the presence of excited pairs, the quasiparticle peaks in the DOS decrease progressively, concomitant with the pair-pair interaction, as a function of temperature and a pseudogap is finally found at $T_c$ up to $T^*$ in the whole doping range. A similar pseudogap is found in the vortex core, in very good agreement with tunneling experiments.

The evolution of the DOS as a function of temperature reveals a mixed state wherein condensed or excited bosons and normal electrons coexist.

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