Critical temperatures in cuprate superconductors

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Abstract.- The order parameter in superconductivity of cuprates is investigated in the framework of the Bogoliubov theory. By using a simplifying assumption about the electronic states, it is predicted an effective critical temperature $T_c^* > T_c$ associated to the coherent gap Δ_0. A connection between Δ_0 and the antinodal pseudogap Δ_{PG} is proposed allowing for a comprehensive picture of the main experimental features of cuprates superconductors.

The high temperature superconductivity (SC) in cuprate based materials is one of the most intensely investigated topics in condensed matter physics. It has been about twenty-four years since the seminal paper of Bednorz and Muller [1] sparked the race to attain the highest SC critical temperature(T_c) [2]. Much efforts have been spent to explain the pairing nature of electrons in the SC phase of cuprates, but yet physicists remain undecided on what model among the ones so far proposed worths general consensus [3]. However, in recent years several features concerning the SC and the normal state have been unveiled so making the matter a little more clear. It is known that, due to high electronic repulsion, undoped CuO_2 planes are Mott insulators turned to antiferromagnetic (AF) states [3]. Injection of small quantities of holes destroys the long-range AF order and give rise to phenomenologically rich electronic systems. Below a temperature T*, depending on the doping level, the normal phase show a gap of width dependent on the electron momentum (pseudogap, PG). As the doping level increases a small doping interval initially is found where the electronic system shows a glassy phase with partial electron and hole localization [4,5]. Further increasing the doping, open Fermi contours appear across the nodal directions in the momentum space, usually referred to as Fermi arcs [6].

By means of ARPES measurements, it was found that the SC gap exhibits the universal form $\Delta_0 \ \cos 2\theta_k$ over an angular range larger than the Fermi arc

[7]. Beyond this, the spectral weight of the SC states decreases against the one of the PG states [7]. Experiments also show that T_c is approximately related both to Δ_0 and to the extension of Fermi arcs by [8,9]

$$2\Delta_0 \ \alpha/(\pi/4) = 4.3 \ k_B T_c \quad , \tag{1}$$

where the angle α spans the half-Fermi arc as measured from the nodal direction [8]. Thus, the bell-shaped curve of T_c versus the hole concentration is strongly dependent on the way the shrinking PG hamper the full expression of the SC gap and the Fermi contour. On this regard, it is worth to point out that available data does not allow to find an unambiguous connection between the competing gaps, because of their very different behaviors [11,12].

In this paper, some points concerning the order parameter are reconsidered on the light of the Bogoliubov theory. By using a simplifying assumption about the electronic state distribution, worthy for semi-quantitative discussion, an effective critical temperature $T_c^* > T_c$ is predicted associated to the coherent gap Δ_0. A connection is proposed between Δ_0 and the antinodal pseudogap Δ_{PG}, consistent with experimental findings in cuprates superconductors. At the end of this paper, a formal construction of the anisotropic pairing matrix is proposed.

According to the Bogoliubov theory, the order parameter satisfies [13,14]

$$\Delta_k = \frac{1}{2} \sum_{k'} \frac{G_{k,k'} \Delta_{k'}}{\sqrt{\xi_{k'}^2 + \Delta_{k'}^2}} \quad , \tag{2}$$

where ξ_k are the energies of quasi-particle states with respect to the Fermi level. Here it is used the convention according to which the minus sign of the pairing interaction is explicitated in the Bogoliubov Hamiltonian [14]. In agreement with the d-like form of Δ_k, we will use $G_{k,k'} = G \ \cos 2\theta_k \ \cos 2\theta_{k'}$ where, for simplicity, G is assumed to be independent of k and k'. This position will be discussed later in more detail. Simple calculus leads to

$$2\Delta_0 = 3.52 \ \Gamma_0 \ kT_c \quad , \tag{3}$$

where for the case of closed Fermi surface $\Gamma = 1.22$ [15].

Differently from the usual approach [15], a reduced angular range will be considered in the sum (2). The reason is that, because of competition with PG states, when approaching the antinodal direction, there may be not enough states allowing for coherent pairing [16]. Thus an effective angle α^* is here introduced, not necessarily coincident with the angular extension α of the half-Fermi arc. On this ground, eq. (3) is replaced by

$$2\Delta_0 = 3.52 \ \Gamma(\alpha^*) \ kT_c^* \quad , \tag{4}$$

where $\Gamma(\alpha^*) \geq \Gamma_0$ ($\Gamma(\pi/4) = \Gamma_0$). Thus, T_c^* is to be distinguished from T_c since the former pertains to the closure of gap Δ_0 [11] and the latter to the drop of the superfluid density [7]. Actually, there are spectroscopic evidences of presence of coherent pairing above T_c [8, 16, 17]. Loss of phase rigidity [17] or gap nucleation in nanoscale regions [11] are invoked to explain the signals of the phase-incoherent superconductivity. However, besides the proposed interpretations, it is reasonable to assume that the vanishing of the residual SC phase is signed by T_c^*, like the main drop of the phase-coherent superconductivity is signed by T_c.

To get into more details, it is convenient to use a simplifying model for the electron states. For this purpose, let us assume that states contributing to pairing lie within an energy span $\pm\delta\varepsilon$ around the Fermi such that $\delta\varepsilon << kT_c^*$. If Ω_0 is the density of states at the Fermi level, eq. (2) leads to

$$\Delta_0 = 8\Omega_0 G\delta\varepsilon \sin^2\alpha^* \quad , \tag{5}$$

$$3.52\ \Theta\left(\alpha^*\right)\ kT_c^* = 2\Delta_0 \quad , \tag{6}$$

$$\Theta\left(\alpha^*\right) = \frac{1}{3.52}\frac{4\sin^2\alpha^*}{\frac{\alpha^*}{2} - \frac{1}{8}\sin 4\alpha^*} \quad , \tag{7}$$

A numerical check shows that $\Theta\left(\alpha^*\right)/\Gamma\left(\alpha^*\right) \simeq 1.2$ within the range $[0,\pi/4]$. It is interesting that for small angles eqs (6) and (7) lead to $(12/\pi)\ kT_c^* \simeq 2\Delta_0\ \alpha^*/(\pi/4)$, which mimics the equation expected for T_c with $\alpha = \alpha^*$.

In the model dealt-with, Δ_0 is related to the pairing strength in a very simple way. If PG and SC shares the same dependence on G, eq. (5) insights what connection may be established between them. It was suggested, on this regard, that competition may be originated by the same microscopic interactions underlying the pairing mechanism [7]. Thus, the pairing strength may enter in the particle self-consistent field to determine the pseudogap amplitude Δ_{PG}. Therefore, it is not meaningless to assume $\Delta_{PG} \propto G$, so that

$$\Delta_0 = \gamma\Delta_{PG}\sin^2\alpha^* \quad , \tag{8}$$

where γ is a suitable factor. Eventually, the latter could also include adjustments required to account for interactions among CuO_2 planes [8]. Since in overdoped cuprates Δ_0 can be larger than Δ_{PG} , it can be expected that $\gamma \gtrsim 2$.

It may be helpful to consider some numerical examples by using data from ARPES detailed investigations of Bi2201 superconductors [7]. The overdoped sample, there labelled as OD29K, was found with $\Delta_{PG} \simeq \Delta_0 \simeq 14\ meV$ and $T_c = 29K$. The half coherence arc was estimated at about 37° measured from the nodal direction. By using this figure as α^*, $\gamma = 2.75$ is obtained so that eq. (6) leads to $T_c^* = 59K$ $(2\Delta_0/kT_c^* = 5.6)$. By using the same γ for the underdoped sample (UD23K, T_c=23K), showing $\Delta_{PG} \simeq 62meV$ and $\Delta_0 \simeq 19\ meV$, we get $\alpha^* = 19.2°$ which is close to the estimated 20.4°. In this case, $T_c^* = 48.5\ K$ $(2\Delta_0/kT_c^* = 9.4)$. Discrepancy is obtained for the optimally doped sample (OP35K, $T_c = 35K$), showing $\Delta_{PG} \simeq 34meV$ and $\Delta_0 \simeq 18\ meV$, which allows $\alpha^* = 26°$ against the estimated 30°.

In place of any further comment, it is convenient to present a comprehensive (but quite qualitative) picture of the obtained results by using the above data.

For this purpose, two hypothetical curves for the coherence and the Fermi angles versus hole concentration, shown in fig. 1, are used in eqs.(1),(5-8). Reference angles α are obtained by means of eq. (1) by using data from ref [7]. In both curves, the zero points are added as an assumption. In fig. 2, the curve for Δ_0 is calculated by using $\gamma = 2.75$ and $\Delta_{PG}(meV) = 75\ (1-x)$ (which is a rough estimation for the material dealt with [8]) where x=0.05+(p-0.05)/0.225 (about the range where $T_c \neq 0$ [8]), symbol p meaning the hole concentration within [0.005,0.275]. For comparison, the typical curve $T_c \propto x(1-x)$ is also drawn by circles. Finally, it is to be noted that fig.2 appears quite similar to the analogous one reported in ref. [8].

As for the interaction matrix, some insights are suggested by experiments according to which pairing take place along the O-Cu-O lattice directions in the CuO_2 plane [18]. Conjugated electrons may interact either along the X or Y directions, reminiscent of the residual AF interaction. Thus, probabilities can be associated to pairs in such a way that the mean interaction matrix can be written as a tensor contraction like

$$G_{k,k'} = \sum_{\lambda_1,\lambda_2,,\lambda'_1,\lambda'_2} G_{k,k'}^{\lambda_1,\lambda_2,,\lambda'_1,\lambda'_2} \rho^{\lambda_1,\lambda_2} \rho'^{\lambda'_1,\lambda'_2} \ , \tag{9}$$

where ρ and ρ' are suitable probability matrices of pairs. The more simplest form for ρ, satisfying Tr(ρ)=1, is the diagonal one

$$\rho = \begin{pmatrix} \cos^2\theta & 0 \\ 0 & \sin^2\theta \end{pmatrix} \quad , \tag{10}$$

For language convenience, let us define the mean polarization of the pair along the direction θ as $P_\theta = \rho^{11} - \rho^{22} = \cos 2\theta$. Thus, polarizations $P_\theta = \pm 1$ merely means pairs capable of interaction along only one of the two main directions O-Cu-O. Nodal directions, $P_\theta = 0$, are the ones where polarization sign changes. Based on these positions, we are allowed to use a 2x2 matrix $G_{k,k'}^{\lambda,,\lambda'}$ where meaning of elements can be easily understood by considering pairs moving along the main directions. The diagonal terms represent processes where incoming and outcoming pairs maintain the same X or Y directions. Since these are expected to be equivalent, the relative terms can be assumed to be equal. The non-diagonal terms correspond to processes where the outcoming pairs are polarized on the direction orthogonal with respect to the ones of the incoming pairs. Depending on the interaction features, a phase factor may be associated to these terms so that, in a little more general way, the anisotropic properties of the pairing matrix can be represented as

$$\begin{bmatrix} G_{k,k'}^{11} & G_{k,k'}^{12} \\ G_{k,k'}^{21} & G_{k,k'}^{22} \end{bmatrix} = g_{k,k'} \begin{bmatrix} 1 & \exp(-i\varphi) \\ \exp(i\varphi) & 1 \end{bmatrix} \quad ,$$

where the s- and d-like cases correspond to $\varphi = 0, \pm 2\pi$ and $\varphi = \pm\pi$, respectively.

In conclusion, by properly handling the Bogoliubov theory with some simplifying assumptions, several points concerning the order parameter and its relation with the critical temperatures can be accounted for. Hopefully, the picture here presented may become an useful canvas for future investigations in the concealed matter of high temperature superconductivity.

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Captions

Figure 1.- Models of coherence and Fermi angle curves versus the hole doping concentration. Triangles and circles are obtained by using data from ref. [7] in eq. 8 and in eq. (1), respectively. The zero points an assumption.

Figure 2.- Pseudogap (Δ_{PG}), coherent gap (Δ_0) and critical temperature curves versus the hole doping concentration: curve of Δ_0 is obtained form eq. (8); curve of T_c^* is obtained from eqs. (6) and (7); curve of T_c is obtained from eqs. (1). Curve drawn by circles shows the typical form $T_c \propto x(1-x)$ where x stands for the normalized hole concentration (see text).