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Correlation of Normal and Superconducting Properties and Unified Approach to the Description of High T_c Oxides

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ABSTRACT

We present a unified approach based on the Fermi liquid picture which allows us to describe the normal as well as the superconducting properties of the doped cuprates.

1. Introduction

The theory presented in this paper is for the doped compounds which are metallic. One can distinguish two interrelated, but nevertheless, different directions in the physics of high T_c [1,2], one involving the problem of carrier doping and the transition to the metallic state and the second being the description of the metallic state. It is important that this metallic phase undergoes the transition into the superconducting state; as a result, our analysis is directly related to the origin of high T_c. We are using a quasi-2D Fermi liquid model to estimate the fundamental parameters of these very interesting materials. We find that this description is able to describe these materials and also that phonons and plasmons play a major role in the mechanism of high T_c.

2. Normal Properties

The most efficient way to analyze the anisotropy and to evaluate the normal parameters is to describe the system in momentum (reciprocal) space; our method is based on the use of Fermiology. The anisotropy of the system is reflected in the topology of the Fermi surface (FS): $\varepsilon(p)=\varepsilon_F$.

Our approach [3] is based on Fermi liquid theory. According to the Fermi liquid theory which has been developed by Landau and describes strongly correlated Fermi systems, the low lying excitation of the system can be classified in the same way as a Fermi gas. It means that such concepts as disper-

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sion relation, Fermi surface and Fermi velocity have a direct meaning. We certainly followed this approach in our previous paper [3]. Recent experimental photoemission data on 1:2:3 [4] shows the presence of a sharp Fermi edge. These data present direct experimental support for an approach based on these concepts.

The usual methods for studying the Fermi surface require the sample to be normal at low temperatures, otherwise the intensive thermal motion smears out the relevant signals. An unconventional and explosive technique to produce very large magnetic fields (megagous) has been successfully utilized to demon-strate De Haas-Van Alphen oscillations in grain-aligned crystals of Y-Ba-Cu-O [F. Mueller et al. 1990] [5]. This result unambiguously demonstrates the exis-tence of a Fermi surface in this material.

The La-Sr-Cu-O system has a layered structure, so that the interlayer distance $d_c >> d_a, d_b$. The dispersion relation $\varepsilon(p)$ is highly anisotropic, where $p=\{k, p_z\}$ is a quasi-momentum (k is a 2D momentum); the Z axis has been chosen to be perpendicular to the layers. As a first approximation, one can assume the Fermi surface to be cylindrically shaped which corresponds to neglecting the interlayer transitions. Of course the interlayer transitions lead to small deviations from the cylindrical shape. It is important that we are not assuming the Fermi curve (the Fermi curve is defined as the cross-section of the FS by the plane p_z = constant) to be a circle. It is appears that one can estimate the values of the Fermi energy ε_F and the effective mass m*(its defin-ition see below, Eq.(2)) without specifying the shape of the Fermi curve. In the case of cylindrically shaped FS the dispersion relation is $\varepsilon(k)$ and does not de-pend on p_z. A large anisotropy of the normal conductivity justifies such an approximation. One should note that this approach is applicable to hole as well as to electron carrier types of materials. For example, the hole surfaces at the corners of the first zone can be viewed in the quasi-2D case as a cylinder as can be seen from a simple translation in momentum space. One can derive the following relations [3].

$$m^* = 3\,(h^2/\pi)\,k_B^{-2}\,d_c\,\gamma \qquad (1)$$

$$\varepsilon_F = (\pi^2 k_B^2/3)\,n/\gamma \qquad (2)$$

Here n is the carrier concentration, and γ is the Sommerfeld constant.

Equations (1) and (2) express m* and ε_F in terms of the experimentally measured quantities d_c, n, and γ. These values of m* and ε_F do not depend on any assumption about the shape of the Fermi curve. On the contrary, these values should be taken into account when reconstructing the Fermi surface.

The values of γ and n can be determined from heat capacity data (see e.g. the review 6) and Hall effect measurements. The comparison of the evaluated major normal parameters of the high T_c material and the usual normal metal can be seen in Table I.

TABLE I. Comparison of normal-state properties of conventional metals with $La_{1.8}Sr_{0.2}CuO_4$.

Quantity	Conventional Metals	$La_{1.8}Sr_{0.2}Cu$-O_4
m*	(1-15) m_e	$5m_e$
$k_{F\ (cm^{-1})}$	10^8	3.5×10^7
$v_{F\ (cm\ sec^{-1})}$	(1-2) x 10^8	8 x 10^6
ε_F (eV)	5-10	0.1

We think that small values of ε_F and v_F along with the anisotropy are key physical properties of the new high T_c oxides.

The cuprates are characterized also by unusual spectra of the collective excitation. Speaking of phonon spectrum, one should stress the existence of low frequency optical nodes and the presence of strong anharmonicily. As a result, one could expect the strong electron-phonon coupling (see below). In addition they contain the quasi-2D low-lying acoustic plasmon branch which has a slope of the same order of magnitude as the Fermi velocity (see e.g.,

Ref. [7]). This small slope of the "electronic sound" makes the branch similar to the usual phonon acoustic branch.

3. Superconducting Parameters

According to our analysis, the Fermi velocity v_F is small relative to the values in conventional metals. For La-Sr-Cu-O (see Table I) $v_F \cong 8 \times 10^6$ c m sec^{-1}. One can see that a such small value along with a large value of T_c leads to a short coherence length. Indeed, if we use the expression $\xi_c = 0.18\, h v_F / k_B T_c$ we obtain $\xi_0 \cong 25$Å.

A small value of the Fermi energy ε_F has also had a strong impact on the superconducting properties. The ratio $\Delta(0)/\varepsilon_F$ in conventional superconductors is small ($\sim 10^{-4}$), whereas in the high T_c oxides ε_F and Δ are comparable ($\Delta(0)/\varepsilon_F \leq 10^{-1}$). A small value of the ratio $\Delta(0)/\varepsilon_F$ means that only a small number of states near the FS are involved in pairing. The picture is different in the oxides. A large value of the ratio corresponds to a situation when a significant fraction of the carriers are paired. This of course means a short coherence length is directly related to the quasi-2D structure of the cuprates. Indeed, in conventional superconductors ($\Delta/\varepsilon_F << 1$) pairing can occur only near the Fermi surface. (Cooper theorem). The states on the Fermi surface form a quasi 2D system in momentum space. This is an important factor because in the 2D case, any attraction leads to the formation of bound states (see e.g. Ref. [8]). The presence of the layered structure makes pairing possible even for states which are distant from the Fermi surface; this corresponds to the picture in the cuprates.

A large value of $\Delta(0)/\varepsilon_F$ leads to an unusual critical behavior near T_c. This has been predicted in Ref. [9] and observed experimentally in Ref. [10]. In addition the observation of a shift in the positron-annihilation lifetime in the high T_c oxides, such as La-Sr-Cu-O, Y-Ba-Cu-O or Tl-Ba-Ca-Cu-O [11] is directly related to the small value of their Fermi energy. The shift $\Delta\tau/\tau$ is equal to [12].

$$\frac{\Delta\tau}{\tau} = \gamma \left(\frac{\Delta}{\varepsilon_F}\right)^2 \ln \frac{\varepsilon_F}{\Delta} \qquad (3)$$

where $\gamma \cong \tau$; in addition $\gamma \sim m^*$. Therefore the sign of the shift is directly related to the sign of the carriers. For conventional superconductors

$(\Delta/\varepsilon_F)^2 \cong 10^{-8}$, whereas for La-Sr-Cu-O $\Delta/\varepsilon_F \cong 10^{-1}$ and this leads to the possibility of observing the shift.

4. Strength of the Coupling

Using heat capacity and neutron spectroscopy data, one can evaluate the strength of the electron phonon coupling: $\lambda = [\gamma(0)/\gamma(T_c)-1]$.

1. Using the data [5], we obtain $\lambda_{\varepsilon-ph} \cong 2.5$ and this means the presence of strong coupling. Nevertheless, based on the expression [13]

$$T_c = \frac{0.25\,\tilde{\Omega}}{[e^{\frac{2}{\lambda}} - 1]^{\frac{1}{2}}} \qquad (4)$$

one can conclude that there is a need for an additional mechanism. We think that the additional attraction is mediated by a peculiar acoustic plasmon branch [12] with weak additional coupling λ_{pl}. A small value of λ_{pl} does not mean that the contribution to T_c is also small. In fact, it depends not only on the strength of the coupling but to its corresponding energy scale. A noticeable contribution of plasmons to T_c arises from the large scale of the plasmon energy relative to the phonon energy. This can be seen directly from the equation [3, 7]

$$T_c = T_c^{ph}\left(\frac{\tilde{\omega}_{pl}}{T_c^{ph}}\right)^{\upsilon} \qquad (5)$$

where $\upsilon = \lambda_{pl}\,(\lambda_{ph} + \lambda_{pl})$. Here T_c^{ph} is described by eq. (12) and λ_{pl} is the electron-plasmon coupling constant and $\tilde{\omega}_{pl} \approx \langle\omega\rangle_{pl}$.

Therefore, a high T_c is due to a generalized phonon mechanism, that is caused by a strong interaction with phonons and low lying phonon-like plasmon mode ("electronic-sound").

5. Multigap Structure

A multigap structure is caused by the presence of overlapping energy bands; each band is characterized by its own energy gap. Differences in densities of states, pairing interactions, etc. lead to distinct values of the gaps. It should be noted that the overlap of the energy bands is a typical situations for conventional metals including superconductors. Nevertheless, the properties of conventional superconductors have been described accurately by a one-gap model. This is due to their large coherence length ξ_o; namely, the inequality $l << \xi_o$ (l is a mean free path) which holds for most conventional superconductors leads to averaging [17], because of interband scattering and as a result to the applicability of a one-band model. One exception is Nb doped $SrTiO_3$, for which a two gap structure was observed [18].

The situation in the high T_c oxides is entirely different. The coherence length is small and the criterion $l > \xi_o$ can be easily met. As a result there is an unique opportunity to observe the effects due to multigap structure.

One should note that La-Sr-Cu-O has a relatively simple band structure and as a result, its properties can be adequately described by the one band model. The situation is different for Y-Ba-Cu-O and Bi-S-Ca-Cu-O. Note also that the effect of the multigap structure is similar to the effect of an energy gap anisotropy. In both cases we are dealing with a deviation of the Fermi surface from a spherical shape. The multiband structure implies the existence of several sections of the Fermi surface even for a fixed direction in momentum space. This effect is stronger than the usual anisotropy and leads to a larger spread of the values of the energy gaps.

Let us consider two overlapping energy bands. The pairing is described by the order parameters $\Delta_1(\vec{p}, \omega_n)$ and $\Delta_2(\vec{p}, \omega_n)$, where $\vec{p}$ is a quasi-momentum, and $\omega_n = (2n + 1)\pi T$. They are solutions of the following equations in an analytical form:

$$\Delta_i(\vec{p}, \omega_n) Z_i = T \sum_{\omega_{n'}} \sum_{l=1,2} \int d\vec{p}' \, \Gamma_{il}(\vec{p}, \omega_n ; -\vec{p}, -\omega_n ; \vec{p}', \omega_{n'} ; -\vec{p}', -\omega_{n'}) \frac{\Delta(\vec{p}', \omega_{n'})}{\sqrt{\omega_{n'}^2 + \Delta^2(\vec{p}', \omega_{n'})}}$$

$i = \{1, 2\}$.

If we study the usual phonon mechanisms, then $\Gamma_{il} = \lambda_{il} D$, where $D = \Omega^2(q)\ [\Omega^2(q) + (\omega_n - \omega_n)^2]^{-1}$; $\vec{q} = \vec{p}\,' - \vec{p}$ and Ω is the phonon frequency; we assume a summation over all phonon branches. As a result, we obtain the Eliashberg equation generalized for the case of several gaps T_c is described by the expression:

where
$$T_c = 1.14\,\tilde{\Omega}\,\exp\left(-1/\tilde{\lambda}\right) \tag{6}$$

$$\tilde{\lambda} = \frac{1}{2}\left\{\lambda_{11} + \lambda_{22} + \left[(\lambda_{22} - \lambda_{11})^2 + 4\lambda_{12}\lambda_{21}\right]^{1/2}\right\} \tag{7}$$

Note also that usually $p_{F1} \neq p_{F2}$, and as a result, one can neglect interband pairing.

6. The Ratios $\varepsilon_i(0)/T_c$

Let us now evaluate the ratio $\varepsilon_1(0)/T_c$ and $\varepsilon_2(0)/T_c$ in a two-gap model. This problem is of definite interest, because these ratios can be determined experimentally. As is well known, the ratio $\varepsilon(0)/T_c$ in a one-gap theory allows one to determine the strength of the coupling.

In the two-band case we have three independent coupling constants (λ_{11}, λ_{22}, λ_{12} ; $\lambda_{21} = \lambda_{12}\,\nu_1/\nu_2$). That's why the correspondence between $\varepsilon_i(0)/T_c$ and λ_{il} is not simple and must be treated carefully one can formulate the following theorem: one of the gaps in a two-gap system is always smaller than the BCS value ($\Delta(0) = 1.76\ T_c$), whereas the other gap is larger. Note that

$$\frac{\Delta_1}{\Delta_2}\Big|_{T_c} = \frac{\Delta_1(0)}{\Delta_2(0)}$$ as has already been shown [16].

Assume for concreteness that $\tau < 1$ ($\varepsilon_1 > \varepsilon_2$). Then

$$(2\varepsilon_1/T_c) > a_{BCS};\ (2\varepsilon_2/Tc) < a_{BCS} \tag{8}$$

Note that the value $2\varepsilon_1/T_c$ exceeds a_{BCS}, but such behavior does not mean strong coupling, as in the one-band case (see Eq. (8)). This deviation from the BCS value is caused by the presence of a multigap structure.

Consider the following example: $\lambda_{11}>>\lambda_{12}, \lambda_{21}; \lambda_{22} = 0$. This means that the superconducting state of the second band is due to the interband transitions only. This model is realistic for cuprates (see below). In this case we obtain:

$$\tau \cong \lambda_{21}/\lambda_{11} << 1 \qquad (9)$$

Therefore, the ratio Δ_2/Δ_1 is small;. This means (see Eq. (14)) that the values of the energy gaps may noticeably differ from each other.
In the strong coupling limit

$$\tau = \frac{\varepsilon_2(0)}{\varepsilon_1(0)} \cong \frac{\lambda_{21}(1+\lambda_{11})}{\lambda_{11}} \qquad (10)$$

In a weak coupling approximation $\lambda_{11} << 1$ and we obtain the expression (9).

The presence of strong coupling leads to the factor $1 + \lambda_{11}$. This factor is important if we are interested in the relative value of the energy gaps. For example, if $\lambda_{11} = 1.5$ and $\lambda_{21} = 0.3$, then the weak coupling approximation (see Eq. (17)) leads to the value $\tau = 0.2$, whereas the correct value obtained with consideration of the strong coupling effects (see Eq. (10)) is $\tau = 0.5$. The strong coupling tends to decrease the relative difference in the values of the energy gaps in order to observe the multigap structure one should meet the criterion $l>\xi_0$. The cuprates are characterized by short coherence length and as a result it is perfectly realistic to observe a multigap structure in the high T_c oxides. Of course, this possibility implies the overlap of different energy bands. Such a situation is realized in Y-Ba-Cu-O system and probably in the Bi-S-Ca-Cu-O. As for the La-Sr-Cu-O compound it is characterized by a relatively simple band structure (see e.g. the review [19]), and its properties can be described by a one- gap model. The weak temperature dependence of the Hall coefficient (see Ref.[20]) is a manifestation of such a structure. A detailed description of this system is given in our paper [4].

The situation with Y-Ba-Cu-O is entirely different and it is connected with presence of the chain structure. As a result, we have two different energy bands; they have a quasi-2D and a quasi-1D nature. The presence of such a two-band picture is manifested in a strong temperature dependence of the Hall effect and it is supported by the band structure calculations [19] The Fermi surface in this system consists of a cylindrical piece and two planar pieces as we have described previously [3].

As a result, one should observe two energy gaps in the Y-Ba-Cu-O superconductor. There were several experimental papers indicating the presence of the two-gap structure. The most convincing evidence comes from NMR experiments [20, 21].

A more recent detailed investigation carried out in [21] and describing the temperature dependence of the Knight shift clearly demonstrated the presence of two energy gaps. Therefore, the Y-Ba-Cu-O compound is characterized by two superconducting subsystems, two different bands with different energy gaps. The authors [21] can definitely distinguish the presence of two gaps; as for their numerical values, there are some experimental uncertainties. For the smaller gap Δ_{ch}/T_c is of the order of 3.5. The value of Δ_{pl}, according to [21] lies between 4 T_c and 6 T_c.

7. The Parameters of $Y_1Ba_2Cu_3O_7$

In our papers [3, 4]we evaluated the major normal and superconducting parameters of the La-Sr-Cu-O system. Based on the two band model, one can estimate the parameters of Y-Ba-Cu-O.

According to heat capacity data the Sommerfeld constant for Y-Ba-Cu-O is equal to $\gamma \cong 16$ mJ/mole K^2. In the presence of two bands $\gamma = \gamma_{pl} + \gamma_{ch}$. The Fermi surface for Y-Ba-Cu-O compound consists of two parts: a cylindrical part and a set of planes. The cylindrical part, which corresponds to the quasi-2D band (planes) is similar to the quasi-2D band of La-Sr-Cu-O. Based on the relation [3] : $\gamma = (\pi/3\ h^2)\ k_B^2\ m^* d_c^{-1}$ and assuming that the value of the effective mass m^* of the carriers in the planes is the same as for La-Sr-Cu-O ($m^* \cong 5\ m_e$) we obtain $\gamma_{pl} \cong 0.04$ mJ/cm^3 K^2. Correspondingly $\gamma_{ch} \cong 0.15$ mJ/cm^3 K^2. Assuming also that the hole concentration is similar to that in the $La_{1.85}Sr_{0.15}CuO_4$ compound ($n_h \cong 3 \times 10^{21}$cm^3) we obtain $k_{F;pl} \cong (2\pi\ n d_c)^{1/2} \cong 4.7 \times 10^7$ cm^{-1} and $v_{F;pl} \cong 10^7$cm/s^{-1}. The Fermi energy appears to be equal to $E_F \cong 0.2$ eV in accordance with a previous calculation by G.

Deutscher and the present authors using a different method[3]. It is remarkable that the photoemission data [4] also gives the same value for the Fermi energy.

A small value of the Fermi energy is a very important feature of the cuprates [3, 21].

Using the values of the parameters obtained above, one can estimate the value of the in-plane coherence length $\xi_{pl} = hv_F/\pi\ \Delta(0)$, and we obtain $\xi_{pl} \cong 10$ Å.

Let us consider the carriers in the quasi-1D band (chains). Using the value of γ obtained above, one can evaluate the Fermi velocity (see [3]) and we obtain $v_{F;ch} \cong 5\ x10^6$ cm s^{-1}. This leads to a very small value of the coherence length $\xi_{ch} \cong 7$Å. The carrier concentration, n_{ch}, is unknown. In the presence of two bands the Hall effect depends strongly on temperature and it cannot be used to determine n directly. It is probable that $m^*_{ch} >> m^*_{pl}$; e.g. if $n_{ch} \cong n_{pl} \cong 3 \times 10^{21}$, we obtain $m^*_{ch} \cong 25\ m_e$.

The nature of the carriers on the chains is a very interesting question. This question can be answered by analyzing the positron annihilation data. According to [11] the shift in the positron annihilation lifetime $\delta\tau \sim m^*$. Therefore the sign of the shift is directly related to the sign of m*. For La-Sr-Cu-O the positron comes to rest near the planes and in Y-Ba-Cu-O the positron comes to rest near the chains [11]. The shifts in the lifetime have opposite signs [11] and we know that the carriers in the Cu-O planes in La-Sr-Cu-O are holes therefore, we are dealing with n-type of conductivity in the chain structure.

8. Conclusion.

We described the unified approach in the theory of high T_c based on strong correlation of normal and superconducting properties. The main results can be summarized as follows:

1. Small values of ε_F and v_F along with high anisotropy are key properties of the oxides.

2. The calculated value of the coherence length (Sec. III.2) appears to be small. A small value of ε_F leads to a peculiar picture of the pairing when a significant part of the carriers are paired. The quasi-2D nature of the system is favorable for the pairing.

3. The small value of ξ_o leads to a unique opportunity to observe the multigap structure.

4. The materials are characterized by strong electron-phonon coupling. However, the coupling is not strong enough to provide such a high T_c. There is a need for an additional attraction, such as a plasmon mechanism.

We think that small values of ε_F and v_F along with the anisotropy are key physical properties of the new high T_c oxides. The cuprates are characterized also by unusual spectra of the collective excitation. Speaking of phonon spectrum one should stress the existence of low frequency optical modes and the presence of strong anharmonicity. As a result, one should expect the strong electron-phonon coupling (see below). In addition, these materials contain a quasi-2D low lying acoustic plasmon branch which has a slope of the same order of magnitude as the Fermi velocity (see, e.g., Refs7). This small slope of the "electronic-sound" makes the branch similar to the usual phonon acoustic branch.

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