Superfluid response in electron-doped cuprate superconductors

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We propose a weakly coupled two-band model with $d_{x^2-y^2}$ pairing symmetry to account for the anomalous temperature dependence of superfluid density $\rho_s$ in electron-doped cuprate superconductors. This model gives a unified explanation to the presence of an upward curvature in $\rho_s$ near $T_c$ and a weak temperature dependence of $\rho_s$ in low temperatures. Our work resolves a discrepancy in the interpretation of different experimental measurements and suggests that the pairing in electron-doped cuprates has predominately $d_{x^2-y^2}$ symmetry in the whole doping range.

Identification of pairing symmetry has been an important issue in the investigation of high-Tc superconductivity. For hole-doped cuprate superconductors, it is commonly accepted that the pairing order parameter has $d_{x^2-y^2}$ wave symmetry. However, for electron-doped cuprate superconductors, no consensus has been reached on the pairing symmetry. A number of experiments, including the angle resolved photoemission (ARPES) and Raman spectroscopy, and the phase-sensitive measurements, suggested that the electron-doped superconductors also have $d_{x^2-y^2}$-wave symmetry. However, the results revealed by other experiments are controversial. In particular, the magnetic penetration depth data measured by Kokales et al. and Prozorov et al. showed that the low temperature superfluid density of electron-doped superconductors varies quadratically with temperature in the whole range of doping, in agreement with the theoretical prediction for a $d$-wave superconductor with impurity scattering. However, the experimental data published by Kim et al. suggested that there is a $d$- to anisotropic $s$-wave transition across the optimal doping. For optimal and overdoped samples, they found that the low temperature superfluid density exhibits an exponential temperature dependence, in favor of an anisotropic $s$-wave pairing state.

The above discrepancy indicates that low lying quasiparticle excitations in electron-doped cuprates behave quite differently than in hole doped ones. To resolve the discrepancy, a thorough understanding of the electronic structure of electron-doped materials is desired. In this regard, the doping evolution of the Fermi surface (FS) revealed by the ARPES of Nd$_{2-x}$Ce$_x$CuO$_4$ (NCCO) is of great interest. At low doping, a small FS pocket first appears around $(\pi, 0)$, in contrast to the hole doping case where the low-lying states are centered around $(\pi/2, \pi/2)$. By further doping, another pocket begins to form around $(\pi/2, \pi/2)$. The presence of the two separate FS pockets may result from the band folding effect induced by the antiferromagnetic correlations. It may also be a manifestation of the lower and upper Hubbard bands. At the mean field level, the theoretical calculations indicate that these two FS pockets can be effectively described as a two-band system. This two-band scenario is consistent with the conjecture made by a number of groups on the existence of two kinds of charge carriers in electron-doped materials.

The interplay between the above mentioned two bands can affect significantly the behavior of superconducting quasiparticles. A generic feature of a weakly coupled two-bands system, as first pointed out by Xiang and Wheatley, is the presence of an upward curvature in the temperature dependence of superfluid density $\rho_s$ near $T_c$. This intrinsic upward curvature in the superfluid density has indeed been observed in electron-doped materials by a number of experimental groups. Not only does it lend further support to the two-band picture, but also sheds light on the understanding of various controversial experimental observations.

In this paper, we propose to use a two-band BCS-like model with $d_{x^2-y^2}$-wave pairing symmetry to account for the low energy electromagnetic response of superconducting quasiparticles in electron-doped materials. This model, as will be shown later, captures the main features of quasiparticle excitations in the superconducting state and gives a unified account for the experimental data. Our result suggests that the superconducting pairing in electron-doped materials is governed by the same mechanism as in hole-doped ones, although their phase diagrams look asymmetric.

The two-band model we study is defined by

$$H = \sum_{i\kappa\sigma} \xi_{ik\kappa\sigma} c_{ik\kappa\sigma}^\dagger c_{ik\kappa\sigma} + \sum_{i\kappa\kappa'} V_{i\kappa\kappa'} c_{i\kappa\sigma}^\dagger c_{i\kappa'\sigma}^\dagger c_{i\kappa\sigma} c_{i\kappa'\sigma}$$

$$+ \sum_{\kappa\kappa'} \left( V_{3\kappa\kappa'} c_{i\kappa'\sigma}^\dagger c_{i\kappa'\sigma}^\dagger c_{2\kappa'\sigma} f_{2k'\sigma} + \text{h.c.} \right) ,$$

where $i = 1, 2$ represents the band around $(\pi, 0)$ and $(\pi/2, \pi/2)$, respectively. $c_{i\kappa\sigma}$ and $c_{i\kappa'\sigma}$ are the corresponding electron operators. $V_{1\kappa\kappa'}$ and $V_{2\kappa\kappa'}$ are the reduced pairing potentials for the two bands. $V_{3\kappa\kappa'}$ is the interband pair interaction. This model has also been used to describe superconducting properties of the two-band superconductor MgB$_2$. In MgB$_2$, the interband coupling is weak since the two relevant bands have different parity symmetry. In the present case, the interband coupling is also weak since the strong antifer-
romagnetic fluctuations do not couple the first band with the second one in electron-doped cuprates.

In electron-doped materials, the superconductivity occurs at much higher doping than in hole doped ones. However, as shown by the ARPES experiments, the appearance of the superconducting phase coincides with the appearance of the second band at the Fermi level. This reveals a close resemblance between electron- and hole-doped materials. It suggests that it is the interaction driving the second band to superconduct that leads the whole system to superconduct in electron-doped materials, and that the pairing potential $V_{2kk'}$ has predominantly $d_{x^2-y^2}$ symmetry, resembling the hole doped case. $V_{1kk'}$ can in principle be different to $V_{2kk'}$. However, if pairing in the first band is originated from the same mechanism as the second band or induced by the second band by the proximity effect, $V_{1kk'}$ should most probably have $d_{x^2-y^2}$ symmetry.

In the calculations below, we assume that $V_{iikk'}$ ($i = 1,2,3$) can all be factorized: $V_{1kk'} = g_1 \gamma_k \gamma_k'$, $V_{2kk'} = g_2 \gamma_k \gamma_{k'}$ and $V_{3kk'} = g_3 \gamma_k \gamma_{k'}$, where $g_1$, $g_2$, and $g_3$ are the corresponding coupling constants, $\gamma_k = \gamma_{2k} = \gamma_k$ is the $d_{x^2-y^2}$-wave pairing function. Here we have implicitly assumed that the first band has the same pairing symmetry as the second one. This assumption can in fact be relaxed. The qualitative conclusion draw below does not depend much on the detailed form of the pairing function for the first band near $(\pi,0)$, provided there are no gap nodes on the FS of this band.

Taking the BCS mean field approximation, the interaction between the two bands is decoupled. It is straightforward to show that the quasiparticle eigenspectrum of the $i^{th}$ band is given by the following expression $E_{ik} = \sqrt{\xi^2_k + \Delta_i^2}$, where $\Delta_i$ is the gap amplitude of the $i^{th}$ band. They are determined by the following coupled gap equations

$$\Delta_1 = \sum_k \gamma_k (g_1 \langle c_{1k} \text{c}_{1k'} \rangle + g_3 \langle c_{2k} \text{c}_{2k'} \rangle)$$

and

$$\Delta_2 = \sum_k \gamma_k (g_2 \langle c_{2k} \text{c}_{1k} \rangle + g_3 \langle c_{1k} \text{c}_{1k} \rangle),$$

where $\langle \cdots \rangle$ denotes thermal average.

The above expression of $E_{ik}$ indicates that there are gap nodes in the quasiparticle excitations of the second band. However, there is a finite excitation gap in the first band since the nodal lines of $\gamma_k$ do not intersect with the FS of that band if the system is not heavily overdoped. Therefore, as far as thermal excitations are concerned, the first band behaves as in a $s$-wave superconductor, although the pairing is of $d_{x^2-y^2}$ symmetry. This indicates that the superconducting state of electron-doped cuprates is actually a mixture of $d$-wave and $s$-wave-like pairing states. Apparently, the low temperature/energy behavior of quasiparticle excitations is governed by the second band since the first band is thermally activated. This would naturally explain why the typical $d$-wave behaviors were observed in quite many experiments. However, the presence of the first band will change the relative contribution of the second band to the superfluid as well as other thermodynamic functions. This will suppress, for example, the temperature dependence of the normalized superfluid density and aggrandize the experimental difficulty in identifying the expected power law behavior for a $d$-wave superconductor.

The superfluid density is inversely proportional to the square of the magnetic penetration depth, i.e., $\rho_s \propto \lambda^{-2}$. Under the BCS mean-field decomposition, the superfluid density of the system is simply a sum of the contribution from each band and can be expressed as

$$\rho_s(T) = \rho_{s,1}(T) + \rho_{s,2}(T),$$

where $\rho_{s,i}$ is the superfluid density of the $i^{th}$ band. It can be evaluated with the formula given in Ref. 24. In low temperatures, since there is a finite gap in the quasiparticle excitations of the first band, $\rho_{s,1}(T)$ is expected to be given by

$$\rho_{s,1}(T) \sim \rho_{s,1}(0) \left(1 - ae^{-\Delta_1 / k_B T}\right),$$

where $\Delta_1$ is the minimum value of $\Delta_1 \gamma_k$ on the FS of the first band and $a$ is a constant. There are gap nodes in the second band, therefore $\rho_{s,2}$ should behave similarly as in a pure $d$-wave superconductor and show a linear $T$ dependence in low temperatures due to the low energy linear density of states:

$$\rho_{s,2}(T) \sim \rho_{s,2}(0) \left(1 - \frac{T}{T_c}\right).$$

Thus, in the limit $T \ll T_c$, the normalized total superfluid density is approximately given by

$$\frac{\rho_s(T)}{\rho_s(0)} \approx 1 - \frac{\rho_{s,2}(0)}{\rho_s(0)} \frac{T}{T_c} - \frac{\rho_{s,1}(0) - \rho_{s,2}(0)}{\rho_s(0)} \frac{T}{T_c} e^{-\Delta_1 / k_B T},$$

where $\rho_s(0) = \rho_{s,1}(0) + \rho_{s,2}(0)$.

For a pure $d$-wave superconductor, as shown by Eq. (4), the slope of the linear $T$ term in the normalized superfluid density is proportional to $1/T_c$. However, for the coupled two-band system considered here, this linear slope is normalized by a factor $\rho_{s,2}(0)/\rho_s(0)$. The zero temperature superfluid density $\rho_{s,2}(0)$ is a measure of the diamagnetic response in the $i^{th}$ band. It is approximately proportional to the ratio between the charge carrier concentration and the effective mass in that band, i.e., $\rho_{s,2}(0) \propto n_i / m_i^*$. It is difficult to estimate this ratio for each individual band. However, as the FS pocket of the first band appears immediately after doping and that of the second band appears only after the long range antiferromagnetic order is completely suppressed, one would expect $\rho_{s,2}(0)$ to be much smaller than $\rho_{s,1}(0)$. This means that $\rho_{s,2}(0)/\rho_s(0) \ll 1$ and the linear $T$ term in $\rho_s(T)$ is greatly suppressed. Thus the low temperature curve of the normalized superfluid density looks much flatter than in a pure $d$-wave system, although $\rho_s(T)$ is
still governed by a power law $T$ dependence at sufficiently low temperatures.

In real materials, the low temperature dependence of $\rho_s(T)/\rho_s(0)$ will be further suppressed by impurity scattering and the linear term will be replaced by a $T^2$ term in the limit $T \ll \Gamma_0$ [27]

$$\rho_{s,2}(T) \sim \rho_{s,2}(0) \left(1 - \frac{k_B T^2}{6\pi \Gamma_0 \Delta_2}\right). \quad (6)$$

where $\Gamma_0$ is the scattering rate. In this case, $\rho_s(T)/\rho_s(0)$ becomes

$$\frac{\rho_s(T)}{\rho_s(0)} \approx 1 - \frac{\rho_{s,2}(0)}{\rho_s(0)} \frac{k_B T^2}{6\pi \Gamma_0 \Delta_2} - \frac{\rho_{s,1}(0)}{\rho_s(0)} \Delta_1^1/k_B T. \quad (7)$$

We believe this formula captures the main feature of low temperature superfluid density. Indeed, by fitting the experimental data with the above equation, we find that it does give a good account for the low temperature superfluid in the whole doping range. This can be seen from Fig. 1 where the fitting curves of Eq. 7 to the measurement data published in Ref. 11 are shown for three representative doping cases in the under-, optimal and over-doping regimes, respectively.

In electron-doped materials, doping will reduce the distance between the FS of the first band and the nodal lines of $\gamma_k$. At low doping, the contribution from the exponential term is small and the $T^2$ term is dominant. By further doping, $\Delta_1^1$ begins to drop (the inset of Fig. 1), the contribution from the exponential term becomes comparable with the $T^2$ term in certain low temperature regime. In this case, the $T^2$ dependence of $\rho_s(T)$ would become difficult to be identified if the exponential term is not clearly separated. In heavily overdoped regime, the FS of the first band will strike over the nodal lines of $\gamma_k$. In this case, $\Delta_1^1 = 0$ and $\rho_s(T)/\rho_s(0)$ should behave similarly as in a conventional d-wave superconductor. This picture for the doping dependence of low temperature $\rho_s(T)/\rho_s(0)$ agrees qualitatively with all experimental observations.

Close to $T_c$, a positive curvature will appear in $\rho_s(T)$. This is a simple but universal property of a weakly coupled two-band system [20]. To understand this, let us first consider the case $\rho_3 = 0$. In this case, the two bands are decoupled and will become superconducting independently. Let us denote their transition temperatures by $T_{c1}^3$ and $T_{c2}^3$ and assume $T_{c1}^3 < T_{c2}^3$. For finite but small $\rho_3$, the superconducting transition will occur at a critical temperature close to $T_{c2}^3$, i.e. $T_c \sim T_{c2}^3$ (Fig. 2). Just below $T_c$, $\rho_s$ is mainly contributed from the second band. However, when $T$ drops below $T_{c1}^3$, the intrinsic superconducting correlation of the first band will appear in addition to the induced one, and the contribution to $\rho_s(T)$ from this band will rise rapidly with decreasing temperature. Consequently, a clear upturn will show up in $\rho_s(T)$ around $T_{c1}^3$. The appearance of a positive curvature in the experimental data of $\rho_s(T)$, as already mentioned, is a strong support to the two-band picture.

To calculate explicitly the temperature dependence of $\rho_s$ in the whole temperature range, one needs to know the band dispersion $\xi_{ik}$. For this purpose, we adopt the expressions first proposed by Kusko et al. [10] $\xi_{ik} = \pm \left(\varepsilon_{i,k} + \varepsilon_{i,k+Q} \pm \sqrt{\varepsilon_{i,k}^2 - \varepsilon_{i,k+Q}^2 + \Delta^2}\right)/2 - \mu_i$ where $\pm$ corresponds to the first/second band, $\varepsilon_{i,k} = -(2t_i \cos k_x + \cos k_y - 4t'_i \cos k_x \cos k_y - 4t''_i \cos^2 k_x + \cos^2 k_y - 1)$, $t'_i = -0.25t_i$ and $t''_i = 0.2t_i$. $Q = (\pi, \pi)$ is the antiferromagnetic wave vector and here $\delta$ is taken as a constant. $\mu_i$ is the chemical potential determined by the occupation number for each band. It was shown that the FS contours determined from this formula agree qualitatively with the ARPES data [15, 16]. Following the suggestion of Ref. [17, 18], we assume that the second band is hole-like. The doping concentration is therefore given by the difference $x = n_e - n_h$, where $n_e$ and $n_h$
are the carrier concentrations of the first and the second bands, respectively. However, it should be emphasized that similar results can also be obtained if both bands are electron-like.

Fig. 3 compares the theoretical results of superfluid density for a pure system with the corresponding experimental data (symbols) for \( x = 0.124, 0.131, \) and \( 0.152 \). The parameters used are \( t_1 = 5, t_2 = 1, (g_1, g_2, g_3, n_e, n_h) = (1.3, 1.082, 0.005, 0.214, 0.09) \) for \( x = 0.124, (1.3, 1, 0.01, 0.231, 0.1) \) for \( x = 0.131, \) and \((1.3, 0.984, 0.001, 0.261, 0.11)\) for \( x = 0.152 \). As can be seen, the overall agreement between theoretical calculations and experimental data is fairly good. It gives a strong support to our picture. In low temperatures, the theoretical curves exhibit stronger temperature dependence than the experimental ones, especially for the case \( x = 0.131 \). This is because the impurity scattering was not included in the theoretical calculations. By including the impurity scattering, the linear temperature behavior \( \rho_s \) will be replaced by a quadratic form. This, as demonstrated in Fig. 4, will reduce the difference between theoretical calculations and experimental data in low temperatures.

Besides the superfluid density discussed above, our model is also consistent with the phase-sensitive, tunneling spectroscopy, and other experiments that support d-wave pairing symmetry in electron-doped cuprates. Recently, the ARPES as well as the Raman spectroscopy showed that the energy gap is highly anisotropic and shows a maximum between the nodal and anti-nodal regions. This non-monotonic variation of the energy gap from the zone diagonal to the zone axis is not what one may expect for a single-band d-wave superconductor, but is compatible with our two-band picture.

More experimental measurements should be done to further detect the gap structure in electron-doped materials. The scanning tunneling measurement that was used for testing the two-band nature of MgB_2 from the vortex core state along the c-axis, for example, can be used to examine the two-gap picture here. Since the interlayer hopping is highly anisotropic and the c-axis tunneling current is contributed mainly from the first band, this measurement would allow us to determine the coherence length of the first band from the spatial extension of the vortex core. Comparing it with the coherence length of the second band which can be determined from the measurement of \( H_{c2} \), this will provide a direct test for our two-band theory.

In conclusion, we showed that the temperature dependence of \( \rho_s \) in electron-doped cuprate superconductors can be well explained by a weakly coupled two-band model. Our work resolves the discrepancy in the interpretation of different measurement results. It suggests that the pairing potential in electron-doped cuprates has \( d_{x^2−y^2} \) symmetry in the whole doping range, same as in hole-doped materials.

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\[ \text{FIG. 3: Comparison between theoretical calculations (lines) and experimental data (symbols) for the temperature dependence of the normalized superfluid density } \rho_s(T)/\rho_s(0) \text{ of PCCO at three different doping levels.} \]

References:
1. C. C. Tsuei and J. R. Kirtley, Rev. Mod. Phys. 72, 969 (2000), and references therein.
2. T. Sato et al., Science 291, 1517 (2001).
3. N. P. Armitage et al., Phys. Rev. Lett. 86, 1126 (2001).
4. G. Blumberg et al., Phys. Rev. Lett. 88, 107002 (2002).
5. C. C. Tsuei and J. R. Kirtley, Phys. Rev. Lett. 85, 182 (2000).
6. B. Chesca et al., Phys. Rev. Lett. 90, 057004 (2003).
7. L. Alf et al., Phys. Rev. Lett. 83, 2644 (1999).
8. J. D. Kokales et al., Phys. Rev. Lett. 85, 3696 (2000).
9. R. Prozorov et al., Phys. Rev. Lett. 85, 3700 (2000).
10. A. Snezhko et al., Phys. Rev. Lett. 92, 157005 (2004).
11. M.-S. Kim et al., Phys. Rev. Lett. 91, 087001 (2003).
12. N. P. Armitage et al., Phys. Rev. Lett. 88, 257001 (2002).
13. T. Yoshida et al., Phys. Rev. Lett. 91, 027001 (2003).
14. H. Matsui et al., cond-mat/0410388 (unpublished).
15. Q.-S. Yuan et al., Phys. Rev. B 69, 214523 (2004).
16. C. Kusko et al., Phys. Rev. B 66, 140513(R) (2002).
17. Z. Z. Wang et al., Phys. Rev. B 43, 3020 (1991).
18. W. Jiang et al., Phys. Rev. Lett. 73, 1291 (1994).
19. P. Fournier et al., Phys. Rev. B 56, 14149 (1997).
20. T. Xiang and J. M. Wheatley, Phys. Rev. Lett. 76, 134 (1996).
21. J. A. Skinta et al., Phys. Rev. Lett. 88, 207003 (2002).
22. J. A. Skinta et al., Phys. Rev. Lett. 88, 207005 (2002).
23. A. V. Pronin et al., Phys. Rev. B 68, 054511 (2003).
24. N. Nakai, M. Ichikawa, and K. Machida, J. Phys. Soc. Jpn., 71, 23 (2002).
25. I. I. Mazin et al., Phys. Rev. Lett. 89, 107002 (2002).
26. T. Xiang, C. Panagopoulos, and J. R. Cooper, Int. J.
[27] P. J. Hirschfeld and N. Goldenfeld, Phys. Rev. B 48, 4219(R) (1993).

[28] M. R. Eskildsen et al., Phys. Rev. Lett. 89, 187003 (2002).