Nodeless d-wave superconducting pairing due to residual antiferromagnetism in underdoped Pr$_{2-x}$Ce$_x$CuO$_{4-\delta}$

Tanmoy Das, R. S. Markiewicz, and A. Bansil

Physics Department, Northeastern University, Boston MA 02115, USA
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We have investigated the doping dependence of the penetration depth vs. temperature in electron doped Pr$_{2-x}$Ce$_x$CuO$_{4-\delta}$ using a model which assumes the uniform coexistence of (mean-field) antiferromagnetism and superconductivity. Despite the presence of a $d_{x^2-y^2}$ pairing gap in the underlying spectrum, we find nodeless behavior of the low-T penetration depth in underdoped case, in accord with experimental results. As doping increases, a linear-in-T behavior of the penetration depth, characteristic of d-wave pairing, emerges as the lower magnetic band crosses the Fermi level and creates a nodal Fermi surface pocket.

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An understanding of the symmetry of the order parameter and its evolution with hole and electron doping is a key to unraveling the mechanism of high-$T_c$ superconductivity in the cuprates. Many experimental and theoretical studies of these fascinating materials demonstrate the presence of antiferromagnetic (AFM) order in underdoping for both hole [1] and electron doping [2, 3, 4]. With hole-doping, the route followed by the AFM phase as it develops into the superconducting (SC) phase involves the intervention of nanoscale phase separations related to stripe or pseudogap physics [1]. The behavior with electron doping, on the other hand, seems to be simpler in that the doped phase appears to be a uniform AFM metal, possibly evolving into a phase with coexisting AFM and SC orders [2, 3, 4].

For the hole doped cuprates it is generally believed that $d$-wave pairing survives up to the edge of antiferromagnetism [1, 5, 6], but the doping dependence of the pairing symmetry with electron doping remains a matter of debate. This symmetry has been studied by low-T penetration depth (PD) measurements [7, 8, 9, 10], point contact spectroscopy [11, 12, 13], tunneling [14], and other phase sensitive probes [10], in a variety of electron-doped cuprates, including Nd$_{2-x}$Ce$_x$CuO$_{4-\delta}$ (NCCO) [7, 8, 9, 10, 11], La$_{2-x}$Ce$_x$CuO$_{4-\delta}$ (LCCO) [11, 12], Pr$_{2-x}$Ce$_x$CuO$_{4-\delta}$ (PCCO) [11, 12, 13, 14]. The results have been contradictory, with some early measurements [7, 8, 9, 10] finding evidence for s-wave pairing, while other experiments suggest a transition from $d$-wave in underdoping to either s-wave [11, 12] or $(d + is)$-wave character [13] in the optimally and overdoped cases. Yet other experiments [12, 13] report only $d$-wave pairing, with the situation further complicated by the presence of non-monotonic SC-gap variations observed in NCCO [17] and Pr$_{1.4}$La$_{0.6}$Ce$_{0.2}$CuO$_{4-\delta}$ (PLCCO) [2].

A recent study approximated the AFM background by treating the resulting partially-gapped Fermi surface (FS) in a two band model [18]. To understand the interplay between AFM and SC orders and the role of AFM order in modifying the pairing [19, 20], in this article we directly evaluate the PD in a model with coexisting AFM and SC order. We assume a SC gap of $d$-wave pairing with a combination of first and third harmonics, which is necessary to incorporate nonmonotonic gap variations [2, 17]. We find that even in the presence of a $d$-wave pairing gap, the PD varies exponentially at low $T$ for most dopings — a behavior characteristic of a nodeless SC-gap, as antiferromagnetism suppresses the spectral weight from the nodal point. In the overdoped case ($x = 0.152$), the PD shows a linear-in-$T$ behavior as the hole pocket forms in the nodal region. Our analysis indicates that with increasing electron doping the position of the maximum leading edge gap on the FS moves away from the antinodal direction and that the nonmonotonic nature of the gap becomes stronger.

Our treatment of the in-plane PD is based on the Hamiltonian

$$H = H_{pair} + H_{int}, \quad (1)$$

where $H_{pair}$ describes the physics of coexisting AFM and SC orders. We take $H_{pair}$ to be a one-band, tight-binding Hubbard Hamiltonian along the lines of Ref. [2] in which the SC gap is of $d$-wave pairing with a combination of first and third harmonics. The tight binding parameters are assumed to be same as for NCCO [3]. The external perturbation is given by the electromagnetic interaction,

$$H_{int} = -\left(\frac{e}{c}\right)\vec{A} \cdot \sum_{k,\sigma} \vec{v}_{k} c_{k,\sigma}^{\dagger} c_{k,\sigma} \quad (2)$$

where $c_{k,\sigma}^{\dagger}$ ($c_{k,\sigma}$) is the electronic creation (destruction) operator with momentum $\vec{k}$, charge $e$ and spin $\sigma$, and $c$ is speed of light. $\vec{A}$ is the Fourier component of the vector potential in momentum space. $\vec{v}_{k} = \partial \xi_{k}/(\hbar \partial k)$ is the band velocity for the noninteracting band $\xi_{k}$ [3].

The PD is obtained by evaluating the induced current parallel to the vector potential, which is proportional to the inverse square of the in-plane PD [21]. We have gen-
eralized the pure BCS result to the mixed AFM-SC case and find [22] 

\[ \lambda_{ij}^2(T) = \frac{4\pi^2}{c^2a^2d} \sum_{\nu=\pm} \sum_{\mathbf{k}} \left( \frac{1}{m_{\nu kij}} \right) \left( 1 - \frac{\tilde{\xi}_{\mathbf{k}}^\nu + \nu E_{0\mathbf{k}}}{E_{\mathbf{k}}^\nu} \right) \tan\left( \frac{\nu E_{\mathbf{k}}^\nu}{2} \right) - \frac{\beta}{2} \frac{\nu_{\mathbf{k}i}^\nu \nu_{\mathbf{k}j}^\nu \sech^2(\beta E_{\mathbf{k}}^\nu/2)}{E_{\mathbf{k}}^\nu} \right). \]  

(3)

Here, \( a \) is the in-plane and \( d \) the out-of-plane lattice constant of PCCO and \( \beta = 1/k_BT \). The prime on the \( \mathbf{k} \) summation means that the sum is restricted to wave vectors in the magnetic zone. The magnetic field is assumed to lie perpendicular to the CuO\(_2\) plane. For a tetragonal lattice \( \lambda_{ij} \) is diagonal, with \( \lambda_{aa} = \lambda_{bb} = \lambda \) within the CuO\(_2\) plane. Interestingly, Eq. 3 displays a form similar to that for a pure \( d \)-wave SC [23, 24], excepting two modifications. Firstly, the FS has components \( \nu = \pm \) associated with the upper magnetic band (UMB) and the lower magnetic band (LMB), respectively:

\[ (E_{\mathbf{k}}^\nu)^2 = \left( \xi_{\mathbf{k}}^\nu + \nu E_{0\mathbf{k}} \right)^2 + \Delta_{\mathbf{k}}^2, \]  

(4)

where \( E_{0\mathbf{k}} = \sqrt{(\xi_{\mathbf{k}}^\nu)^2 + (U_Q S)^2} \) and \( \xi_{\mathbf{k}}^\nu = (\xi_{\mathbf{k}}^\nu + \xi_{\mathbf{k}+Q})/2 \). \( \Delta_{\mathbf{k}} \) is the SC gap and \( U_Q S \) the AFM gap in terms of the AFM repulsion \( U_Q \) and the commensurate magnetisation \( S \) at the nesting vector \( Q = (\pi, \pi) \). Secondly, the band masses \( m_{\nu kij} \) and quasiparticle velocities \( v_{\mathbf{k}ij}^\nu \) have magnetic correlation corrections: \( 1/m_{\nu kij} = \partial^2(\xi_{\mathbf{k}}^\mu + \nu E_{0\mathbf{k}})/(h^2\partial k_i\partial k_j) \), \( v_{\mathbf{k}ij}^\nu = \partial(\xi_{\mathbf{k}}^\mu + \nu E_{0\mathbf{k}})/(h\partial k) \).

We obtain the AFM and SC gaps self-consistently as a function of \( T \) for a series of doping levels over the range \( x = 0.115 - 0.152 \), using doping dependent interaction parameters [4], before proceeding with the PD calculation from Eq. 3. The effective AFM interaction given by \( U_Q \) is taken from our earlier work on NCCO [2] and decreases from a value of 3.33 at \( x = 0.115 \) to 3.1 at \( x = 0.152 \); the resulting self-consistent magnetization \( S \) decreases linearly from 0.2 to 0.13 over this doping range, in agreement with earlier results [2], despite the presence of the SC order.

The two terms on the right hand side of Eq. 3 correspond to the conventional diamagnetic (first term) and paramagnetic [22] (second term) currents of electrons. In a London picture, \( \lambda^2(T) \) is proportional to the SC electron density \( n_s \), and hence vanishes as \( T \to T_c \), while at \( T = 0 \) all the electrons are superconducting. Here we find a similar result, but only the electrons in the AFM pockets condense. Similarly, as \( T \to 0 \), the linear-in-\( T \) PD found in overdoped samples reveals the presence of gap nodes, where normal quasiparticles persist to zero energy.

Figure 1 compares the theoretical and experimental values of the inverse square of the PD in PCCO [20] over the doping range \( x = 0.115 - 0.152 \). The results are normalized to the computed \( T = 0 \) value for the \( c \)-axis lattice constant \( d = 12.2 \text{ Å} \) [27] in order to highlight \( T \)-dependences. The overall agreement is quite good, allowing us to adduce the doping dependence of the AFM and SC properties as discussed below. A discrepancy is found at the lowest and highest dopings, where the PD shows a tail extending beyond \( T_c \), possibly associated with sample inhomogeneities [28].

Turning to the inset in Fig. 1, note first that the theoretical values (red line) of \( \lambda^{-2}(T)/\lambda^{-2}(0) \) as a function of \( T \) for different dopings \( x \); the corresponding experimental data for PCCO [26] is shown by symbols of the same color (see legend). Inset: Computed (red line) and experimental (blue dots) values of \( \lambda^{-2}(0) \) as a function of doping. Green arrow points to the kink associated with the opening of the nodal pocket in the theory curve.
We do not find a second regime of linear-in-doping of the gap PD in the strongly underdoped regime\cite{19}. These results suggest that on the underdoped side AFM fluctuations are more deleterious than expected from the mean field BCS model underlying our computations. The reappearance of bad metal behavior on overdoping is puzzling and its origin is unclear—it may be related to increasing doping-induced disorder.

We discuss the doping and $T$-dependencies of the preceding theoretical PD results with reference to Figures 2-4. In Fig. 2(a), we emphasize that the contribution of the UMB is nodeless since the PD is dominated by energies near the Fermi level and the UMB pocket is far from the nodal region. An exponential form, $1 - C \exp (-\beta D)$, is seen to produce an excellent fit in the low-$T$ regime in Fig. 2(a). The values of the SC-gap $D$ in Fig. 3(a) so obtained for the UMB (blue dots) are quite close to the SC-gap (red open squares) at the electron pocket tip, marked by yellow diamonds on the FS plots of Figs. 3(b)-(d). The value of $C$ is approximately 4.4, essentially independent of doping. Only at the highest doping $x = 0.152$ do we find a significant linear-in-$T$ ($d$-wave) contribution to the PD as shown in Fig. 2(b), which coincides with the appearance of the hole pocket near $(\pi/2, \pi/2)$ at high dopings as the LMB crosses the Fermi level (see Fig. 4(d)). A linear equation of the form, $1 - aT$, fits the LMB contribution very well up to $T = 1.5K$ as shown by blue line in Fig. 2(b)\cite{31}. We do not find a second regime of linear-in-$T$ PD in the strongly underdoped regime\cite{19}.

Figure 3 examines the doping dependence of the SC gap parameters. The dome-like shape as a function of doping of the gap $D$ in Fig. 3(a) is reflected in the behaviors of the first and third harmonics of the pairing gap in Fig. 3(b) as well. Fig. 3(c) delineates the doping dependence of the first and third harmonics of the pairing interaction, which display a maximum near $x \approx 0.13$ where $T_c$ is optimal. The doping dependence of the SC gap parameters $\Delta_1$ and $\Delta_3$ is compared with various experimental results in Figs. 3(b) and (d). Some disagreement with Raman experiments on NCCO (green filled squares) and PCCO (green open squares)\cite{32} is due to sample variations, reflected in $T_c$ variations, while the ratio $2\Delta_1/k_BT_c$ is essentially constant and agrees well with experiment. If we scale the experimental gap to fit the calculated maximum at optimal doping, we can reproduce the dome-like behavior of the SC gap as shown by the green dashed line in Fig 3(b) for NCCO. The tunnelling data (magenta diamonds)\cite{13, 14} do not show a maximum, because tunnelling is sensitive to the total gap obtained by combining AFM and SC gaps, and this combined gap in our computations does not have a maximum near optimal doping. Similarly, the larger gap seen by Raman\cite{32} in under- and optimally doped samples can be understood since the $B_{2g}$ channel measures the total spectral gap near the $(\pi,0)$ point\cite{33}, and hence is strongly coupled to the AFM order.

Fig. 3(d) shows that the ratio $2\Delta_1/k_BT_c$ possesses a nearly constant value of 4.1, close to the BCS value for a $d$-wave gap. In contrast, for fixed ratio of $V_1/V_3\cite{34}$, the third harmonic ratio $-2\Delta_3/k_BT_c$ increases linearly.
symmetry becomes more pronounced as one goes from low resolution. The nodal pocket is fully formed in the overdoped regime. In underdoping, where the FS only consists of the (π, 0)-centered electron pockets, λ−2 varies in a nodeless manner, even though the pairing interaction is of d-wave symmetry, because the electron pocket lies far from the nodal region. Our analysis indicates that the SC electron density (n_e(0)) is suppressed in a non-BCS fashion as one goes away from optimal doping to either under- or overdoping. Interestingly, we find that the SC interaction (V_1 and V_3) also peaks at optimal doping.

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