Theory of point contact spectroscopy in electron-doped cuprates

C. S. Liu$^{1,2}$ and W. C. Wu$^1$

$^1$Department of Physics, National Taiwan Normal University, Taipei 11650, Taiwan
$^2$Institute of Theoretical Physics, Chinese Academy of Sciences, Beijing 100080, China

In the hole-doped $d_{x^2-y^2}$-wave cuprate superconductor, due to the midgap surface state (MSS), a zero bias conductance peak (ZBCP) is widely observed in [110] interface point contact spectroscopy (PCS). However, ZBCP of this geometry is rarely observed in the electron-doped cuprates, even though their pairing symmetry is still likely the $d_{x^2-y^2}$-wave. We argue that this is due to the coexistence of antiferromagnetic (AF) and the superconducting (SC) orders. Generalizing the Blonder-Tinkham-Klapwijk (BTK) formula to include an AF coupling, it is shown explicitly that the MSS is destroyed by the AF order. The calculated PCS is in good agreement with the experiments.

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Pairing symmetry is an important issue towards the development of an understanding the mechanism of superconductivity. For hole-doped high-$T_c$ cuprate superconductors, it is generally accepted that the pairing symmetry is $d_{x^2-y^2}$-wave \cite{1}. Among many supporting experiments, PCS measurement shows a ZBCP due to the existing MSS in the [110] direction \cite{2,3,4}. On the electron-doped side of cuprates, although no consensus has been reached yet, more and more recent experiments have found results also consistent with a $d_{x^2-y^2}$-wave pairing symmetry \cite{5,6,7,8,9,10}. Thus one expected to see a similar ZBCP for the electron-doped cuprates. The situation is more subtle than this naive expectation however. The ZBCP has been consistently observed in the underdoped samples. In the optimally- and overdoped samples, in contrast, two doping-dependent coherence peaks were generally observed \cite{11,12,13,14}. This has been taken to indicate that the excitation gap in electron-doped cuprates might switch from $d$- to $s$-wave when the doping is increased – a phenomenon consistent with what was observed in the magnetic penetration depth measurement \cite{15}.

The clues towards an understanding of the complicated PCS of the electron-doped cuprates lie in the doping evolution of the two (often called $\alpha$ and $\beta$) pocket Fermi surfaces (FS) and the nonmonotonic $d_{x^2-y^2}$-wave excitation gap, as revealed by angle resolved photoemission (ARPES) measurements \cite{16,17}. These phenomena have been interpreted in terms of a phenomenological two-band model \cite{18}, which in turn led to a successful account for the magnetic penetration depth measurement \cite{17} and Raman scattering \cite{18} data. The key feature of the two-band model is that $\alpha$- and $\beta$-band superconducting (SC) gaps are both monotonic $d_{x^2-y^2}$-wave, but with a different (doping dependent) amplitude. Thus it was originally expected that [110] MSS should also exist in electron-doped cuprates. The difficulty in describing the experiments suggests that there may be some other physics intervening in the system in the SC state.

The most promising candidate (for this absence) is the coexistence of an AF order with the SC order. This scenario finds support in ARPES as the data has been well explained in terms of a $k$-dependent band-folding effect due to an existing AF order \cite{19,20,21,22,23}. Apart from the ARPES data, no other direct evidence indicates that AF order does indeed exist in these materials. Therefore, it is highly desired that some other experiments provide more definitive information regarding the possible existence of AF order in the electron-doped cuprates. When a normal electron is incident into a superconductor, it will induce the excitation of single quasi-particles (QPs) corresponding to all possible order parameters to which the proximity effect is ignored \cite{2}. For $d_{x^2-y^2}$-wave superconductor of interest, the interface is manipulated to be perpendicular to the $k_x$ axis (along the [110] direction). When both SC and AF orders exist, QP excitations of an inhomogeneous superconductor have a coupled electron-hole character associated with the coupled $k$ and $k+Q$ \cite{$\mathbf{Q}= (\pi, \pi)$ subspaces. Correspondingly QP states can be described by the generalized Bogoliubov-de Gennes (BdG) equations \cite{24}}

\begin{align}
E_{u1} &= h_0 u_1 + \Delta k v_1 + \Phi v_2 \\
E_{v1} &= \Delta k u_1 - h_0 v_1 + \Phi v_2 \\
E_{u2} &= \Phi u_1 + h_0 v_2 - \Delta k + Q v_2 \\
E_{v2} &= \Phi v_1 + \Delta k + Q u_2 - h_0 v_2,
\end{align}

where $h_0 \equiv -\hbar^2 \nabla^2_z/2m - \mu$ with $\mu$ the chemical poten-
tial, $\Phi$ is the AF order parameter, and $\Delta_k = (\Delta_0 \sin 2\theta)$ is the $d_{xy}$-wave SC order parameter with $\Delta_{k+Q} = -\Delta_k$. Here the two-component wave functions $u_1$ and $v_1$ are related to $k$ subspaces, while $u_2$ and $v_2$ are related to $k + Q$ subspaces. In arriving at Eq. (1), the pairing potential is assumed to be $\sim \Delta_k \Theta(x)$ with $\Theta(x)$ the Heaviside step function and $\Delta_k$, given above, the Fourier transform of the Cooper pair order parameter in the relative coordinates.

To better describe the effect of an AF order, the FS will be approximated by a square (see Fig. 1). Thus at nearly half-filling, the FS matches the MBZ boundary. Under the WKBJ approximation (25), the formal wave function for the normal metal overlayer

$$
\begin{pmatrix}
  u_1 \\
v_1
\end{pmatrix} = \begin{pmatrix}
e^{ik_F x} u_1 & e^{-ik_F x} u_1 \\
ev^{-i k_F x} v_1 & e^{i k_F x} v_1
\end{pmatrix}
$$

with $\gamma$ being the attenuation constant for $|E(k_F)| < |\Delta(k_F)|$ and $k_F = (k_x, k_y, k_z)$. Eq. (1) becomes the Andreev equation in the $k_x$ direction

$$
E \begin{pmatrix}
  \hat{u}_1 \\
  \hat{u}_2
\end{pmatrix} = \begin{pmatrix}
  \epsilon & \Delta_k & \Phi & 0 \\
  \Delta_k & \Phi & 0 & -\Delta_k \\
  \Phi & 0 & -\epsilon & \Delta_k \\
  0 & \Phi & \epsilon & \Delta_k
\end{pmatrix} \begin{pmatrix}
  \hat{u}_1 \\
  \hat{v}_1 \\
  \hat{u}_2 \\
  \hat{v}_2
\end{pmatrix}
$$

for the superconductor overlayer ($x > 0$). Here $\epsilon = \epsilon(k_x) = i\gamma k_x/m$. The wave-vector components parallel to the interface are conserved for all possible processes.

Solving Eq. (2), one obtains eigenvalues $E = \pm \sqrt{\Delta_k^2 + \Phi^2 + \epsilon^2}$ where $+$ ($-$) corresponds to the electron- (hole-) like QP excitation. Since $\epsilon(-k_x) = -\epsilon(k_x)$ and $\Delta(-k_x) = -\Delta(k_x)$, states for $k_x = k_x$ and $-k_x = k_x$ are actually degenerate. Thus for $k_x = k_x$, one can have two degenerate eigenstates for electron-like QP excitation, while for $k_x = -k_x$, one can have another two degenerate eigenstates for electron-like QP excitation. Superposition of these four eigenstates thus gives a formal wave function for the superconductor overlayer

$$
\psi_S(x) = \begin{pmatrix}
  c_1 & \Delta_k & 0 & E_+ \\
  0 & \Phi & \Delta_k & 0 \\
  -\Delta_k & 0 & \Phi & -E_+
\end{pmatrix} e^{-i k_x x} + \begin{pmatrix}
  0 & E_- & 0 & \Phi \\
  E_+ & 0 & 0 & \Phi \\
  0 & 0 & -\Delta_k & 0
\end{pmatrix} e^{i k_x x}.
$$

FIG. 1: Schematic plot shows all possible reflection and transmission processes for a normal electron incident into an NIS junction, where an AF order exists in the SC side. The inset shows the incident wave vector $k_F = (k_{x0}, k_y, k_z)$ and its corresponding AF wave vector $k_F + Q \equiv k_{FQ} = (-k_{x0}, k_y, k_z)$ due to an AF coupling. Both vectors are tied to the FS, which is approximated by a square (thick line). For convenience, $k_x$ axis is chosen to be along the [110] direction.

Considering the effect of free boundary at $x = -d$, it requires that $\psi_N(x = -d) = 0$. We then obtain the following eigencondition for the surface bound states:

$$
e^{-2ik_x d} E_+ + e^{2ik_x d} E_- = 2\Phi.
$$

Eq. (5) represents one of the major result in this paper. When the AF order $\Phi = 0$, there exists a zero-energy state which is responsible for the ZBCP widely observed in hole-doped $d_{x^2-y^2}$-wave cuprate superconductors.

In order to compare the theory with experiments, we next consider a superconductor [110] surface in point contact with a normal metal (STM) tip. In this case, a thin insulating layer is considered to exist between the normal
the integration over the angle between \( \theta \)
mensionless quantities \( \Phi \)out, to which the FS is absent. In the following the di-
the ARPES data [16].
are characterized by the cutoff angle
are monotonic
The gap is piecewise: both segments are fitted to the
Fig. 2(a) is a typical SC gap for electron-doped cuprates.
AF and SC orders are crucial. Shown in the inset (I) of
cuprates, the issues concerning their doping dependent
side (with an angle \( \theta \)), four possible reflections and their
related coefficients are detailed as follows: (a) Normal
reflection (reflected as electrons) with the coefficient \( r_s \).
(b) Andreev reflection (reflected as holes, due to electron
and hole coupling in the \( k \) subspace) with the coefficient
\( r_{AF}^n \). (c) AF reflection (reflected as electrons, due to the \( k \)
and \( k + Q \) subspace coupling) with the coefficient \( r_{AF}^b \).
(d) Andreev-AF reflection (reflected as holes, due to elec-
tron and hole coupling in the \( k + Q \) subspace) with the
coefficient \( r_{AF}^* \). In terms of these coefficients, the
formal wave function for the normal-metal side can then be
written as
\[
\psi_N(x) = \left[ \exp(i k_{x0} x) + r_s \exp(-i k_{x0} x) \right] r_{AF}^n \exp(i k_{x0} x) + \exp(-i k_{x0} x) + \exp(-i k_{x0} x)
\]
The four reflection coefficients are determined by the boundary conditions:
\[
\psi_N(x)|_{x=0^+} = \psi_N(x)|_{x=0^-}
\]
\[
\frac{2mH}{\hbar^2} \psi_N(x)|_{x=0^+} = \frac{d\psi_N(x)}{dx}|_{x=0^+} - \frac{d\psi_N(x)}{dx}|_{x=0^-}
\]
The normalized tunneling conductance is then given by
\[
\widehat{\sigma}(E, \theta) = 1 - |r_s(E, \theta)|^2 + |r_{AF}^n(E, \theta)|^2 + |r_{AF}^b(E, \theta)|^2 - |r_{AF}^b(E, \theta)|^2.
\]
Actual tunneling conductance is intimately determined by the junction properties. When the tip and the
superconductor are in an ideal point contact, i.e., when the effective potential barrier \( Z \equiv 2mH/\hbar^2 \) is sufficiently
low and narrow, the wave functions at the interface meet
good condition of continuity. Consequently Andreev and
AF reflections are important. For non-ideal point con-
tacts, in contrast, only the normal reflection is impor-
tant. In the following, we focus on the case of low
and narrow barrier height, i.e., the, PCS.
Since the theory is aimed to the electron-doped
cuprates, the issues concerning their doping dependent
AF and SC orders are crucial. Shown in the inset (I) of
Fig. 2(a) is a typical SC gap for electron-doped cuprates.
The gap is piecewise: both segments are fitted to the
monotonic \( d_{x^2-y^2} \)-wave \( (\Delta_0 \sin 2\theta) \), with different amplitudes
\( \Delta_{0\beta} \) and \( \Delta_{0\alpha} \). The \( \beta \)- and \( \alpha \)-band FS segments
are characterized by the cutoff angle \( \theta_1 \) and \( \theta_2 \). The
values of doping-dependent \( \theta_1 \) and \( \theta_2 \) were extracted from the
ARPEs data [16].
In a real NIS junction experiment, the total tunnel-
ner conductance is given by \( \sigma(E) = \int \hat{\sigma}(E, \theta) d\theta \). Here
the integration over the angle between \( \theta_1 \) and \( \theta_2 \) is ruled
out, to which the FS is absent. In the following the di-
mensionless quantities \( \Phi_\beta \equiv \Phi/\Delta_{0\beta} \) and \( \Phi_\alpha \equiv \Phi/\Delta_{0\alpha} \),
which play the determining role on the actual PCS, will
be given from the fitting calculations. The actual values
of \( \Phi, \Delta_{0\alpha} \), and \( \Delta_{0\beta} \) can also be obtained through the
fitting processes. Moreover in the calculation, theQP
energy \( E \) will be replaced by \( E - i\Gamma \) with \( \Gamma \) characterizing
the finite lifetime of the QPs. The parameters from the
best fittings are summarized in TABLE I. As a matter of
fact, only parameters associated with the \( \beta \) band FS
(i.e., associated with the nodal region) are sensitive to the
fitting.
Figure 2(a) compares the theoretical calculations with
the conductance-voltage \( (G-V) \) curve of PCS data [26]
on underdoped \( \text{Pr}_{2-x}\text{Ce}_x\text{CuO}_4 \) (PCCO) \( (x = 0.13) \). For
this case, \( Z = 0.05 \) is used to simulate a low resistance
\( (R = 9.80) \). The result is shown to be in good quan-
titative agreement with the data, to which \( (\Phi_\beta, \Phi_\alpha) = (0.1, 0.2) \) are obtained. The smallness of \( \Phi_\alpha \) and \( \Phi_\beta \) indicates that the effect of AF order is unappreciable. As
a consequence, a strong ZBCP appears, revealing the dom-
inance of the \( d_{x^2-y^2} \)-wave symmetry of the gap. This is

| \( \Phi_\beta \) | \( \Phi_\alpha \) | \( Z \) | \( \Delta_{0\beta} \) | \( \Delta_{0\alpha} \) | \( \Phi \) |
|---|---|---|---|---|---|
| (a) | 0.10 | 0.20 | 0.05 | 1.88 | 0.94 | 0.19 |
| (c) | 0.75 | 1.00 | 1.50 | 3.00 | 2.25 | 2.25 |
| (d) | 0.70 | 0.75 | 0.75 | 1.33 | 1.24 | 0.93 |

(c) 0.75 1.00 1.50 3.00 2.25 2.25

(d) Undoped \( \text{Nd}_{2-x}\text{Ce}_x\text{CuO}_4 \) (\( x = 0.17 \))

(b) Underdoped \( \text{Pr}_{2-x}\text{Ce}_x\text{CuO}_4 \) (PCCO) (\( x = 0.13 \))

(a) Optimally doped \( \text{Pr}_{2-x}\text{Ce}_x\text{CuO}_4 \) (PCCO) (\( x = 0.15 \))

in full support to the conclusion drawn in Ref. \[26\] that the paring symmetry for the underdoped samples is consistent with \(d_{x^2-y^2}\)-wave. To explore the AF effect in more details, the \(G-V\) curve is recalculated for an ideal point contact (\(Z, \Gamma \to 0\)). In this limit [see inset (II) in Fig. 2(a)], the zero-bias "peak" is actually a mix with a narrow plateau. The plateau, that resembles the feature of an s-wave superconductor, arises simply because a small but finite AF order exists near the nodal region.

The evolution of the AF order can be understood from the doping-dependent FS. In underdoped electron-doped cuprates, due to their more distant FS from the MBZ, the scattering about \(Q = (\pi, \pi)\) is weak. This results a small AF order. With increasing the doping, FS approaching and crossing to the MBZ, the scattering about \(Q\) becomes more important which leads to a more important AF order \([21, 27]\). Upon further increase of the doping, long-range order is destroyed such that the AF order decreases and vanishes eventually.

A similar plateau (with a dip) structure has also been observed in PCS on underdoped \(Nd_{2-x}Ce_xCuO_4\) \[12\]. To fit this set of data, \((\Phi_\beta, \Phi_\alpha) = (0.7, 0.9)\) and \(\hat{Z} = 0.25\) are obtained [see Fig. 2(b)]. Comparing the result with that in inset (II) of Fig. 2(a), the \(G-V\) curve changes from a plateau to a two-peak structure. The latter results from much higher \(\Phi_\beta\) and \(\Phi_\alpha\) and a slightly higher resistance \(\hat{Z}\). The dip at zero bias is an evidence that the ZBCP does not exist in this case.

Consider more closely how the FS segments evolve as the doping changes. At low doping, \(\alpha\)-band FS first emerges in the antinodal direction before the superconductivity sets in. When the doping is increased, \(\beta\)-band FS appears simultaneously with the appearance of superconductivity. Since MSS is the signature for a superconductor which has symmetrically a positive and a negative portion of the gap, as long as \(\Phi\) is inappreciable, the ZBCP can still be observed in underdoped samples no matter how the FS segments emerge, or even in the (unrealistic) case without the nodal (\(\beta\)-band) FS.

PCS with high resistance \(\hat{Z}\) has been observed on optimally-doped PCCO \((x = 0.15)\) \[26\]. In the best fitting [Fig. 2(c)], large ratios \((\Phi_\beta, \Phi_\alpha) = (0.75, 1.0)\) and \(\hat{Z} = 1.5\) (for \(R = 18\Omega\)) are obtained. The strong effect of the AF order \(\Phi\) leads to a clear two-peak feature, consistent with the case of a dominant s-wave gap. Nevertheless, theoretical curve deviating from the data at higher biases confirms that a higher \(\hat{Z}\) is in use and the wave functions at the interface do not meet good condition of continuity.

In Fig. 2(d), fairly good fitting is also made with the PCS data on overdoped PCCO \((x = 0.17)\) \[26\], to which large \((\Phi_\beta, \Phi_\alpha) = (0.7, 0.75)\) and a relatively smaller \(\hat{Z}\) (for \(R = 2.6\Omega\)) are used. Again, a two-peak feature consistent with an s-wave gap manifests the largeness of \(\Phi\). In Ref. \[26\], the \(G-V\) curve in Fig. 2(d) was also fitted using the BTK model. Various pairing models were tested and it is the \(d + i s\)-wave symmetry that leads to the best result. This does support the scenario discussed in the current paper that single particle excitation is gapped by both SC and AF orders, \(\Delta_{\text{eff}} = |\Delta_d + i\Phi| = \sqrt{\Delta_d^2 + \Phi^2}\). The actual PCS is indeed the competitive result between the SC and AF contributions.

In summary, PCS of the electron-doped cuprates is investigated. It is shown explicitly that MSS of the \(d\)-wave superconductor can be destroyed by the presence of an AF order \(\Phi\). Due to the smallness of \(\Phi\), ZBCP occurs in the underdoped sample, consistent with the \(d_{x^2-y^2}\)-wave pairing. A more important effect of \(\Phi\) results a two-peak feature in optimally and overdoped samples. The phenomenon that the peak energy first increases and then decreases as doping increases is soundly explained.

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