Andreev and Single Particle Tunneling Spectroscopies in Underdoped Cuprates

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We study tunneling spectroscopy between a normal metal and underdoped cuprate superconductor modeled by a phenomenological theory in which the pseudogap is a precursor to the undoped Mott insulator. In the transparent tunneling limit, the spectra show a small energy gap associated with Andreev reflection. In the Giaever limit, the spectra show a large energy gap associated with single particle tunneling. Our theory semi-quantitatively describes the two gap behavior observed in tunneling experiments.

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It has long been argued that the highly anomalous pseudogap phase of underdoped (UD) cuprates holds the key to the physics of high $T_c$ superconductors \cite{1-3}. A variety of models have been proposed to describe this phase. At present a consensus is lacking and the merits of the different models are being vigorously debated. Some models propose the partial truncation of the Fermi surface in the pseudogap phase is due to the presence of order, which breaks translational symmetry. However in the absence of experimental evidence for broken translational symmetry \cite{5}, models without this property have gained traction. These in turn can be divided into two classes. One emphasizes the reduction of the superconducting (SC) $T_c$ by strong phase fluctuations due to the reduced superfluid density in UD cuprates. This allows the larger SC energy gaps, which in the d-wave form are maximal in the antinodal directions on the Fermi surface, to remain finite at temperatures $T > T_c$ due to preformed Cooper pairs but without off-diagonal long range order \cite{6}. Nernst effect and diamagnetism experiments confirm the presence of SC fluctuations in an extended temperature range above $T_c$ in the UD region of the phase diagram but the range ends substantially below the temperature scale of the onset of pseudogap behavior \cite{7,8}. Alternative models interpret the anomalous properties of the pseudogap phase as precursors to the Mott insulator at zero doping \cite{1}. Since Mott insulating behavior \textit{per se} is not associated with translational symmetry breaking, precursor behavior may not be associated with it either.

Andreev tunneling has been proposed as a distinguished tool to discriminate between SC pairing fluctuations and precursor insulating in the pseudogap phase in an early paper by Deutscher \cite{9}. (For a review of Andreev reflection of pure d-wave superconductor see Ref\cite{10} ) It was pointed out that the voltage (or energy) scale in Andreev tunneling experiments on UD cuprates in the pseudogap phase \cite{11} was substantially below that observed in Giaever or single particle tunneling experiments. The two voltage scales however were the same in the overdoped (OD) region. In a subsequent review of the Andreev experiments Deutscher concluded that “the balance was tilted somewhat against the preformed pairs scenario” \cite{12}. However, the opposite conclusion, namely that higher pseudogap energy scale reflects the pairing strength while a second lower scale the SC condensation energy, was argued for in a later review by Hufner and coworkers which examined many experimental results using different techniques\cite{13}. To make progress in this debate one needs to move beyond qualitative arguments about many individual experiments and on to more explicit models which can be used to consistently analyze a whole range of experiments.

In this letter, we perform such solid analysis by using the model proposed by Yang, Rice and Zhang (YRZ), which has successfully been applied to explain many other experiments, to study both Andreev reflection and Giaever type tunneling for the UD cuprates. Good agreements are achieved, with both the Andreev reflection where a small SC gap $\Delta_s$ is reported, and Giaever type tunneling experiment where a large pseudogap is reported. Our theory provides a semi-quantitative description of the two gap scenario.

In the YRZ model, a single particle propagator was proposed for the pseudogap phase\cite{14}. The YRZ propagator was inspired by an analysis by Konik, Rice and Tsvelik \cite{15} of a 2D array of lightly doped 2-leg Hubbard ladders which gave a set of hole pockets with an energy gap on fixed lines in $k$-space connected by elastic Umklapp scattering processes. The adaptation of this analysis to a 2D Hubbard model for a square lattice lightly doped away from half-filling was influenced by the functional renormalization group results at weak to moderate interaction strength of Honerkamp, Salmhofer and coworkers \cite{16} and by Zhang \textit{et al} \cite{17} early analysis of Anderson’s resonant valence bond (RVB) proposal \cite{18,19}. The strong coupling t-J model was ana-
analyzed using a Gutzwiller renormalized mean field theory (RMFT). In this phenomenological approach the single particle gap at the antinodes is controlled by the RVB gap which truncates the tight-binding Fermi surface into 4 pockets centered on the nodal directions (see Fig[1a]). The d-wave SC energy gap opens up primarily on these Fermi pockets.

This phenomenological propagator gives a consistent description [14] of angle resolved photoemission spectroscopy (ARPES) experiments which followed the evolution of the Fermi surface from 4-disconnected Fermi arcs centered on the nodal directions in UD to the full Fermi surface in OD cuprates [20]. The model has been used to explain a range of other spectroscopic measurements [21], e.g. ARPES results showing increasing particle-hole asymmetry as one moves away from the nodal directions [22], angle integrated photoemission electron spectroscopy (AIPES) experiments measuring the doping, x, dependence of the density of states (DOS) [23] and scanning tunneling microscopy (STM) measurements of the coherent Bogoliubov quasiparticle dispersion at low temperatures [24]. The YRZ form was also used by Carbotte, Nicol and coworkers to successfully describe the T and x dependences of a wide range of properties in the pseudogap phase including specific heat [25], optical conductivity [26], London penetration depth [27] and symmetry dependent Raman scattering spectra [28]. The latter was also analyzed in a similar way by Valenzuela and Bascones [29].

In the YRZ model [14], the incoherent part of the single particle Green’s function contributes a smooth spectral background with a tiny real component at low energies, and the coherent part reads,

\[ G^0(k, \omega) = g_t \left[ \omega - \epsilon_k - \Sigma^0(k, \omega) \right] \]  

(1)

where \( g_t = 2x/(1+x) \) is a renormalization factor [17, 19]. We use the result from the RMFT for the RVB state as the “bare” dispersion \( \epsilon_k \) [30]. \( \Sigma^0 \) is the self energy, which is zero for the OD cuprates (x > x_c = 0.2). For the UD cuprates, \( x < x_c \), \( \Sigma^0(k, \omega) = \left[ \Delta_{RVB}^{RVB} \right]^2 / (\omega + \epsilon_k^0) \) with \( \epsilon_k^0 = -2t(\cos k_x + \cos k_y) \) [30], and \( \Delta_{RVB}^{RVB} = \Delta_0(1 - x/x_c)(\cos k_x - \cos k_y) \), with \( \Delta_0 = 0.3 \). All energies are in unit of \( t_0 = 0.3eV \). Note that \( \epsilon_k^0 = 0 \) at the antiferromagnetic reduced Brillouin zone boundary, where the Umklapp scattering is strongest [10]. Eq[1] predicts four Fermi pockets in the pseudogap phase, consistent with the recent laser ARPES data [31]. Fig[1b] shows one of these Fermi pockets.

Here we consider a d-wave superconducting gap function, \( \Delta_{sc}^y = \Delta_{sc}^x (\cos k_x - \cos k_y) \) for the states around the Fermi surface within a small energy shell. Several previous work proposed similar SC pairing form of YRZ model [14, 21, 27]. We choose \( \Delta_{sc}^0 = 0.08t_0 \) for UD (x = 0.1), and \( \Delta_{sc}^0 = 0.04t_0 \) for OD (x = 0.25). These gap parameters lead to the SC gap \( \Delta_s \) (maximum \( \Delta_{sc}^y \) on Fermi surface) comparable to those observed in the Andreev reflection (~15 and 21 meV, respectively) [11], and to those reported in the recent STM data [24].

The Green’s functions for the SC state in the UD and OD cuprates take the following form in Nambu spinor representation,

\[ G_{UD}^{sc}(k, \omega) = g_{t1} \sum_{i=1,2} \frac{Z_{ki,i} \omega + E_{ki,i} \tau_z - \Delta_{sc}^x \tau_x}{\omega^2 + E_{ki,i}^2 - (\Delta_{sc}^x)^2}, \]  

(2)

\[ G_{OD}^{sc}(k, \omega) = g_{t2} \frac{\omega + \epsilon_k \tau_z - \Delta_{sc}^x \tau_x}{\omega^2 + \epsilon_k^2 - (\Delta_{sc}^x)^2}, \]

where \( \tau_x/\tau_z \) are the Pauli matrices, and the label \( i = 1, 2 \) denotes the lower and higher energy quasiparticle bands given by Eq[1] for the UD region with spectral weight \( g_{t1} Z_{ki,i} \), and dispersion \( E_{ki,i} \). \( G_{OD}^{sc} \) has a BCS form. In the UD region, the quasiparticle energy of the band \( i = 2 \) is well above the chemical potential, which supports our choice \( \Delta_{sc}^x = 0 \). The typical profile of DOS of the SC state is shown in Fig[1b]. In the UD case, the peaks at \( \pm 90 \text{ meV} \) are related to the RVB gap around the antinodes.

We use the Keldysh formalism to study Andreev reflection of a NS junction, consisting of a normal metal lead at the left and a superconductor lead at the right as
shown in Fig[2]. We approximate the connection area or line interface as a scattering center. The tunneling of an electron from the left (L) to the right (R) via the scattering center can be described by the hybridization Hamiltonian, \( H' = \sum_{k,\sigma} t^\alpha_{k,\sigma} c_k^\dagger c_{-k,\sigma} + h.c. \) with \( c_k, c_{-k} \) and \( d \) the electron annihilation operators at lead \( \alpha = L, R \) and on scattering center, respectively. In our following calculations, we assume \( t^\alpha_k = t^\alpha \) for simplicity. In an Andreev reflection process (for a review see Ref[32]), an electron in the normal metal moving along the \( y \)-direction to the scattering center may be reflected back as a hole due to the proximal superconductivity in the scattering center. In the tunneling process, \( k_x \) is conserved. As studied by Meir et al. [33] for NN junction, and by Sun et al. [34] and Wang et al. [35] for NS junction, the total current can be given by (setting \( h = 1 \)),

\[
I = \sum_{s=\pm} e s \int d\omega \frac{dk_x}{2\pi} \left\{ T_N^{s}\left(k_x,\omega\right)\left[f_L^s\left(\omega + seV\right) - f_R^s\left(\omega\right)\right]
+ T_A\left(k_x,\omega\right)\left[f_L^s\left(\omega + seV\right) - f_L^s\left(\omega - seV\right)\right]\right\}
\]  

(3)

where \( f^\alpha \) is the Fermi function at lead \( \alpha \). \( T_N^{s}, T_A \) are the diagonal components of the single particle tunneling matrix \( T_N \) and the Andreev reflection coefficient, respectively. \( s = (+) \) corresponds to the electron (hole) channel. With the frequency-dependence implicitly implied we have,

\[
T_N\left(k_x\right) = G^c_{\sigma}(k_x)\Gamma^L(k_x)G^c_{\sigma}(k_x)\Gamma^R(k_x)
\]  

(4)

\[
T_A\left(k_x\right) = [G^c_{\sigma}(k_x)]_{12}\left[\Gamma^L(k_x)\right]_{22}[G^c_{\sigma}(k_x)]_{21}\left[\Gamma^L(k_x)\right]_{11}
\]  

where \( G^{\alpha}_{\sigma} \) for \( \alpha = r, t \) refers to the retarded or advanced Green’s function, \( G_{\sigma}(k_x) = 1/\left[\omega - \Sigma^L(k_x) - \Sigma^R(k_x)\right] \) is the Green’s function in the scattering center [36]. The self energies \( \Sigma^\alpha(k_x) = (t^\alpha)^2\tau_5G^c_{\sigma}(k_x)\tau_5 \) and lifetime broadening \( \Gamma^\alpha(k_x) = -i\Sigma^\alpha(\Sigma^\alpha - \Sigma^{\alpha\dagger}(k_x)) \), with \( G^c_{\sigma} \) the Green’s functions on the metal side or on the superconductor side given by Eq[12] at their edges to the scattering center. Spin rotational invariance leads to \( T_N^{s\pm}(\omega) = T_N^{s\mp}(\omega) \) and \( T_A(\omega) = T_A(-\omega) \).

The conductance at zero temperature is given by

\[
\sigma_s(\epsilon_V) = \int_{-\pi}^{\pi} \frac{dk_x}{2\pi} e^2 \sum_{s=\pm} \left\{ T_N^{s\pm}(k_x, \epsilon_V) + 2T_A(k_x, seV) \right\}
\]  

(5)

In our calculations, we consider the tunneling along an antinodal direction of the CuO₂ plane, and assume a parabolic dispersion on the normal metal, \( \epsilon_k^F = (k^2 - k_F^2)/2m \), setting \( k_F = \pi/2, m = \pi/2 \) in unit of \( 1/t_0 \).

We now discuss the tunneling conductances in our model and compare them with experiment. There are two parameter regions in the tunneling. At large \( t^R/L \), we have transparent tunneling. Andreev reflection is dominant within the SC gap \( \Delta_s \). At small \( t^R/L \), the Andreev reflection is strongly suppressed, and single particle tunneling dominates.

We first discuss the OD case, which is similar to the conventional BCS superconductor. In this case, the normal state is a metal with a full Fermi surface shown in Fig[1a]. The RVB gap vanishes, leaving only a SC gap \( \Delta_s \). The calculated conductance \( \sigma_s \) in a typical transparent region is shown in Fig[2a]. The conductance in the single particle tunneling region is shown in Fig[2b] in a good agreement with STM data [37], where the contribution from the Andreev reflection is essentially vanishing.

For the UD cuprates, there are two energy scales, a larger RVB gap or pseudogap, and a smaller SC gap \( \Delta_s \). We expect two distinct energy scales in the tunneling conductance. \( \sigma_s \) in the transparent region is plotted in Fig[3a]. The contribution from the Andreev reflection is only substantial within the SC gap on the remnant region of the Fermi surface. \( \sigma_s \) shows a clear peak-edge feature at the SC gap energy \( \Delta_s \). Our result is in good agreement with the reported Andreev tunneling experiment [31], which is reproduced here for comparison. In a single gap scenario, it is not clear that the relative contributions of Andreev and single particle processes to tunneling, into the ordered SC state should change between OD and UD.

The voltage-dependent conductance in the single particle tunneling region is plotted in Fig[3b] for UD samples. In this case, the Andreev reflection is substantially suppressed, so that voltage-dependence of \( \sigma_s \) is similar to that of DOS (Fig[1b]). In both \( \sigma_s \) and DOS in the SC phase, there are two energy scales. The lower energy peak is associated with the SC gap \( \Delta_s \), and the higher energy peak with the RVB gap. The overall profile we obtained is very close to the recent STM experimental data on Bi2212 [38]. Note that the tunneling conductance we study here does not include a strong electron-hole asymmetry in the spectral weight associated with the asymmetry of injecting an electron or a hole in the strongly correlated systems, as examined by Anderson and Ong [39] and
by Randeria et al. [10]. We argue that the relatively low energy tunneling spectral is weakly affected by this strong asymmetry [10] so that our model calculations of the tunneling conductance remain valid in the relevant energy region.

One point worth noting concerns the asymmetry in the single particle tunneling spectra between positive and negative voltages. This is much more pronounced in the DOS calculations based on the YRZ propagator than in the tunneling experiments. The asymmetry in the YRZ DOS comes from the Dirac point at positive energies in the lower quasiparticle band. Interestingly a linear dependence of the DOS at the chemical potential on the hole density was reported in AIPES [23], which is consistent with the approaching to a Dirac point as the hole density is reduced. The quasiparticle DOS calculations do not include the effects of lifetime broadening of the coherent quasiparticle spectra. This could be important in view of the evidence for strong inelastic scattering processes. These could act to smear out signs of a Dirac point at finite energies above the chemical potential and so reduce the asymmetry in the DOS. This discrepancy requires further study.

In summary, we have theoretically studied the tunneling spectroscopy of the underdoped cuprates. The single particle pseudogap in our theory appears as a precursor to the Mott insulator at zero doping. Our theory semi-quantitatively explains the two gap scenario at underdoping revealed in tunneling experiments: a small energy gap associated with Andreev reflection in the transparent limit and a large gap associated with single particle tunneling, which are in contrast with the same scales at overdoping [9, 12]. Although the onset of long range superconducting order on the remaining Fermi pockets (or arcs) induces a reduced pairing amplitude also in

FIG. 4: Conductance for UD cuprate ($\varphi = 0.1$). Panel (a) transparent limit. Red curve is the NS conductance $\sigma_n$, $\sigma_n^\Lambda$ in blue denotes the Andreev reflection contribution, black curve is experimental Andreev reflection data on UD YBCO samples [11]. The SC gap ($\Delta_s \sim 15$ meV) is indicated with green lines. Panel (b) Giaever tunneling limit. Blue curve is $\sigma_n$ for NN junction. Black curve is $dl/dv$ curve for UD Bi-2212 ($T_c = 45$ K) observed in STM [35]. The two energy gaps are marked by arrows. The same parameters as OD shown in Fig. 3 are used.

these antinodal regions through Cooper channel scattering processes, the corresponding Andreev signal is found strongly suppressed. Since the tunneling experiments, per se, do not address the origin of this two gap behavior, from broader viewpoint, our calculations support all models in which the pseudogap at underdoping is due to the partial truncation of the Fermi surface through an insulating gap in the antinodal regions, but not due to preformed Cooper pairs.

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We use a “bare” dispersion from the RMFT for the t-J model, \( \epsilon_k = -2t(\cos k_x + \cos k_y) - 4gt' \cos k_x \cos k_y - 2gt'' \cos 2k_x \cos 2k_y - \mu \) with parameters \( t = (g_{\ell}t_0 + \frac{3}{8}g_sJ\chi), \frac{t'}{t_0} = -0.4, \frac{t''}{t_0} = 0.2, J/t_0 = 0.3, \chi_0 = 0.338, g_s = 4/(1 + x)^2, t_0 \) is about 0.3 eV.

In Giaever limit, the scattering center has a uniform tunneling channel at all energies in our calculation.

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