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Theory of tunnelling into and from cuprates

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Abstract

A single-particle spectral density is proposed for cuprates taking into account the bipolaron formation, realistic band structure, thermal fluctuations and disorder. Tunnelling and photoemission (PES) spectra are described, including the temperature independent gap observed both in the superconducting and normal states, the emission/injection asymmetry, the finite zero-bias conductance, the spectral shape in the gap region and its temperature and doping dependence, dip-hump incoherent asymmetric features at high voltage (tunnelling) and large binding energy (PES).

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The strong-coupling extension of the BCS theory based on the $1/\lambda$ multi-polaron perturbation technique firmly predicts the transition to a charged Bose liquid in the crossover region of intermediate values of the BCS coupling constant λ [1]. There is a fundamental difference between the bipolaron theory of high-T_c cuprates [2] and other theories involving real-space pairs (bosons) tightly bound by a field of a pure electronic origin. As emphasised by Emery *et al* [3] such 'electronic' theories are *a priori* implausible due to the strong short-range Coulomb repulsion between two carriers. The direct (density-density) repulsion is usually much stronger than any exchange interaction. On the other hand, the $Frohlich$ electron-phonon interaction can provide *mobile* intersite bipolarons in the CuO_2 plane condensing at high T_c [4]. The (bi)polaronic nature of carriers in cuprates explains a very small coherence volume in the superconducting state, the mid-infrared conductivity [5], the isotope effect on the carrier mass [6].

Although the charged Bose liquid of bipolarons describes anomalous thermodynamics and kinetics of cuprates [7], finite frequency/momentum response functions of bipolaronic superconductors remain to be established. In this letter we derive a single-particle spectral function of strongly coupled carriers in a random potential which provides a quantitative description of recent tunnelling spectra [8,9] and explains some photoemission features (see [10] and references in [8–10]).

In the framework of our theory the ground state of cuprates is a charged Bose-liquid of intersite bipolarons with single polarons existing only as excitations with the energy $\Delta/2$ or larger. Different from the BCS description the pair binding energy Δ is temperature independent. Hence, there is no other phase transition except a superfluid one at $T = T_c$. The characteristic temperature T^* of the normal phase is a crossover temperature of the order of $\Delta/2$ where the population of the upper polaronic band becomes comparable with the bipolaron density. Along this line the theory of tunnelling in the bipolaronic superconductors was developed both for two-particle [11] and single- particle [12] transitions through a dielectric contact. It allowed us to understand the temperature independent gap and the asymmetry of the current-voltage characteristics, observed already in the earlier

tunnelling experiments [13]. However, an attempt to fit the conductance structure led us to a very narrow (bi)polaronic band with a bandwidth of the order or even less than T_c [11,12]. Such a bandwidth is not compatible with the experimental estimate of the effective carrier mass, $m^* \simeq 2-10m_e$ (depending on doping) from the London penetration depth [7]). It is also incompatible with the theoretical estimate [4] of the (bi)polaron bandwidth (c.a. $100meV$ or larger) based on the well-established value of the Frohlich interaction. Moreover, any description based on the Bloch representation is hardly justifiable for cuprates with the mean free path often comparable with the lattice constant. One has to consider a random potential and thermal fluctuations along with a strong pairing potential and band-structure effects.

We apply a single-particle tunnelling Hamiltonian describing the injection of an electron into a single hole polaronic state P with the matrix element $P_{\mathbf{k},\nu}$ and into a paired hole (bipolaronic) state B with the matrix element $B_{\mathbf{k},\nu,\mu}$ (Fig.1),

$$H_{tun} = \sum_{\mathbf{k},\nu} P_{\mathbf{k},\nu} a_{\mathbf{k}} p_\nu + \sum_{\mathbf{k},\nu,\mu} B_{\mathbf{k},\nu,\mu} a_{\mathbf{k}} p_\nu^\dagger b_\mu + H.c. \tag{1}$$

Here $\mathbf{k}$, ν and μ are the quantum numbers describing the electron in a tip (Fig.1) (annihilation operator $a_{\mathbf{k}}$) a hole polaron (p_ν) and a hole bipolaron (b_μ) in the CuO_2 plane in a random field, respectively. If the eigenstates $|\nu\rangle$ and $|\mu\rangle$ are known, the matrix elements $P_{\mathbf{k},\nu}$ and $B_{\mathbf{k},\nu,\mu}$ are derived by the use of the site representation and the canonical polaronic transformation as discussed in detail in Ref. [11,12]. They are almost independent of $k \simeq k_F, \mu, \nu$ in a wide voltage and binding energy range, $P_{\mathbf{k},\nu} \simeq P = constant$, $N^{1/2} B_{\mathbf{k},\nu,\mu} \simeq B = constant$, N is the number of cells in the sample volume. In general, B and P are different [12] because the second hole in a small coherence volume changes the potential barrier of the contact for the tunnelling B compared with P.

The injection rate is given by the Fermi Golden Rule as

$$\begin{aligned} W_{in} = {} & 2\pi P^2 \sum_{\mathbf{k},\nu} f(\xi_{\mathbf{k}}) f(\xi_\nu) \delta(\xi_{\mathbf{k}} + eV + \xi_\nu + \Delta/2) \\ & + \frac{2\pi B^2}{N} \sum_{\mathbf{k},\nu,\mu} f(\xi_{\mathbf{k}}) n_\mu [1 - f(\xi_\nu)] \delta(\xi_{\mathbf{k}} + eV + \xi_\mu - \xi_\nu - \Delta/2), \end{aligned} \tag{2}$$

and the emission rate is

$$W_{em} = 2\pi P^2 \sum_{\mathbf{k},\nu} [1 - f(\xi_{\mathbf{k}})][1 - f(\xi_\nu)]\delta(\xi_{\mathbf{k}} + eV + \xi_\nu + \Delta/2) + \frac{2\pi B^2}{N} \sum_{\mathbf{k},\nu,\mu} [1 - f(\xi_{\mathbf{k}})][n_\mu + 1] f(\xi_\nu)\delta(\xi_{\mathbf{k}} + eV + \xi_\mu - \xi_\nu - \Delta/2). \quad (3)$$

Here $f(\xi) = [exp(\xi/T) + 1]^{-1}$ is the Fermi-Dirac distribution function for electrons in the tip and hole polarons in the sample, n_μ is the bipolaron distribution [14], $\xi_{\mathbf{k},\nu,\mu}$ is the energy spectrum of electrons, polarons and bipolarons, respectively, V is the sample voltage, e is the elementary (positive) charge, and $\hbar = k_B = 1$. Taking the difference of the injection and emission rates multiplied by e and differentiating it with respect to V we obtain the conductance $\sigma = dI/dV$ as

$$\sigma(V,T) = \frac{\pi N_{tip} P^2}{T} \int_{-\infty}^{\infty} d\xi \rho(\xi) sech^2 \left[\frac{\xi + eV + \Delta/2}{2T}\right] + \frac{\pi N_{tip} B^2}{TN} \int_{-\infty}^{\infty} d\xi \rho(\xi) \sum_\mu [n_\mu + f(\xi)] sech^2 \left[\xi - \xi_\mu - eV + \Delta/2 \; over 2T\right], \quad (4)$$

with N_{tip} and $\rho(\xi)$ the density of states (DOS) per spin in the tip near the Fermi level and the polaronic DOS in the sample, respectively. To arrive at the analytical result we assume that the Coulomb bipolaron-bipolaron repulsion [7] is relatively weak, and temperature is small compared with Δ and the characteristic energy scale ϵ_0 of the polaronic DOS (see below). Then the bipolaron distribution n_μ is narrow [14] and the population of the polaronic states is low. That allows us to integrate out the bipolaronic states taking $\xi_\mu = f(\xi) = 0$ in the second term of Eq.(4). The derivative of the Fermi distribution, $sech^2(x)$ cuts the integrals at $|x| = 1$. As a result we obtain

$$\sigma(V,T) = \frac{\pi e^2 N_{tip} P^2}{T} [N(-eV - \Delta/2 + 2T) - N(-eV - \Delta/2 - 2T)] + \frac{\pi e^2 x N_{tip} B^2}{T} [N(eV - \Delta/2 + 2T) - N(eV - \Delta/2 - 2T)], \quad (5)$$

with $N(E) = \int_{-\infty}^{E} dE' \rho(E')$ the cumulative polaronic DOS, and x the bipolaron density per cell proportional to the doping. The first term in Eq.(5) proportional to P^2 contributes to the emission, while the second one describes the injection. They have different values

because, in general, we have $B \geq P$ and $x \leq 1$, so that $A \equiv P^2/B^2 x$ differs from unity [12]. We notice that the spectral shape of the emission and the injection might be also different if the bipolaron distribution is sufficiently wide. There is an additional integration in the second term in Eq.(4), describing the injection compared with the emission. Hence, a fine spectral structure like the dip found in the emission [10,9] (and references therein) can be nearly washed out from the injection as observed [8,9].

The tunnelling (or PES) spectrum, Eq.(5) is defined if the polaronic cumulative DOS is known. It depends on the band structure, dressing and scattering. While high frequency phonons and magnetic fluctuations are responsible for the high-energy spectral features in the region of the order of the Franck-Condon (polaronic) level shift (> 100 meV) [7], the low energy spectral function is determined by the band structure and by the thermal lattice, spin and random fluctuations. The p-hole polaron in cuprates is almost one-dimensional due to the large difference in the $pp\sigma$ and $pp\pi$ hopping integrals and the effective 'one-dimensional' localisation by the random potential as described in Ref. [4]. This is confirmed by the angle-resolved PES [17] with no dispersion along certain directions of the two-dimensional Brillouin zone. Because the amount of disorder is high and the screening radius is about the lattice constant, we can describe the effect of disorder and of the thermal fluctuations as 'white Gaussian noise'. The relevant spectral density $A(k, E)$ for a one-dimensional particle in a random Gaussian potential was derived by Halperin [15] and the density of states, $\rho(E)$ by Frish and Lloyd [16]. Halperin found the spectral function both for a 'Schrodinger' particle (i.e. in the effective mass approximation) and for a 'discrete' particle (tight-binding approximation). The estimated polaronic bandwidth is about 100 meV or larger, so we consider the effective mass (m^*) approximation for the spectral density, given by [15]

$$A(k, E) = 4 \int_{-\infty}^{\infty} p_0(-z) Re p_1(z) dz, \tag{6}$$

with $p_{0,1}(z)$ obeying two differential equations

$$\left[\frac{d^2}{dz^2} + \frac{d}{dz}(z^2 + 2E) \right] p_0 = 0, \tag{7}$$

and

$$\left[\frac{d^2}{dz^2}+\frac{d}{dz}(z^2+2E)-z-ik\right]p_1+p_0=0. \tag{8}$$

The boundary conditions are to be found in Ref. [15]. Here the energy E and the momentum k are measured in the units $\epsilon_0=(D^2m^*)^{1/3}$ and $k_0=(D^{1/2}m^*)^{2/3}$, respectively. The constant D describes the second moment of the Gaussian potential comprising thermal and random fluctuations as $D=2(V_0^2T/M+n_{im}v_0^2)$, where V_0 is the amplitude of the deformation potential, M is the elastic modulus, n_{im} is the impurity density, and v_0 is the coefficient of the δ- function impurity potential. Then the cumulative DOS

$$N(E)=(2\pi)^{-1}\int_{-\infty}^{E}dE'\int_{-\infty}^{\infty}dkA(k,E') \tag{9}$$

is expressed analytically in terms of the tabulated Airy functions $Ai(x)$ and $Bi(x)$ as

$$N(E)=\pi^{-2}\left[Ai^2(-2E)+Bi^2(-2E)\right]^{-1}. \tag{10}$$

Substituting Eq (10) into Eq.(5) we obtain the expression for the tunnelling and PES spectra in the voltage (energy) region, where the high-frequency phonon shake-off is forbidden by the energy conservation. In particular, we find for $T=0$

$$\frac{\sigma(V,0)}{\sigma_0}=A\rho\left(\frac{eV-\Delta/2}{\epsilon_0}\right)+\rho\left(\frac{-eV-\Delta/2}{\epsilon_0}\right), \tag{11}$$

with

$$\rho(x)=\frac{4}{\pi^2}\times\frac{Ai(-2x)Ai'(-2x)+Bi(-2x)Bi'(-2x)}{[Ai^2(-2x)+Bi^2(-2x)]^2*} \tag{12}$$

and the constant $\sigma_0=2\pi k_0\epsilon_0^{-1}e^2xN_{tip}B^2$.

We compare the conductance, Eq.(11) with the scanning tunnelling microscope (STM) [8] and point-contact tunnelling (PCT) [9] measurements in an overdoped and optimally doped $Bi_2Sr_2CaCu_2O_{8+\delta}$ (Bi-2212) in Fig.2 and Fig.3, respectively. The bipolaron theory describes quantitatively the spectra in the gap region, including the zero-bias conductance at $T=0$, the asymmetry, and the decreasing background at higher voltages which are inconsistent with the classic BCS theory, no matter s or d-wave. The zero-bias conductance

at $T = 0$ is explained by the presence of the impurity tails of the polaronic DOS inside the gap, while the decreasing background, proportional to $|V|^{-1/2}$ for $|V| >> \Delta/2$ is explained by the one-dimensional band dispersion of polarons. The peak amplitudes and the zero-bias conductance are determined by the ratio of the bipolaron binding energy Δ to the characteristic scattering rate ϵ_0. The position of two peaks and their amplitudes relative to the zero-bias conductance allow us to determine the relevant parameters Δ, ϵ_0 and the asymmetry A with an error bar less than five percent. The doping dependence of Δ agrees with that found from the uniform magnetic susceptibility and explained by us [18] as resulting from the screening of the Frohlich interaction by free carriers.

An essential feature of the bipolaron theory is the temperature independent gap with the ratio Δ/T_c, which might be quite different from the BCS one, $2\Delta_{BCS}/T_c \simeq 3-5$. We obtain a very large ratio, $\Delta/T_c \simeq 9$ for both overdoped, Fig.2 and optimally doped, Fig.3, samples. Such a large ratio is difficult to understand in the framework of the BCS theory including its canonical strong-coupling extension. Renner *et al* [8] emphasised that the evolution of the STM spectra with temperature was very different from the classic BCS behaviour, both s and d-wave. The 'superconducting' gap was found temperature independent evolving into the 'normal' gap above T_c. In our theory this is one and the same gap, which is the bound energy of real-space bipolarons. It does not disappear at any temperature, neither at T_c nor at T^*. The theoretical evolution of the spectrum with temperature described in Eq.(5), Fig.3 (inset), reproduces well the experimental features. In particular, the zero-bias conductance increases with temperature and there is no sign that the gap closes at a given temperature, in agreement with the experiment [8]. The latter observation rules out any role of superconducting phase or spin fluctuations in the normal gap. We notice that the theoretical peaks shift to higher energies above T_c, Fig.3 (inset), as observed (see Fig.2 in Ref. [8]).

There is some characteristic voltage (binding energy) V_c, (Fig.2 and Fig.3), above which the experimental STM and PCT conductance deviate from the theoretical one. We believe that a hump observed above V_c is due to a polaronic cloud, as discussed in Ref. [7]. The

high-frequency phonons and magnetic fluctuations contribute to the excess spectral weight with a maximum around twice the Franck-Condon shift. The dip of the spectral weight at V_c is explained by the electron-collective excitation coupling as suggested by Shen and Schrieffer [10] for PES and discussed by DeWilde *et al* [9] for STM and PCT. We have shown earlier that a similar dip structure appears in the electronic DOS as a result of the electron-Einstein phonon interaction [19]. With the established DOS, Eq.(12) we can quantify this feature. If we determine $V_c \simeq 70meV$ in the overdoped sample, Fig.2, and $V_c \simeq 80meV$ in the optimally doped, then the relevant polaron kinetic energy, $E_c = eV_c - \Delta/2$, appears to be about $39meV$ and $42meV$, respectively. Hence, the emission of any dispersionless phonon of that energy can produce a dip in the polaronic DOS as described in Ref. [19]. However, E_c is also close to the estimated energy of the magnetic fluctuations thought to be responsible for the spin-flip neutron scattering at $q = (\pi, \pi)$ ($41meV$ peak observed in $YBa_2Cu_3O_7$ [20]). These magnetic fluctuations, should they be found in Bi2212, might contribute to the dip as well. The polaron-bipolaron inelastic collisions also contribute to the dip in a manner similar to the polaron-phonon interaction [19] because V_c is close to Δ. The polaronic DOS is finite in the middle of the gap, as discussed above. Hence, the polaron with the kinetic energy E_c can break a bipolaron into two single polarons with the energy about $\Delta/2$ each.

The present theory of tunnelling and PES can be generalised to describe SIS junctions, $c-axis$ current at high voltage and the angle-resolved photoemission (ARPES). In particular, SIS current-voltage characteristics are obtained by a convolution of the polaronic DOS with itself. As a result we get two peaks around the temperature independent $|eV| = \Delta$, and the symmetric shape of the SIS conductance, as observed [9]. We expect an S-shape $I - V$ for the $c - axis$ current *both* in the superconducting and normal state as a result of the bipolaron-breaking at high voltage. The S shape c-axis $I - V$ characteristics were measured in Bi2212 and interpreted as a 'subgap resistance of intrinsic Josephson junctions' between *superconducting* CuO_2 planes [21]. We believe, that while the notion of 'subgap' is perfectly correct, one cannot refer the observed nonlinearity to the Josephson junctions. The nonlinearity is still found at temperatures as high as $140K$ (Fig.4 of Ref. [21]) where

the CuO_2 planes are definitely in the normal state, as expected in the framework of the bipolaron theory. Therefore, there is no doubt that the true normal state $c-axis$ resistivity and the upper critical field H_{c2} were measured in Ref. [22] by applying an external magnetic field. ARPES can be described with the spectral function $A(k, E)$, determined numerically from Eqs (7,8). While such a feature of ARPES as the normal state gap is understood within the present analysis, the k dispersion will be presented elsewhere.

In summary, we propose a single-particle spectral function for cuprates, which describes the spectral features observed in tunnelling and photoemission, in particular the temperature independent gap and the anomalous gap/T_c ratio, injection/emission asymmetry both in the magnitude and in the shape, zero-bias conductance at zero temperature, and the spectral shape inside and outside the gap region. The dip-hump features and the temperature/doping dependence of the tunnelling conductance and PES are discussed as well.

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REFERENCES

[1] A.S. Alexandrov, Zh.Fiz.Khim. **57**, 273 (1983) (Russ.J.Phys.Chem.**57**, 167 (1983)); Phys. Rev. B**46**, 2838 (1992).

[2] A.S. Alexandrov, Pis'ma Zh. Eksp.Teor.Fiz. (Prilozh.) **46**, 128 (1987) (JETP Lett Suppl. **46**, 107 (1987)).

[3] V.J. Emery, S.A. Kivelson, and O. Zachar, Phys. Rev. B**56**, 6120 (1997).

[4] A.S. Alexandrov, Phys.Rev. B**53**, 2863 (1996).

[5] for a review see D.B. Tanner and T. Timusk, in 'Physical Properties of High-Temperature Superconductors III', ed. D.M. Ginsberg, World Scientific, Singapore (1992) and E.K.H. Salje, A.S. Alexandrov, and W.Y. Liang (eds), 'Polarons and Bipolarons in High-T_c Superconductors and Related Materials', Cambridge University Press, Cambridge (1995) .

[6] G. Zhao, M.B. Hunt,H. Keller, and K.A. Müller, Nature **385**, 236 (1997).

[7] A.S. Alexandrov and N.F. Mott, Rep. Prog. Phys. **57** 1197; 'High Temperature Superconductors and Other Superfluids' (Taylor and Francis, London) (1994).

[8] Ch. Renner *et al*, Phys. Rev. Lett. **80**, 149 (1998).

[9] Y. DeWilde *et al*, Phys. Rev. Lett. **80**, 153 (1998).

[10] Z.-X. Shen and J.R. Schrieffer, Phys. Rev. Lett. **78**, 1771 (1997).

[11] A.S. Alexandrov, M.P. Kazeko and S.G. Rubin, Zh. Eksp. Teor. Fiz. **98**, 1656 (1990) (JETP **71**, 1656 (1990)).

[12] G.G. Melkonian and S.G. Rubin, to be published.

[13] J. Geerk, X.X. Xi and G. Linker, Z. Phys. B**73**, 329 (1988).

[14] Within the Bogoljubov approximation $n_\mu \simeq n\delta_{\mu,0}$ for $T = 0$, where $\mu = 0$ refers to the

mobility edge [7], n the bipolaron density.

[15] B.I. Halperin, Phys. Rev. **139**, A104 (1965).

[16] H.L. Frisch and S.P. Lloyd, Phys. Rev. **120**, 1175 (1960).

[17] D.M. King *et al*, Phys. Rev. Lett. **73**, 3298 (1994); K. Gofron *et al*, *ibid* 3302 (1994).

[18] A.S. Alexandrov, V.V. Kabanov and N.F. Mott, Phys. Rev. Lett. **77**, 4796 (1996).

[19] A.S. Aleksandrov (Alexandrov), V.N. Grebenev, and E.A. Mazur, Pis'ma Zh. Eksp. Teor. Fiz. **45**, 357 (1987) (JETP Lett. **45**, 455 (1987)).

[20] J. Rossat-Mignod *et al*, Physica Scripta **45**, 74 (1992).

[21] A. Yurgens *et al*, Phys. Rev. Lett. **79**, 5122 (1997).

[22] Y. Ando *et al*, Phys. Rev. Lett **75**, 4662 (1995); A.S. Alexandrov *et al*, Phys. Rev. Lett. **76**, 983 (1996).

Figure Captures

Fig.1 SIN tunnelling into a single polaron state P and into a bipolaron state B.

Fig.2 Theoretical tunnelling conductance (line) compared with the STM conductance ($T = 4.2K$) in overdoped $Bi2212$ ($T_c = 74.3K$ [8]).

Fig.3 Theoretical tunnelling conductance (line) compared with the PCT conductance ($T = 4.2K$) in optimally doped $Bi2212$ ($T_c = 95K$ [9]). Inset shows the temperature dependence of the conductance calculated with a constant ϵ_0 in the gap region.

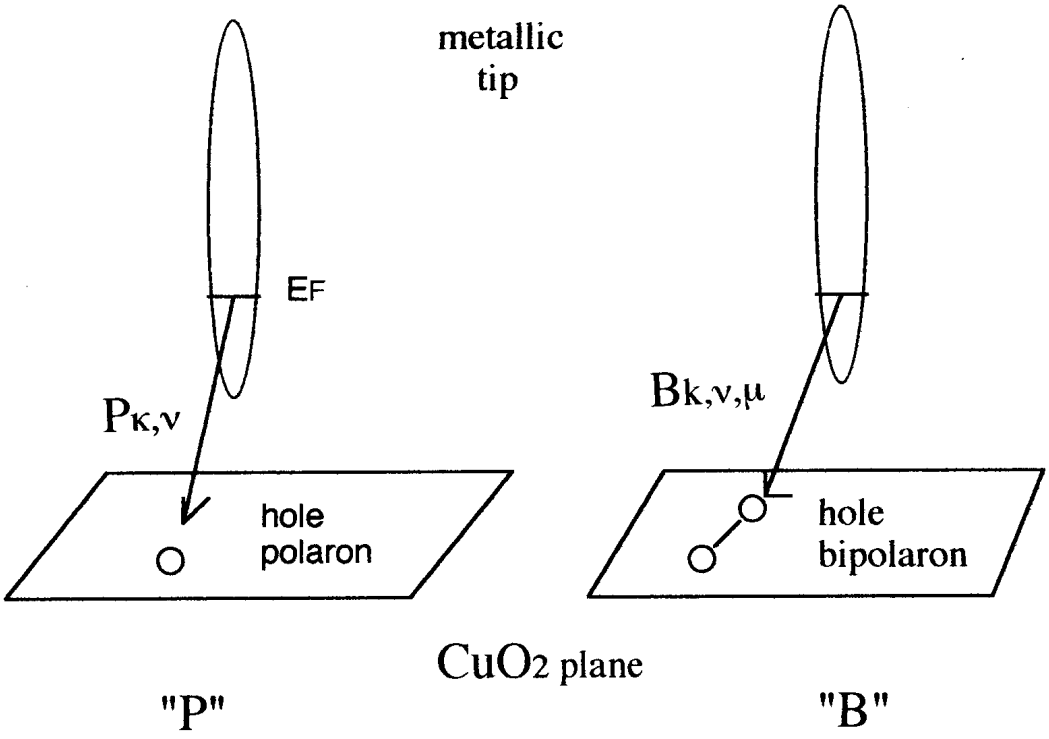

metallic
tip
EF
Pκ,ν
hole
polaron
Bk,ν,μ
hole
bipolaron
CuO2 plane
"P"
"B"

Fig. 1

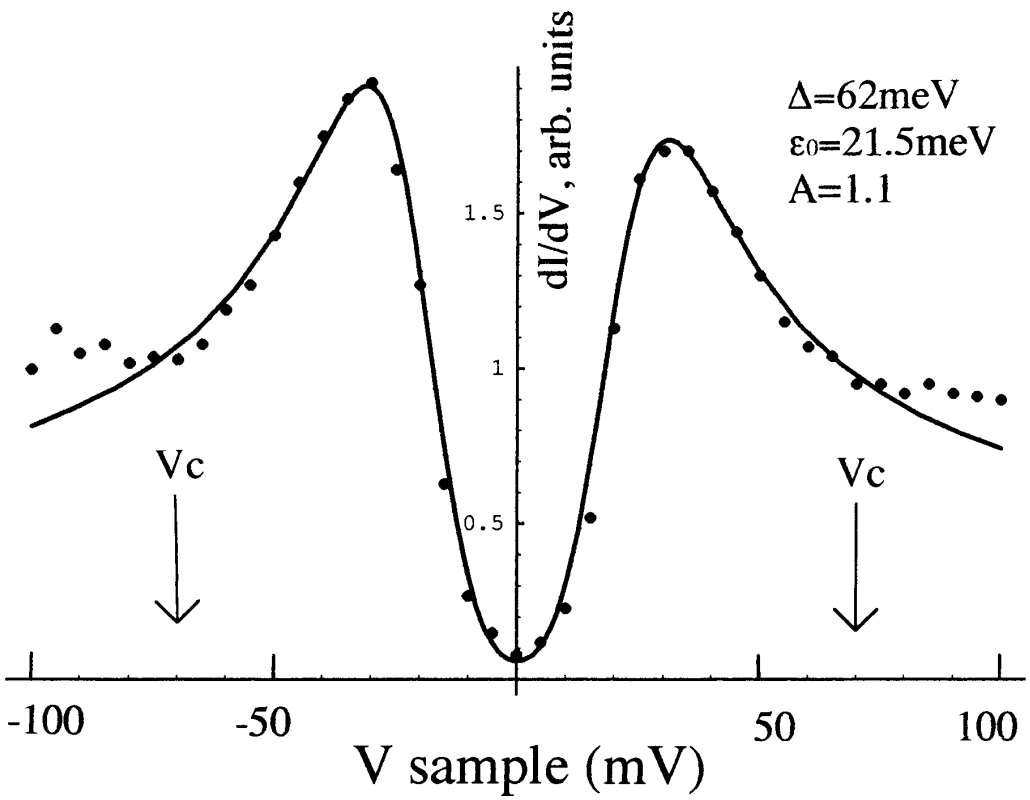

Δ=62meV
ε0=21.5meV
A=1.1
dI/dV, arb. units
1.5
1
0.5
Vc
Vc
-100
-50
50
100
V sample (mV)

Fig. 2

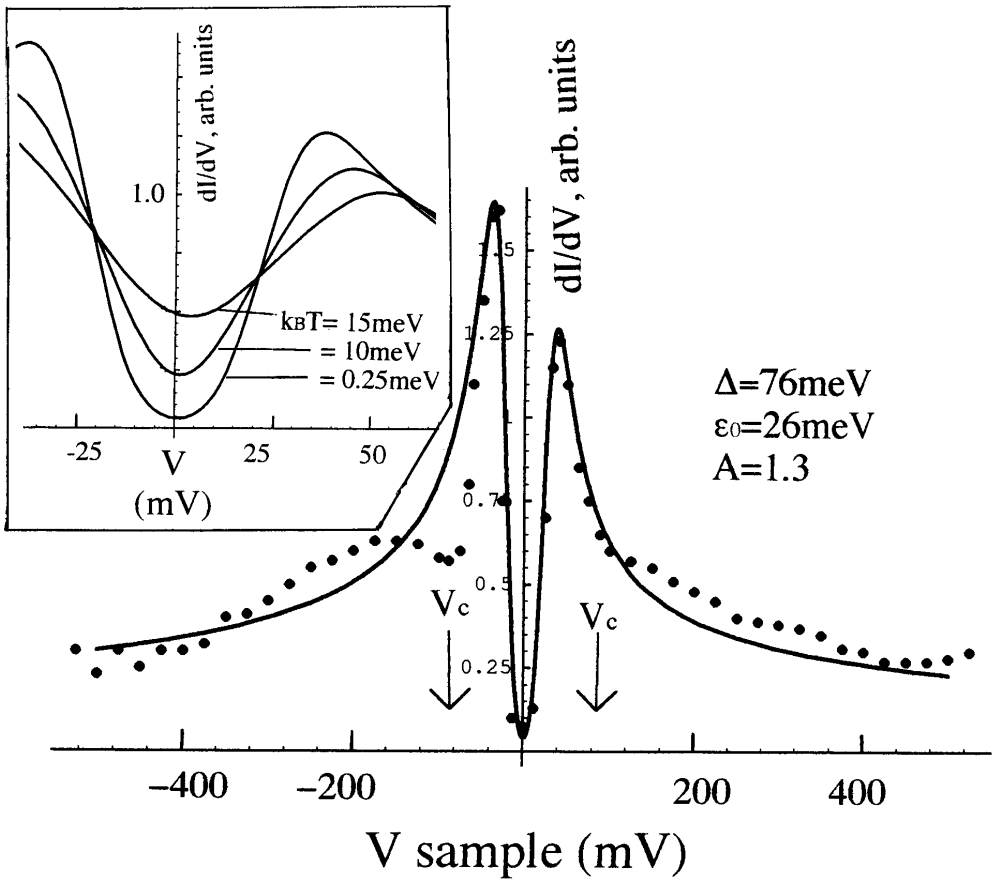

dI/dV, arb. units
1.0
kBT= 15meV
= 10meV
= 0.25meV
-25
V
(mV)
25
50
dI/dV, arb. units
Δ=76meV
ε0=26meV
A=1.3
Vc
Vc
0.25
0.5
0.7
1.25
1.5
-400
-200
200
400
V sample (mV)

Fig. 3