Unusual Quasiparticle Tunneling in High-$T_c$ Cuprate Superconductors: Evidence for the BCS and Polaronic Multi-Gap Effects on Tunneling Spectra

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We propose a model of quasiparticle tunneling across the high-$T_c$ superconductor-insulator-normal metal junction based on the different mechanisms for tunneling of electrons at positive bias and dissociating polaronic Cooper pairs and large polarons at negative bias, and the gap inhomogeneity (i.e., multi-gap) picture. We show that the main features of the tunneling spectra such as low-bias U- and V-shaped features, asymmetry and high-bias dip-hump features, their temperature and doping dependences, and shoulders inside the conductance peaks observed in high-$T_c$ cuprates arise naturally from the model. The experimental tunneling spectra of Ba$_2$Sr$_2$CaCu$_2$O$_{8+x}$ are fitted quite well by taking into account the distribution of BCS and polaronic gap values.

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In conventional superconductors, superconductivity arises from the binding of electrons into Cooper pairs and the BCS gap opening in the electronic excitation spectrum at the superconducting (SC) transition temperature $T_c$ serves as the SC order parameter. In contrast, in high-$T_c$ cuprate superconductors the precursor Cooper pairing of carriers occurs in the normal state and the BCS-like gap is manifested as a pseudogap (PG) opening at a temperature $T^* > T_c$, at which the Cooper pairs condense into a superfluid (SF) Bose-liquid state $\uparrow\downarrow$. As argued in Refs. [1, 2], in these materials the Cooper pairing is only a necessary but not a sufficient condition for the occurrence of superconductivity and the BCS-like gap might be different from the SC order parameter appearing below $T_c$. Other alternative PG scenarios were also proposed (for a review, see, e.g., Refs. [3, 6]), among which the SC fluctuation scenario suggests that the PG appearing below $T^*$ is related to superconductivity as a form of precursor pairing and evolves smoothly into the SC gap at $T_c$. It is still highly debated whether the PG observed by various experimental techniques originates from SC fluctuations above $T_c$ [7, 9] or from the precursor non-SC Cooper pairing below $T^*$ [1, 3] or from some other effects (see Refs. [10–12]).

Scanning tunneling microscopy and spectroscopy (STM and STS) [13, 17] and angle-resolved photoemission spectroscopy (ARPES) [18, 21] have made significant progress in the studies of PG phenomena in high-$T_c$ cuprates and other materials. Progressive investigations of tunneling and ARPES spectra have provided important information on single-particle excitation gaps in the cuprates. The STM and STS techniques are very sensitive to the quasiparticle density of states (DOS), with the unique capability to measure any excitation gaps at the Fermi energy, and to the electronic (or gap) inhomogeneities that are intrinsic to the cuprates [13, 17, 22, 24]. These tunneling studies of the cuprate superconductors have revealed a rich variety of tunneling spectra (differential conductance-voltage ($dI/dV - V$) characteristics) of high-$T_c$ cuprate superconductor (HTSC)-insulator (I)-normal metal (N) (called SIN) junctions. Two distinctive features of the $dI/dV$ spectra are: (i) asymmetric conductance peaks [24, 30], (ii) dip-hump structures appearing outside the conductance peak on the negative bias side [13, 27, 28, 30], (iii) suppression of the peak on the negative bias side with increasing temperature and its vanishing somewhat below $T_c$ or near $T_c$, leaving the hump feature (i.e., linearly increasing conductance) and the second conductance peak (on the positive bias side) [13, 27, 28], and (iv) shoulders inside the conductance peaks [22, 24]. Similar peak-dip-hump feature and its persistence above $T_c$ were also observed in ARPES spectra [18, 31].

The unusual features of the tunneling spectra of high-$T_c$ cuprates are neither expected within the simple s-wave BCS model nor within the BCS models based on the d-wave gap symmetry. For example, the tunneling spectra showing more flatter, BCS-like feature is difficult to reproduce in the d-wave model. While the other type of tunneling spectra showing more V-shaped feature might be expected either within the d-wave gap model (which fails to reproduce quantitatively the conductance peak height and shape [13, 15, 24]) or within the s-wave multi-gap model proposed in the present work. The origins of the peak-dip-hump feature and the asymmetry of the conductance peaks have also been the subject of controversy. These features of the tunneling spectra have been attributed either to extrinsic (band-structure) effects (i.e., the van Hove singularity and bilayer splitting) [32, 33] or to intrinsic effects such as particle-hole asymmetry [34, 35] and strong coupling effects (which originate from the coupling to a phonon mode [36] or to a collective electronic mode [37]). Although several theoretical models were successful in reproducing some tunneling...
spectra with the peak-dip-hump features and asymmetric or nearly symmetric peaks observed in cuprates, the well-established experimental tunneling spectra with different peak-dip-hump features \[13, 15\] (e.g., high-bias conductances, which are nearly flat, linearly increasing at negative bias or decreasing at positive bias, temperature- and doping-dependent peaks, dip-hump features and asymmetry of the conductance peaks) characteristic of high-$T_c$ cuprates were not explained yet. The quantitative fits of the experimental spectra of Ba$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ (Bi-2212) to a BCS d-wave gap and a T-independent gap functions \[15\] have been unsuccessful in reproducing the asymmetry (which is opposite to that of the observed tunneling spectra) and the temperature-dependent conductance curves. For underdoped Bi-2212, the asymmetry of the conductance peaks and its doping dependence found in Ref. \[30\] are also inconsistent (i.e., in contrast) with other experimental data \[15, 27, 28\]. Further, STM and STS studies have shown that the electronic system \(\text{Bi-2212}\) is inhomogeneous and the gap distribution (i.e., inhomogeneity) has a strong effect on the tunneling spectra \[22, 24, 37\]. It is necessary for any theoretical model to explain not only the asymmetry and peak-dip-hump features in tunneling conductance but also their evolution with temperature and doping, a flat (i.e., U-shaped) and more V-shaped subgap conductances, the gap-inhomogeneity-induced shoulders inside the conductance peaks that are observed recently by STM in tunneling spectra of Bi-2212 \[23, 24\].

In this paper, we propose a simple and quite effective model of quasiparticle tunneling based on the different mechanisms for tunneling of charge carriers across the SIN junction at negative and positive biases and the multi-gap (i.e., gap inhomogeneity) picture. The proposed model reproduces the well-established experimental tunneling spectra of high-$T_c$ cuprates and their nearly U and V-shaped features, asymmetry, peak-dip-hump structure and shoulder-like features inside the conductance peaks. We focus on the Bi-2212 system (which has been well studied experimentally) and show that the main experimental features of the tunneling spectra and their temperature and doping dependences can be well reproduced by using a BCS DOS at positive bias voltages ($V > 0$) and the combined BCS DOS and quasi-free-state DOS (originating from the dissociation of large polarons) at negative bias voltages ($V < 0$), and taking into account the distribution of BCS and polaronic gap values. There is now ample reason to believe that the electron-phonon interaction in cuprates is strong enough and the relevant charge carriers in these systems are large polarons \[3, 8, 39\]. Therefore, the precursor Cooper pairing of large polarons may occur above $T_c$ with opening the energy gap $\Delta$ in their excitation spectrum \[13, 15\]. As argued in Ref. \[40\], the binding energies of large polarons $\Delta_p$ and Cooper-like large polaron pairs are manifested as the two distinct non-SC gaps in high-$T_c$ cuprates, one a temperature independent PG and the other a BCS-like gap. Two gap-like features observed in ARPES and tunneling experiments are often misinterpreted as the coexisting PG and SC gap.

**Unconventional SIN tunneling.** — We consider the model which describes two specific mechanisms for quasiparticle tunneling across the SIN junction at $V < 0$ and $V > 0$, and explains the asymmetry of the tunneling current taking into account the different tunneling DOS existing in these cases. The first mechanism describes the $S \rightarrow N$ tunneling processes associated with the dissociation of Cooper-like polaron pairs and large polarons at $V < 0$. In this case the Cooper pair dissociates into an electron in a normal metal and a polaron in a polaron band of the HTSC. This $S \rightarrow N$ tunneling is allowed only at $|eV| > \Delta$. The dissociation of large polaron occurs at $|eV| > \Delta_p$ and the carrier released from the polaron potential well can tunnel from the quasi-free state into the free states of the normal metal. Such a $S \rightarrow N$ transition gives an additional contribution to the tunneling current. The other mechanism describes the electron tunneling from the normal metal to the BCS-like quasi-particle states in HTSC at $V > 0$, while the quasi-free states appearing only at the polaron dissociation are absent. Therefore, at $V > 0$ the tunneling current across SIN junction is proportional to the BCS DOS of HTSC given by

\[
D_{BCS}(E, \Delta) = \begin{cases} 
D(\varepsilon_F) \frac{|E|}{\sqrt{|E|^2 - \Delta^2}} & \text{for } |E| > \Delta, \\ 
0 & \text{for } |E| < \Delta.
\end{cases}
\]

where $D(\varepsilon_F) = m_p^{3/2} \varepsilon_F / \sqrt{2\pi} \hbar^3$ is the normal state DOS, $m_p$ and $\varepsilon_F$ are the mass and Fermi energy of large polarons.

In the case $V < 0$, the total current is the sum of two tunneling currents and proportional to the square of the tunneling matrix element, $|M|^2$ \[11\], the $D_{BCS}(E, \Delta)$ and the quasi-free state DOS. This current flows from HTSC to normal metal at the dissociation of Cooper pairs and large polarons. In HTSC, the quasi-free carriers appearing at the dissociation of large polarons have the effective mass $m^*$ and energy $E = \Delta_p + \hbar^2 k^2 / 2m^*$. Then the quasi-free state DOS is defined as

\[
D_f(E, \Delta_p) = \begin{cases} 
D(\varepsilon_F) \sqrt{|E| - \Delta_p}/|\varepsilon_F| & \text{for } |E| > \Delta_p, \\ 
0 & \text{for } |E| < \Delta_p,
\end{cases}
\]

where $\varepsilon_F$ is the Fermi energy of quasi-free carriers, $D(\varepsilon_F) = (m^*)^{3/2} \sqrt{\varepsilon_F} / \sqrt{2\pi} \hbar^3$. For the normal metal, the DOS at the Fermi energy $E_F$ is independent of energy $E$, i.e., $D(E) \approx D(E_F)$. Thus, at $V > 0$ the tunneling current from the normal metal to HTSC is

\[
I_{N \rightarrow S}(V) = C |M|^2 D(E_F) D(\varepsilon_F) \\
\times \int_{-\infty}^{+\infty} \frac{|E + eV|}{\sqrt{(E + eV)^2 - \Delta^2}} [f(E) - f(E + eV)] dE \\
= \frac{G}{e} \int_{-\infty}^{+\infty} \frac{|\varepsilon|}{\sqrt{\varepsilon^2 - \Delta^2}} [f(\varepsilon - eV) - f(\varepsilon)] d\varepsilon,
\]

(3)
\[ dI_{N \rightarrow S}/dV = G(A_1(\Delta_T, a_V) + A_2(\Delta_T, a_V)), \]

where

\[ A_1(\Delta_T, a_V) = \int_{-\infty}^{+\infty} \frac{x \exp[-x - a_V]}{\sqrt{x^2 - \Delta_T^2}(\exp[-x - a_V] + 1)^2}, \]

\[ A_2(\Delta_T, a_V) = \int_{-\infty}^{+\infty} \frac{x \exp[x - a_V]}{\sqrt{x^2 - \Delta_T^2}(\exp[x - a_V] + 1)^2}, \]

\[ x = \varepsilon/k_BT, \quad a_V = eV/k_BT. \] At negative bias voltages \( V < 0 \), the tunneling current and differential conductance are given by

\[ I_{S \rightarrow N} = \frac{G}{e} \left\{ \int_{-\infty}^{+\infty} |\varepsilon|d\varepsilon [f(\varepsilon) - f(\varepsilon + eV)] \right\}, \]

\[ + \frac{D(\varepsilon_F')}{D(\varepsilon_F)\sqrt{\varepsilon_F'}} \int_{-\infty}^{+\infty} |\varepsilon| - \Delta_p \left[ f(\varepsilon) - f(\varepsilon + eV) \right]d\varepsilon \right\}, \]

and

\[ \frac{dI_{S \rightarrow N}}{dV} = \frac{G}{e} \left\{ A_1(\Delta_T, -a_V) + A_2(\Delta_T, -a_V) \right\} \]

\[ + a_F(T) \left\{ B_1(\Delta_p^*, a_V) + B_2(\Delta_p^*, a_V) \right\}, \]

where \( \varepsilon = E - eV, \)

\[ B_1(\Delta_p^*, a_V) = \int_{-\Delta_p^*}^{+\infty} \sqrt{|x| - \Delta_p^*} \frac{\exp[x + a_V]}{\exp[x + a_V] + 1} \]

\[ B_2(\Delta_p^*, a_V) = \int_{-\Delta_p^*}^{+\infty} \sqrt{|x| - \Delta_p^*} \frac{\exp[-x + a_V]}{\exp[-x + a_V] + 1} \]

\[ a_F(T) = [D(\varepsilon_F')/D(\varepsilon_F)]\sqrt{k_BT/\varepsilon_F}, \quad \Delta_p^* = \Delta_p/k_BT. \]

The SIN tunneling conductance curve calculated at \( T=30K \) for the single-gap case (concerning both the polaronic gap \( \Delta_p \) and the s-wave BCS gap \( \Delta \)) is shown in Fig.1(main panel). In this simple model, the absence of gap distribution would lead to the U-shaped spectral behavior at low bias and such a more flatter subgap conductance would be expected for homogeneous high-\( T_c \) cuprates. As can be seen in Fig.1, there are dip-hump feature and asymmetric peaks, with the higher peak in the negative bias voltage. The model is compared with one of the best tunneling spectra measured at \( T \approx 4.8K \) in Bi-2212 \(^{13}\), as shown in the inset of Fig.1.

Multi-gap model. – One can expect that the electronic inhomogeneity in HTSC may produce regions with a distribution of gap amplitudes (\( \Delta(i) \) and \( \Delta_p(i) \)) and variation in the local DOS. Recent STM and STS experiments on Bi-2212 and other high-\( T_c \) systems indicate that the gap inhomogeneities commonly exist in these materials regardless of doping level \(^{22,24,37}\). Therefore, in order to reproduce the main features of the tunneling spectra of high-\( T_c \) cuprates, we have to consider the multi-gap case and the multi-channel tunneling processes, which contribute to the total tunneling current. At positive bias voltages \( V > 0 \), the tunneling of electrons from the normal metal into many regions of HTSC with different BCS DOS takes place and the resulting conductance is

\[ \frac{dI_{N \rightarrow S}}{dV} = \sum_{i} G_i [A_1(\Delta_T(i), a_V) + A_2(\Delta_T(i), a_V)]. \]
In the case $V < 0$, the total current is the sum of tunneling currents from many areas of HTSC with different local DOS ($D_{BCS}(E, \Delta(i))$ and $D_f(E, \Delta_p(i))$) to the normal metal. Then the resulting conductance is

$$\frac{dI_{S\rightarrow N}}{dV} = \sum_1 G_1(A_1, (\Delta_T(i), -aV)) + A_2(\Delta_T(i), -aV) + aF(T)[B_1(\Delta_p(i), aV) + B_2(\Delta_p(i), aV)]. \tag{8}$$

In such a multi-gap model, the tunneling spectra exhibit a more V-shaped behavior at low bias, the peak-dip-hump feature at negative bias and the asymmetry of the conductance peaks. With increasing temperature, the dip and peak on the negative bias side gradually disappear (see Fig.2a), leaving the hump feature and the second conductance peak (on the positive bias side), as observed in tunneling experiments \[15\]. Figure 2b shows that the conductance peaks become more asymmetric with increasing doping, as seen in experiments \[27,28\].

Comparison with the experiment. -The parameters entering into Eqs. 7 and 8 can be varied to fit experimental data. The comparison of the theoretical results with the different experimental data on underdoped, slightly underdoped and overdoped Bi-2212 is presented in Fig.3.

We obtained the best fits to the experimental spectra by taking only two or three terms in Eqs. (7) and (8). In this way, we succeeded in fitting almost all of experimental conductance curves by taking different gap values. The way, we succeeded in fitting almost all of experimental conductance curves by taking different gap values. The comparison of the theoretical results with the different experimental data on underdoped, slightly underdoped and overdoped Bi-2212 is presented in Fig.3. Further, the conductance curve calculated using the multi-gap model (inset in Fig.4) is similar to that in Fig.1c of Ref. [24] measured on inhomogeneous Bi-2212.

We now discuss the relation between the BCS tunneling gap and the SC order parameter. The unusually large reduced-gap values $2\Delta/k_BT_c \approx 7 - 22$ observed in Bi-2212 \[13\] compared to the BCS value 3.52 give evidence that the BCS gap determined by tunneling and ARPES measurements does not close at $T_c$ and it is not related to the SC order parameter. While the peak suppression on the negative bias side near $T_c$ observed in Bi-2212 is due to a spectral superposition of the tunneling conductances associated with the BCS DOS and quasi-free state DOS (originating from the polaron dissociation). The persistence of the conductance peak on the positive bias side well above $T_c$ is evidence for the opening of a non-SC BCS gap at $\varepsilon_F$ (for which the ratio $2\Delta/k_BT^*$ remains constant and close to the value 3.52 \[2,3\]). The preformed Cooper pairs condense into a SF Bose-liquid state at $T_c$ (at which the SC order parameter appears) and the BCS pairing gap persists as the non-SC gap both below $T_c$ and above $T_c$ \[1,2\]. The optical measurements (including tunneling spectroscopy and ARPES) are mainly sensitive to the excitation gaps at $\varepsilon_F$, but such experimental probes compared with the thermodynamic methods \[42,43\] and the methods of critical magnetic field \[44\] and current \[45\] measurements are insensitive to the identification of the SC order parameter as the SF condensation energy or as the energy needed for destruction of a SF Bose-condensate (see also Refs. \[1,2,46\]).

![FIG. 3: Main panel: SIN tunneling spectrum measured on overdoped Bi-2212 at 43.1 K fitted by using two-gap model, with $\Delta=31$ and 18 meV; $\Delta_p=22$ and 15 meV. Left inset: fits of SIN tunneling spectra measured on underdoped Bi-2212 by using three-gap model, with $\Delta_p=44$, 28 and 20 meV and the set of gap values $\Delta=38$, 26 and 17 meV for 46.4 K, $\Delta=37$, 25 and 16 meV for 63.3 K and $\Delta=36$, 24 and 15 meV for 76 K. Right inset: fit of SIN tunneling spectrum measured on slightly underdoped Bi-2212 at 50 K by using three gap model, with $\Delta=36$, 24 and 15 meV; $\Delta_p=56$, 50 and 39 meV.](image1)

![FIG. 4: Comparison of the tunneling conductance data on inhomogeneous Bi-2212 (dashed line) with the tunneling conductance calculated at 30 K (main panel) using the multi-gap model ($\Delta=52$, 45, 36, 27, 19 and 12 meV; $\Delta_p=78$, 65, 47, 34, 23 and 15 meV). Inset represents the conductance curve with pronounced shoulder-like feature, calculated at 30 K using the multi-gap model ($\Delta=59$, 43, 34, 25 and 16 meV; $\Delta_p=64$, 52, 44, 28 and 18 meV).](image2)
Conclusion. – We have proposed a model describing the distinctive mechanisms of quasiparticle tunneling across the SIN junction at negative and positive biases. The model incorporating effects of the BCS DOS and quasi-free state DOS (appearing at the polaron dissociation) at negative bias, and the gap inhomogeneity (i.e., multi-gap effects) reproduces the nearly U- and V-shaped and shoulder-like subgap features, peak-dip-hump structure and asymmetry of the conductance peaks and their evolution with temperature and doping as seen in tunneling spectra of Bi-2212. In this model, many unusual features of the tunneling spectra observed in Bi-2212 on the negative bias side arise from the spectral superposition of the tunneling conductances associated with the BCS DOS, quasi-free state DOS and multi-channel tunneling.

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Abstract
