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Modeling study of the dip-hump feature in $Bi_2Sr_2CaCu_2O_{8+\delta}$ tunneling spectroscopy

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The tunneling spectra of high-temperature superconductors on $Bi_2Sr_2CaCu_2O_{8+\delta}$ (Bi-2212) reproducibly show a high-bias structure in the form of a dip-hump at voltages higher than the gap voltage. Of central concern is whether this feature originates from the normal state background or is intrinsic to the superconducting mechanism. We address this issue by generating a set of model conductance curves—a "normal state" conductance that takes into account effects such as the band structure and a possible pseudogap, and a pure superconducting state conductance. When combined, the result shows that the dip-hump feature present in the experimental conductance curves cannot be naively attributed to a normal state effect. In particular, strong dip features found in superconductor-insulator-superconductor data on optimally doped Bi-2212, including negative dI/dV, cannot be a consequence of an extrinsic pseudogap. However, such features can easily arise from state-conserving deviations in the superconducting density of states, e.g., from strong-coupling effects.

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Tunneling spectroscopy of conventional superconductors produces a direct, high-resolution measurement of the quasiparticle density of states (DOS). The fine structures seen in such measurements have been linked directly to the superconducting mechanism in the conventional superconductors.[1] The same technique has also been applied to high-T_c superconductors (HTSs). Among HTS cuprates, $Bi_2Sr_2CaCu_2O_{8+\delta}$ (Bi-2212) is one of the most extensively studied by tunneling and other surface-sensitive experiments. This is due to the ability to easily cleave the single crystals along the *a-b* plane as well as the possibility of obtaining large single crystals with various doping concentrations.

Unfortunately, the sheer diversity of tunneling spectra from tunneling measurements have led to a variety of interpretations of the spectral features. One example is the debate on the nature of a dip-hump structure observed in the tunneling spectra. The dip is a strong deviation from tunneling conductance beyond the quasiparticle peak, which is followed by a hump first observed in 1989.[2] There are two schools of thought on the origin of this structure. The first is that, similar to what has been learned from conventional superconductors, this feature is intrinsic to the superconducting mechanism and is analogous to the phonon fine structure.[3] Thus, a thorough analysis of tunneling spectra including this feature should produce the necessary parameters in unveiling the nature of superconductivity in HTSs. The other argument points to the idea that the dip-hump feature is simply a normal state or background effect independent of the superconducting mechanism. The explanations range from the hump being the remnant of the Van Hove singularity to the dip as being due to the presence of the pseudogap.[4–6] This means that the hump is the pseudogap peak while the dip is simply the "valley" between the pseudogap peak and the superconducting peak. Under this assumption, the dip-hump feature is a distraction from the intrinsic superconducting properties and can be normalized away from the tunneling conductance.

We will address this last point by generating a model conductance curve that includes the normal state features and show that these normal state effects are insufficient in reproducing the salient characteristics of the dip-hump structure, especially the very strong dip feature found in break junctions. In this study, the presented tunneling conductance of break junctions in Bi-2212 is an extreme case that shows even negative tunneling conductance in the dip voltage. We show using a simple model of strong-coupling effects that such strong dips are easily obtained. Moreover, using neutron scattering data, a model is also suggested by Eschrig and Norman[7] which can produce negative tunneling conductance in the dips of superconductor-insulator-superconductor (SIS) junctions. This strongly suggests that the dip structure in the tunneling conductance spectra has a superconducting origin, and is likely tied to the mechanism of pairing.

We review and consider tunnel junctions that have been fabricated on Bi-2212, using scanning tunneling microscopy and spectroscopy, point contact, break junctions, and fully intercalated intrinsic *c*-axis junctions.[5,8–10] Since SIS data enhance spectral features, we have focused specifically on break junction experiments in this study. We do not include intrinsic Josephson junctions because they are severely affected by Joule heating.[11] For such junctions, the intercalation of Bi-2212 with $HgBr_2$ increases the barrier thickness between the CuO_2 layers and reduces the heating caused by overinjection.[12] Only then are the dip and hump features recovered in the intrinsic density of states.

The main features commonly observed in the tunneling conductance spectra of break junctions are (i) energy gap at voltages $\pm 2\Delta/e$ with Δ ranging from as low as 10 meV for highly overdoped to as high as 60 meV for highly underdoped samples and (ii) high-bias structures in the form of dips and humps at voltages higher than $\pm 2\Delta/e$. The strong dependence of the magnitude of the energy gap on doping concentration is well known.[13] For optimally doped samples of Bi-2212, the value of the energy gap is now understood to be about 37 meV. The overall shape of tunneling spectra is also very reproducible, and for this reason Bi-2212 is a good candidate to understand the mechanism of superconductivity in the cuprates.

The reproducible presence of the dip-hump just above the gap feature has been observed not only in Bi-2212, but also in $Tl_2Ba_2CuO_{6+\delta}$ (Ref. 14) and $(Cu,C)Ba_2Ca_3Cu_4O_{12+\delta}$ cuprates.[15] In SIS junctions, the dip appears at a voltage $(2\Delta+\Omega)/e$, where the mode energy Ω is proportional to T_c.[16] Arguments have been made that this dip-hump structure is purely nonsuperconducting in nature.[17] It is the result of the presence of two energy gaps in the total DOS, one from the superconducting gap in the superconducting DOS, and the other from the pseudogap, which is present even above T_c, and thus, is considered as part of the normal state DOS effect. It has been argued that the product of these two DOSs should produce the identical dip-hump structure seen in the tunneling conductance. If this is true, then in principle one can normalize the conductance data to obtain the pure superconducting DOS, a practice that has been successfully employed for conventional superconductors. The focus of this paper is to investigate this claim. We do this by generating model conductance data that are a product of a “pure” superconducting DOS having the superconducting energy gap and quasiparticle peaks, and a purely normal state DOS incorporating the band structure and an extrinsic pseudogap.

In principle, at zero temperature, the tunneling conductance from a superconductor-insulator-normal metal (SIN) junction gives a direct measure of the DOS.[1] In conventional superconductors, a normalization procedure of the tunneling conductance removes the normal state effects. What is left behind is essentially the superconducting DOS that has been shown to match the BCS DOS. Therefore, to generate our model conductance for comparison with the experimental SIN tunneling conductance, we need to generate two separate components, the normal state DOS and the superconducting DOS. The normal state DOS is obtained from the momentum-averaged single-particle Green’s function, i.e., $N(E)=\frac{1}{\pi}\Sigma_k \mathrm{Im}G(k,E)$. Our model incorporates several important parameters: (i) a realistic band structure for the CuO_2 plane that is derived from angle-resolved photoemission spectroscopy measurement on Bi-2212;[18] and (ii) a d-wave pseudogap order parameter $\Delta_p(k)=\Delta_p[\cos(k_x a)-\cos(k_y a)]/2$ to include the presence of any normal state gap (pseudogap). The pseudogap is modeled by introducing a very large scattering rate $\Gamma_p \sim \Delta_p$. The model is described in detail in Ref. 19. In this work, we assume that the tunneling matrix is constant. The superconducting DOS is obtained from the model used by Won and Maki,[20]

$$\sigma(E)=\mathrm{Re}\left(\frac{E-i\Gamma_s}{\sqrt{(E-i\Gamma_s)^2-\Delta_s(k)^2}}\right) \quad (1)$$

with $\Delta(k)=\Delta\cos(2\phi)$, i.e., having the same symmetry as the d-wave gap with ϕ measured from the Cu-O bonding direction in the a-b plane. Here, Γ_s is the lifetime broadening term for superconducting quasiparticles and is assumed small, $\Gamma_s \ll \Delta_s$. To account for the anisotropic band structure in the cuprate layer, a small directionality factor has been included to the superconducting DOS,[10] which provides a better fit of the subgap region of high-quality scanning tunneling microscopy data.[21]

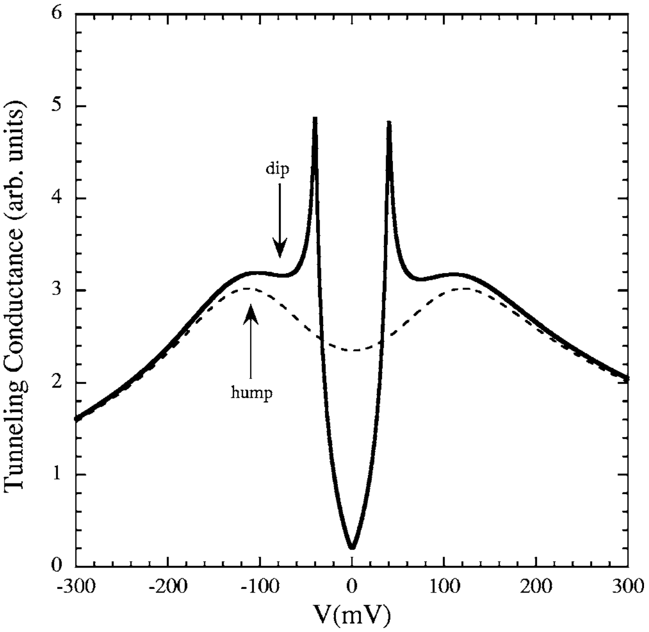

FIG. 1. Dashed line: normal state DOS generated using $\Delta_p=120$ meV and $\Gamma_p=90$ meV. Solid line: the model tunneling DOS using the normal state DOS and superconducting DOS (Won and Maki model).

A “normal state” DOS has been generated with $\Gamma_p=90$ meV and a d-wave pseudogap magnitude $\Delta_p=120$ meV as shown by the dashed line in Fig. 1. These parameters give a qualitative agreement to the estimated background conductance from a SIN data at high positive bias. It reproduces the often seen weakly decreasing background in most SIN spectra. The pseudogap also broadens the Van Hove singularity found in the negative bias side of the DOS, making it undetectable. Next, a superconducting d-wave DOS has then been generated using Eq. (1) with $\Delta_s=30$ meV, $\Gamma_s=1.5$ meV. These parameters were chosen to reproduce the typical SIN data in the gap region, which include the shape of the tunneling gap and the quasiparticle peaks often seen in the experimental data.[10,14,16,21]

The product of normal state DOS and superconducting DOS produces the tunneling DOS, which is shown as the solid curve in Fig. 1. This model tunneling conductance appears to have the generic features of typical SIN data, including the dip-hump structure. We proceed a step further by using the model conductance to generate a SIS conductance. This is shown in Fig. 2 along with the convoluted background conductance. The most important observation of the model SIS curve is that, even though the dip-hump feature is more pronounced, the minimum of the dip is never below the background value. This is a crucial outcome of the model that incorporates the pseudogap as part of the normal state background, and is contradictory to temperature-dependent tunneling studies,[5,13] which clearly show that the dip minimum is far below the normal state conductance.

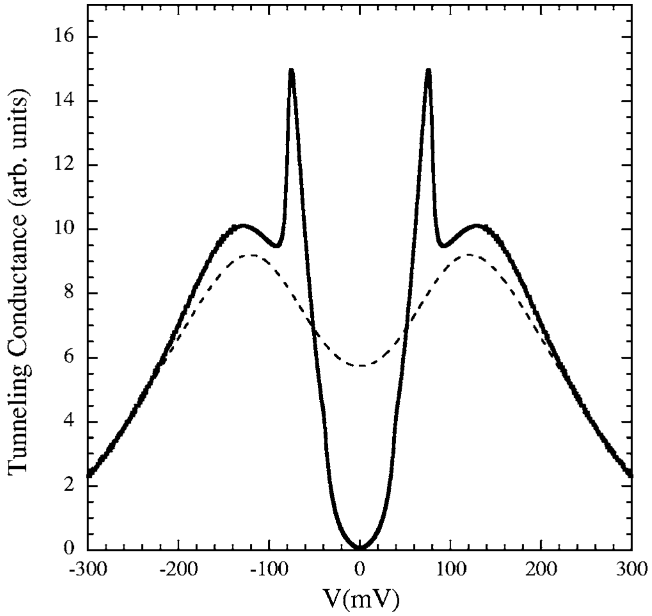

FIG. 2. SIS tunneling DOS generated by convoluting the model DOS from Fig. 1 with itself.

We demonstrate the significant discrepancy between the model SIS curve of Fig. 2 and the two experimental SIS data curves shown in Fig. 3.[13] The two curves are from two different optimally doped Bi-2212 crystals obtained at 4.2 K. Josephson current peaks have been deleted for clarity. Both experimental data presented here are the extreme cases where the dip minima are close to zero. In fact, the lower SIS curve even shows negative conductance values for the dip minima. Such features cannot be found from the model conductance curve. We conclude that attributing the dip as simply the valley between an extrinsic pseudogap peak and the superconducting peak is incompatible with experimental observations.

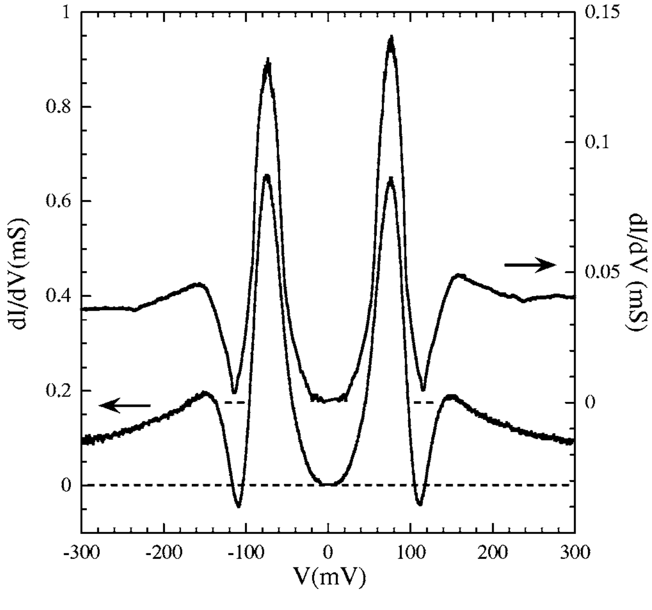

FIG. 3. Experimental SIS tunneling data of optimally doped Bi-2212 at 4.2 K. Note the severe drop of the dip amplitude, even reaching negative values.

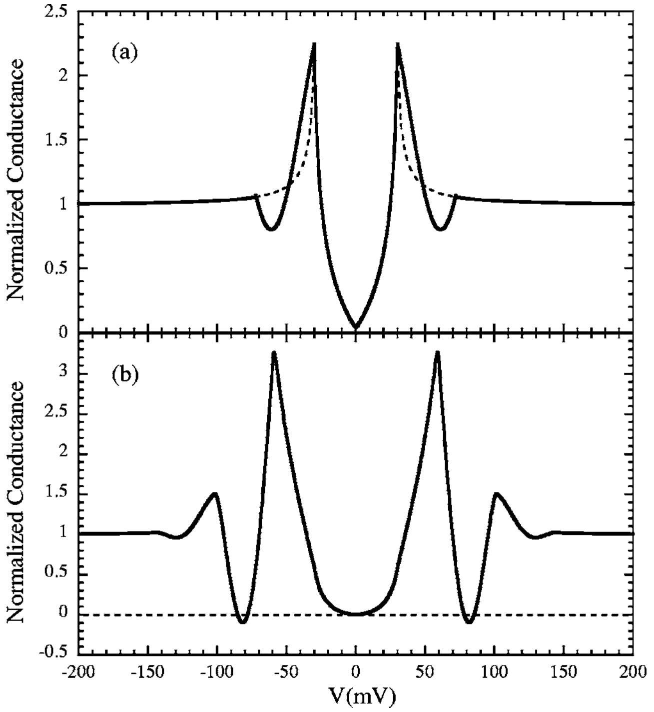

FIG. 4. (a) The dip is introduced as a removal of states from the model superconducting DOS (solid line). The dashed line is the *d*-wave model without the dip. (b) Self-convolution produces the model SIS DOS. It has the identical feature of the dip-hump seen in the experimental data of Fig. 3.

On the other hand, if the dip is incorporated into the superconducting DOS in a similar manner as the phonon structure seen in the tunneling conductance of a conventional superconductor,[3] then all aspects of the experimental dip-hump feature can be reproduced. Figure 4(a) shows the dip as a removal of states from the unperturbed (dashed curve) BCS superconducting DOS. To conserve states, an excess or pile-up of states is placed near the gap edge. This was obtained by multiplying the *d*-wave DOS by one wavelength of a sine function, which guaranteed that the number of states would be conserved. The resulting model DOS was then convoluted to again generate the model SIS tunneling conductance. As shown in Fig. 4(b), the dip minimum is significantly enhanced and even reaches negative values. The dip clearly extends below the background in contrast to the model conductance of Fig. 1. This produces a better agreement with the experimental observations of Fig. 3.

The dip-hump feature observed in tunneling conductance experiments cannot be accurately attributed to normal state effects of an extrinsic pseudogap. The model conductance incorporating such normal state effects, while producing a dip-hump structure, cannot accurately reproduce the important characteristics of this structure, especially in the SIS tunneling spectra. In particular, the pseudogap model shows that the dip minimum always lies above the normal state conductance, a feature that is contradicted by several experiments. More importantly, the model can never produce a negative dynamic conductance, an effect which has been observed experimentally. On the other hand, a dip which drops below the normal state and produces a negative dI/dV is easily reproduced and understood within the framework of a state-conserving deviation from a BCS DOS, as is found with strong-coupling effects.

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