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Analysis of the pseudogap-related structure in tunneling spectra of superconducting $Bi_2Sr_2CaCu_2O_{8+\delta}$ revealed by the break-junction technique

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The tunnel conductance $G(V)$ for break junctions made of single-crystal as-grown $Bi_2Sr_2CaCu_2O_{8+\delta}$ samples with $T_c \approx 86-89$ K were measured and clear-cut dip-hump structures (DHSs) were found in the range 80–120 mV of the bias voltage V. A theory of tunneling in symmetrical junctions between inhomogeneous charge-density-wave (CDW) superconductors, considered in the framework of the s-pairing model, has been developed. CDWs have been shown to be responsible for the appearance of the DHS in the tunnel current-voltage characteristics and properly describe the experimental results.

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Tunneling spectra of superconductor-insulator-superconductor (SIS) structures constitute a rich source of information concerning electronic properties of their electrode materials, which has been evident starting from the famous studies of Giaever, McMillan, and Rowell and up to recent investigations of unconventional materials.[1,2] In particular, tunneling studies of high-T_c oxides reveal predominant $d_{x^2-y^2}$ -wave or extended s-wave (V-shaped) forms of the voltage V dependences of the quasiparticle conductance $G \equiv dJ/dV$ in the vicinity of the $V=0$ point,[3–5] with an anomalously large—in comparison with the characteristic value of the Bardeen-Cooper-Schrieffer (BCS) theory—ratio between the energy gap amplitude Δ and the critical temperature of the superconducting transition, T_c.[6] Here, J is the quasiparticle tunneling current.

On the other hand, tunneling spectra of cuprates have extra peculiarities, such as dip-hump structures (DHSs),[2] a pseudogap- (PG-) like depletion[7] of the electron density of states (DOS), and smaller-scale series of $G(V)$ ripples.[8] Their nature still remains a point of issue. In any case, additional features of the current-voltage characteristics (CVCs) might either be somehow linked to superconductivity[9] or comprise manifestations of totally different phenomena.[10–15] The final solution of the global problem concerning the origin of the PG can be expected only from phase-sensitive experiments,[4] also extremely important to distinguish between various superconducting order parameter symmetries.[16]

It should be noted that DHSs and PGs are observed both for superconductor-insulator-normal metal[2,7] (SIN) and SIS junctions. Nevertheless, additional problems of the overall CVC asymmetry[6,17,18] and the preferential DHS appearance in one polarity branch of $G(V)$ are typical of the former.[2,6] Those difficulties can be avoided for SIS break junctions, symmetrical by definition, if not for the symmetry-breaking phenomenon appropriate to superconductors with charge-density waves (CDWs).[11,14] In addition, such junctions are a more sensitive tool to probe the gap-edge structures, because in this case the CVCs involve a convolution of DOSs from both sides of the junction barrier.[1,2] The break-junction technique[19] is especially suitable to study tunneling in entirely high-T_c-based sandwiches with emphasis on the very nature of PGs and DHSs rather than on the accompanying symmetry violation. The measurements are carried out *in situ*, so that clean and fresh interfaces are studied. Therefore, we have carried out experimental research using break junctions of $Bi_2Sr_2CaCu_2O_{8+\delta}$ (BSCCO) together with theoretical investigations based on the concept of the Fermi surface (FS) partial CDW gapping.[13,14,20,21] The tunnel conductance $G(V)$ was obtained using the four-probe, ac modulation technique.[22] It is important to stress that our theoretical calculations take into account the inherent electronic inhomogeneity of the cuprate superconductors.[6,17,18,23,24] Hence, all superconducting and CDW characteristics are averaged over certain distributions.[12,25]

Single-crystal samples of BSCCO were grown by a standard flux method in the 1 atm air environment. Resistively found T_c values were in the range 86–89 K. Differential CVCs were measured by the modulation method. A typical experimental dependence for an as-grown slightly overdoped crystal at the temperature $T=4.2$ K is shown in Fig. 1. The presented CVC pattern for this highly symmetric junction undoubtedly demonstrates the availability of a nonsymmetric contribution of unknown nature and magnitude, although the nonsymmetry is much less than in the case of truly nonsymmetric junctions.[2,7,18,23,26] One can see well-developed dip-hump structures beyond the coherent superconducting peaks. The unusually strong DHS cannot be associated with conventional strong electron-phonon coupling typical of low-T superconductors.[27] On the other hand, the basic version of the DHS description by a very strong electron coupling to an extremely narrow boson spectrum[2,28] results in a symmetric CVC, although the observed DHS $G(V)$ features appear mostly at one voltage polarity for SIN junctions.[6,7] Thus the strong-coupling approach *per se* cannot describe a certain body of experimental data. One could improve the situation by additionally assuming the existence of a strong Van Hove singularity,[29] but coupling to a resonance mode becomes then at least superfluous, since the Van Hove scenario (related to ours) alone might be responsible for the DHS.[30]

In contrast to the approaches discussed, we propose to fit

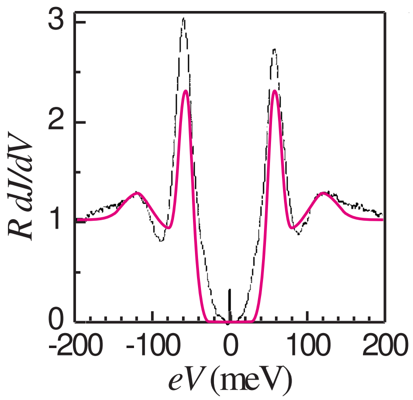

FIG. 1. (Color online) Points denote a normalized experimental curve of the differential conductance $G=dJ/dV$ for a BSCCO break junction measured at $T=4.2$ K, where J is the quasiparticle tunnel current and V the bias voltage across the junction, versus the eV value, where e is the elementary charge. The amplitude of voltage modulation δV for calculating G was 1 meV. A solid curve corresponds to the calculated eV dependence of the dimensionless differential conductance RG of a tunnel junction between two identical inhomogeneous charge-density-wave superconductors. Here, R is the resistance of the junction in the normal state. The parameters of the CDW superconductors are $\Delta_0=30\pm15$ meV, $\Sigma_0=90\pm35$ meV, the Fermi surface CDW gapping parameter $\mu=0.08$, and the temperature $T=4.2$ K. The interval of numerical differentiation $\delta V=1$ meV.

the found dependence with a theoretical curve calculated on the basis of two assumptions; namely, (i) we consider the DHSs as remnants of the smeared peaks due to the CDW (PG) gapping, and (ii) there are no fixed values of the superconducting, Δ, and dielectric (CDW), Σ, gaps, because all BSCCO samples, whatever their quality, turn out to be intrinsically inhomogeneous. The second assumption is a well-established experimental fact,[6,17,18,23,24] whereas the first one is a plausible hypothesis[14] resting upon the observations of regular domains with stripe order[31] and the analysis of the dissimilarities between genuine superconducting phenomena and PG manifestations.[11,13–15,32,33]

In our self-consistent approach,[21] which is an extension of the Bilbro-McMillan model,[20] the quasiparticle tunnel current J between two electronically homogeneous partially CDW-gapped superconductors (CDWSs) is a sum of several terms, $J(V)=\Sigma_i J_i(V)$, each combining two FS sections from different electrodes across the barrier and making allowance for the existence of the CDW-pairing Green's function (see details in Refs. 11, 12, and 14). The input parameters of the problem include "bare" zero-T energy gaps Δ_0 and Σ_0 related to superconducting (Cooper) and CDW (electron-hole) s-wave pairings, respectively, appropriate to hypothetical cases where either of the competing interactions is switched off. The portion of the CDW-distorted FS is described by the dielectric gapping degree parameter $0<\mu<1$. At $T\neq0$, each ith electrode is characterized by two gaps S_i [$\Delta_i(T)$ and $D_i(T)=\sqrt{\Sigma_i^2+\Delta_i^2}>\Delta_i(T)$]. Planck's constant $\hbar$ and the Boltzmann constant k_B amount to unity. In particular, the position of the larger gap, $D_i(T)$, is governed, besides the temperature, by the parameter Σ_0, and that of the smaller one, $\Delta_i(T)$, by all three parameters Δ_0, Σ_0, and μ. The CVC singularities are observed at bias voltages equal to linear combinations $S_1\pm S_2$. Examples of theoretical CVCs for CDWS-I-CDWS junctions with homogeneous electrodes can be found elsewhere.[14] The difference between the results of our pairing model and those of a true pairing state in high-T_c oxides, which has not yet been ultimately identified,[2–5,7] can be substantial only in the voltage range $eV<\Delta_1(T)+\Delta_2(T)$. Here, $e>0$ is the elementary charge.

In the case of inhomogeneous electrodes, the spread δx of each of the electrode parameters $x=(\Delta_0,\Sigma_0,\mu)$ results in a smearing, to a certain extent, of the gap-driven singularities. Every CVC point becomes an average of weighted contributions from different SIS junctions. If we are interested in differential CVCs, the following speculation is of importance. The raw experimental data are no more than a $J(V)$ dependence. That or another method of device-assisted differentiation is reduced to the calculation of a finite difference $\delta J/\delta V$ in some voltage interval δV rather than the true dJ/dV value. Then, the sequence of averaging and differentiating operations is a matter of concern. Really, a bias-induced aligning of the edges of two BCS-like gaps of whatever nature in homogeneous electrodes of the junction gives rise to the appearance of a jump or a cusp in the $J(V)$ dependence with *finite* derivatives dJ/dV on both sides of the feature point. Therefore, in the corresponding dJ/dV versus V dependence, there is also a finite jump here. For inhomogeneous electrodes, the position of the singularity is no longer unique, but averaging over those positions cannot result in anything different from a smeared, distorted step in the $\langle dJ/dV\rangle$ versus V dependence.

On the other hand, averaging the $J(V)$ dependence also brings about something like a smeared jump in the vicinity of this voltage, but the following differentiation can and does produce a high peak rather than a smeared step. The more pronounced coherent peaks for $d\langle J\rangle/dV$ than for $\langle dJ/dV\rangle$ stem from the amplification of the gap singularity in the former dependence, because the finite effective width δS of the gap edge makes it possible for the singularity to be reflected in the apparent calculated $G(V)$ if $\delta S>\delta V$. At the same time, as has been pointed out above, the infinitely thin original jump is "overlooked" while differentiating.

Hence, to obtain a differential CVC, which would reproduce experimental ones obtained by some kind of a modulation technique, one should first calculate the averaged dependence $\langle J(V)\rangle$ and then differentiate it to obtain $d\langle J\rangle/dV$. In the case where one of the electrodes is a normal metal and the counterelectrode is a homogeneous CDWS or a BCS superconductor, the derivative dJ/dV on one side of the jump diverges, which provides the existence of gaplike coherent peaks, although slightly varied, for both operation sequences. All that remains valid for CDW-driven gaps as well, because their DOSs have the same structure due to similarity between relevant coherent factors.[34] The results of our simulations, which will be presented elsewhere, confirm the aforesaid.

In what follows, we numerically differentiated the averaged $\langle J(V)\rangle$ dependence using the interval of differentiation $\delta(eV)=1$ meV. The procedure of averaging $J(V)$ over each

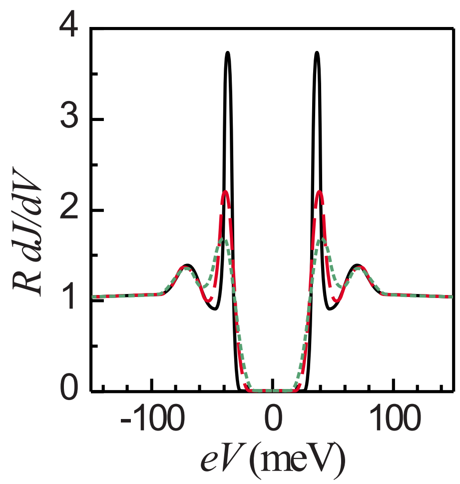

FIG. 2. (Color online) The dependences $RG(V)$ for $\mu=0.1$, $\Sigma_0=50\pm20$ meV, and $\Delta_0=20$ meV with various $\delta\Delta_0=5$, 10, and 15 meV (solid, dashed, and short-dashed curves, respectively). The temperature $T=4.2$ K. The interval of numerical differentiation $\delta V=1$ meV.

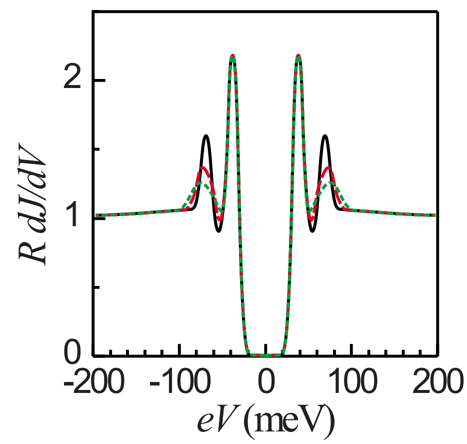

FIG. 3. (Color online) The same as in Fig. 2 but for $\Delta_0=20\pm10$ meV, $\Sigma_0=50$ meV, and various $\delta\Sigma_0=10$, 20, and 30 meV (solid, dashed, and short-dashed curves, respectively).

averaged parameter x was carried out using the weight function $W(x)\propto[x-(x_0-\delta x_0)]^2[x-(x_0+\delta x_0)]^2$, which is bell shaped within the corresponding dispersion interval $[x_0-\delta x_0, x_0+\delta x_0]$ and is equal to zero beyond it. The specific form of the function $W(x)$ does not matter much, however.

Before proceeding to the general case, we would like to emphasize that the roles of electrode parameters $x=(\Delta_0,\Sigma_0,\mu)$ and their corresponding spreads δx in the formation of final CVCs are not equivalent. For instance, the parameter μ is mainly responsible for the ratios between the amplitudes of various CVC features but has little effect on their positions. In addition, the procedure of averaging even over two parameters Δ_0 and Σ_0 (actually, over four parameters, because Δ_0 and Σ_0 for each electrode were varied independently) turned out to be time consuming. Therefore, we selected a dispersionless case $\mu=0.1$ for simulations, as a typical value of CDWSs.[14] We note that for larger μ the dips become deeper. Nevertheless, our theoretical $G(V)$ cannot become negative for any μ. It results from our assumption of incoherent tunneling (tunnel matrix elements $T_{qp}=\text{const}$). For a coherent one with anisotropic T_{qp}, $G(V)<0$ can be obtained, in principle.[29] It is disputable whether the coherent regime can really be achieved in break-junction experiments for cuprates. In our measurements, $G(V)$ was always positive, in contrast to those of Ref. 2. The origin of this discrepancy is unclear. In any case, we restrict ourselves to experimentally justified small values of μ, appropriate not only to BSCCO but also to $La_{2-x}Sr_xCuO_{4-\delta}$.[35]

Figure 2 illustrates the influence of the Δ_0 spread on $G(V)$ for a fixed $\delta\Sigma_0$. This figure demonstrates that all non-zero-temperature S_1-S_2 features are effectively flattened out. Furthermore, the relationship between the magnitudes of characteristic features at 2Δ, $\Delta+D$, and $2D$ is roughly $1:\mu:\mu^2$. Thus, the latter feature is also effectively smoothed out for the selected $\mu=0.1$ and cannot be distinguished in the chosen scale. Therefore, two well-pronounced features, a coherent superconducting peak and a DHS, are observed in each CVC branch, which correspond to experimental observation. The increase of $\delta\Delta_0$ leads to the smearing of the coherent peaks and the lowering of their height. Nevertheless, even at $\delta\Delta_0=0.75\Delta_0$ the peaks remain conspicuous and preserve the BCS-like appearance. It agrees with the observations of unambiguously superconducting patches in over- and optimally doped samples of BSCCO,[6,18,23,24] $Ca_{1.88}Na_{0.12}CuO_2Cl_2$, and $Bi_2Sr_2Dy_{0.2}Ca_{0.8}Cu_2O_{8+\delta}$.[17] At the same time, the smeared singularities at $eV=\Delta+D$ (DHSs) remain almost immovable, changing their profiles only owing to the influence of the larger coherent peak.

A similar situation is observed when $\delta\Sigma_0$ varies but $\delta\Delta_0$ remains fixed (Fig. 3): the variation of $\delta\Sigma_0$ leaves not only the position of the coherent peak almost intact but its amplitude as well (the latter owing to the smallness of the parameter μ), affecting only the DHS. But now, the DHS magnitude is affected much more effectively, being substantially depressed and smeared already at $\delta\Sigma_0=0.6\Sigma_0$. Therefore, one can draw a conclusion that the form and position of coherent peaks on the one hand and DHSs on the other hand are to a large extent independent of one another. To some extent, it reflects the different nature of Cooper and electron-hole pairings in cuprates.

The illustrative materials given above demonstrate that making allowance for the dispersion of each parameter of inhomogeneous CDWS electrodes brings the theoretical differential CVCs closer to experimental ones. On the basis of these considerations, we simulated the "normalized" experimental dependence $G(V)$ (Fig. 1, points) by a theoretical one for a junction between identical CDWSs (solid curve), where both dispersions $\delta\Delta_0$ and $\delta\Sigma_0$ were allowed for. The "normalization" consisted in that, on the basis of the analysis of calculation results, including those depicted in Figs. 2 and 3, we assumed the point at $V=\pm200$ meV to be close enough to the high-voltage asymptotic value. The procedure of exact fitting would require an enormous time of calculation. Moreover, the availability of a small unknown background, which we did not take into consideration, would make the exact fitting senseless. So we confined ourselves to a quantitative modeling. The specific parameters of calculation were selected to reflect the position of the coherent peak and the position and magnitude of the DHS. One sees that all main features of the tunnel spectra are well reproduced except the intragap region, which is the consequence of the adopted isotropic *s*-wave model. There is only one DHS for each voltage sign, corresponding to biases $\pm(\Delta+D)$; the peculiarities at $eV=\pm 2D$ are lost in the calculation uncertainties. Thus, the model of the partially gapped CDW superconductor[13,14,20,21] can easily and adequately describe the DHSs, treating them as low-T PG manifestations. Since we assume a symmetrical junction, the calculated superconducting coherent peaks in all demonstrated figures turned out equal by height. Different experimental peak heights may be due to the experimental uncertainties and the differentiation of raw data $J(V)$, the latter being already *averaged* over various patches of the oxide surface. Those patches with differing properties were found earlier for various cuprates.[17,26] Of course, the disparity seen by us varies from measurement to measurement at random.

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