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METALS AND SUPERCONDUCTORS

Effect of Charge Density Waves on the Tunnel Spectra of the $Bi_2Sr_2CaCu_2O_{8+\delta}$ Superconductor

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Abstract—The differential tunnel conductance G_S of the junction between a normal metal and a superconductor with a charge density wave (CDW) is calculated as a function of the voltage V across the junction. The results are averaged over the spread of superconducting and CDW energy gaps in the nanoscale-inhomogeneous superconductor. It is shown that, if both order parameters are nonzero, a dip–hump structure is formed beyond the superconducting gap of $G_S(V)$. If the phase of the CDW order parameter is not equal to $\pi/2$, a dip–hump structure will appear solely or mainly for one sign of the bias polarity. The results agree with the experimental data for $Bi_2Sr_2CaCu_2O_{8+\delta}$ and other high-temperature oxides

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1. INTRODUCTION

The superconducting oxide $Bi_2Sr_2CaCu_2O_{8+\delta}$ (BSCCO) is a compound in which all typical superconducting and normal-state properties of cuprates are most pronounced [1–3]. In particular, in addition to the superconducting gap Δ, a so-called pseudogap Π is observed, the nature of which remains a highly controversial subject [4–7]. In some samples, the pseudogap feature of the quasiparticle energy spectrum coexists with Δ below the critical temperature T_c and is also preserved above this temperature. For other samples, it is impossible to distinguish the peaks corresponding to Δ or Π below T_c. The overlapping and broadening of the peaks can be attributed to many reasons; the main reasons are, probably, the inhomogeneous electronic properties [3, 8–13], intrinsic even in the best of samples (see below), and heating effects [14]. It should be noted that the presence of a pseudogap Π is typical not only for BSCCO but also for other high-temperature superconductors, for example, $Tl_2Ba_2CuO_{6+\delta}$ [15] and $(Cu,C)Ba_2Ca_3Cu_4O_{12+\delta}$ [16].

The photoemission, point-contact, and tunnel spectra of BSCCO have another typical feature, namely, a very prominent dip–hump (DH) structure (in addition to the usual gap profile) observed at energies (bias voltages) dependent on the experimental setup but always larger in absolute value than the typical energy of the quasiparticle peak. For instance, for asymmetric SIN structures (S is a superconductor; I, an insulator; and N, a normal metal), a feature in the current–voltage characteristic is developed at energies near 2Δ, and for SIS structures (in particular, for break-junctions), at energies near 3Δ (see, e.g., [17]). It should be noted that the positions of the features are only roughly related to the magnitude of the superconducting gap; therefore, there is a freedom for one to choose a possible origin of the DH feature. A number of explanations have been suggested (see references in [5, 18]).

We would not list here all existing interpretations of the DH structure in detail. We just note that they could be divided into two groups. According to one group of interpretations, this structure is intrinsic in the normal-state electronic spectrum of BSCCO serving as a background for superconductivity. The other point of view is that both obviously superconductivity-related and extra features are actually of the same superconducting origin. Both of these interpretations (and all versions of them) can be supported by various arguments. However, the authors of [18] claim that a nonsuperconducting origin of the DH structure is impossible in principle, because it inevitably comes at odds with several experimental facts. For example, according to the calculations performed in [18], which take into account both a pseudogap order parameter (OP) of unknown nonsuperconducting origin and its superconducting counterpart (with both being assumed to have the d-wave symmetry), the magnitude of the tunnel density of states (TDOS) for SIN and SIS junctions is such that the minimum of the dip is never below the background value of the normal-state dynamic electrical conductance of the tunnel junction $G_N \equiv (dJ/dV)_N$, let alone the occasionally observed negative values in the minimum [17, 19] (which, however, can be related to overheating effects [20, 21]). Here, J is the tunnel current and V is the bias voltage. It is maintained in [18] that the calculation of the TDOS with inclusion of the interaction with a bosonic mode [22, 23], similarly to strong-coupling approximation calculations for phonons, gives a fairly satisfactory fit to the experimental data.

Another TDOS feature (appearing only in SIN junctions) is that the function $G_S \equiv (dJ/dV)_S$ (subscript S denotes that the oxide bank is in the superconducting state) is asymmetric with respect to DH structure, which is usually observed for only one sign of the voltage applied to the junction (see Fig. 1, borrowed from [17]; here, all $G_S(V)$ dependences were measured at T = 4.2 K and the temperatures shown on the graphs are the critical transition temperatures of the samples). Such asymmetry of the DH feature is typical not only of BSCCO [17, 24, 25] but also of $Bi_{2-x}Pb_xSr_2CaCu_2O_{8+\delta}$ [26], $Bi_2Sr_2Ca_2Cu_3O_{10+\delta}$ [27], $(Cu,C)Ba_2Ca_3Cu_4O_{12+\delta}$ [16], $Tl_2Ba_2CuO_{6+\delta}$ [15], and $HgBa_2Ca_{n-1}Cu_nO_{2n+2+\delta}$ [28]. In some cases, however, the DH structure is also observed for the other voltage polarity, though it is less prominent. For example, for nonuniform $Bi_{2-x}Pb_xSr_2CaCu_2O_{8+\delta}$ samples, observations are strongly dependent on the choice of a nanosized region where the tunneling current flows [26]. Tunneling measurements on BSCCO [29] revealed DH structures for both signs of V, though there was a preferred polarity. In all cases, the preferred polarity corresponds to the tunneling of quasiparticles of the superconductor from the states below the Fermi level into the normal contact.

Within the approach developed in [22], the asymmetry is explained in terms of the breaking of the particle–hole symmetry in the electronic band structure of BSCCO. In [30], this asymmetry is even attributed to an artifact due to the interference of the contributions to the tunnel current coming from different defect regions of the nonuniform superconducting nanostructure of the oxide compound established previously in [26].

In the present paper, we propose an alternative explanation of the tunneling conductance of SIN junctions (SIS junctions will be discussed in a separate paper), which is based on the assumption that the pseudogap Π is actually the insulating gap Σ that accompanies a charge density wave (CDW). Numerous experimental facts support this hypothesis [5]. We demonstrate that the difficulties [18] related to the alleged insufficient dip depth do not actually exist in this scenario. In order to explain the experimental data, it is necessary to take into account the appreciable spatial inhomogeneity of the CDW order parameter $\tilde{\Sigma}$, which requires averaging over the corresponding distribution functions. Moreover, the asymmetry of the function $G_S(V)$ with respect to the size of the DH structure is easily explained.

2. FORMULATION OF THE PROBLEM

The starting point for describing the BSCCO cuprate is the model of a partially gapped superconducting CDW metal (CDWS) [5, 31]. Within this

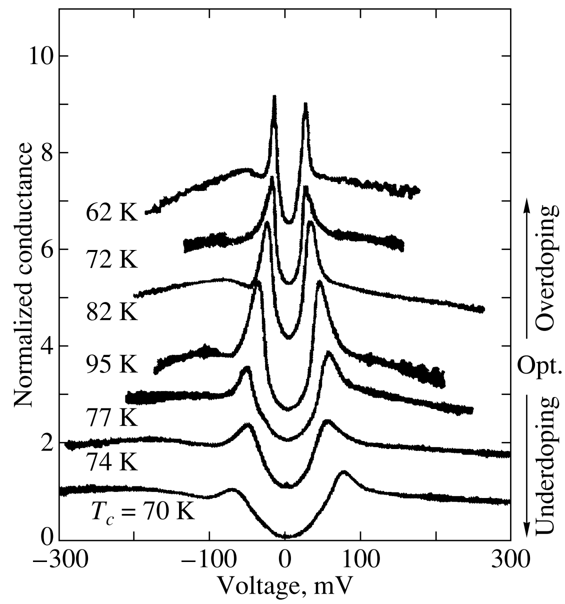

Fig. 1. Normalized tunnel conductances of SIN junctions for various doping levels of the superconducting oxide $Bi_2Sr_2CaCu_2O_{8+\delta}$ (from [17]).

model, the Fermi surface (FS) is divided into two congruent regions (i = 1, 2) where the quasiparticle spectrum is degenerate (d) and one remaining part (i = 3) where the spectrum is nondegenerate (n). In the former case, the bare branches of the quasiparticle energy spectrum $\xi_{1,2}(\mathbf{p})$ reckoned from the common Fermi level are related as

$$\xi_1(\mathbf{p}) = -\xi_2(\mathbf{p}+\mathbf{Q}), \tag{1}$$

where $\mathbf{Q}$ is the CDW wave vector. Due to the attraction of the quasiparticles from the different d regions of the FS, a dielectric order parameter $\tilde{\mathbf{\Sigma}} = \mathbf{\Sigma}\cos\varphi$ arises below the critical temperature of the structural transition $T_d > T_c$ and an energy gap Σ opens on both the regions. Here, T_c is the superconducting transition temperature and φ is the phase of $\tilde{\Sigma}$. If the attraction is of Coulomb origin and the branches $\xi_{1,2}(\mathbf{p})$ describe electrons and holes, respectively, then an excitonic insulator is formed [32]. A similar opportunity also appears for a strongly anisotropic quasi-one dimensional spectrum with flat regions of the FS where the attraction between the quasiparticles is due to the electron–phonon interaction. In this case, a Peierls insulator state appears [33]. The remaining part of the FS is undistorted and described by the n branch of the spectrum, $\xi_3(\mathbf{p})$. The separation of the FS into gapped and gapless parts is often described in terms of the parameter

$$\mu = N_{d0}(0)/N_0(0), \tag{2}$$

where

$$N_0(0) = N_{n0}(0) + N_{d0}(0) \tag{3}$$

is the total bare (above T_d) DOS and $N_{d0}(0)$ and $N_{n0}(0)$ are its components, i.e., the DOSs in the d and n regions of the FS, respectively.

A superconducting OP Δ, the same for the whole FS, appears below $T_c < T_d$. In the d regions of the FS, a combined energy gap $D = (\Sigma^2 + \Delta^2)^{1/2}$ arises, whereas in the n region the gap is equal to Δ. In an excitonic insulator, the phase φ is always fixed (0 or π) [34]. On the other hand, in a Peierls insulator, the CDW can be pinned with an arbitrary phase φ [33].

Quasiparticle tunnel current J flowing through a SIN junction is a functional of temporal Green's functions $G_{ij}(\omega)$, where subscripts i, j = 1, 2, 3 indicate the regions of the FS. For our purposes, it is important that the current has a contribution proportional to $\tilde{\Sigma}$ determined by the Green's function $G_{12} = G_{21} \equiv G_c$. It is this function that describes electron–hole pairing. Technically, we follow the classical work [35].

In spite of still standing controversies [2], it is generally accepted that the superconductivity in cuprates (at least, in hole compounds) is better described by an OP with $d_{x^2-y^2}$ symmetry [1]. The symmetry of the dielectric OP is completely unknown. However, simulation of even the main observed superconducting features of $G_S(V)$ based on a d-wave OP encounters difficulties. In particular, it is impossible to describe the shape of $G_S(V)$ inside the gap, the amplitude of the coherent peaks near the gap edges, and the DH structure [36] even using an ad hoc weight function $g(\theta)$ [18, 27, 36, 37] for integration over the angle θ, which is the argument of the OP function $\Delta(\theta) \equiv \Delta_0\cos(2\theta)$. Therefore, it is reasonable to assume that both OPs have s-wave symmetry. As is demonstrated below by numerical results, this assumption turns out to be fairly satisfactory in practice.

For definiteness sake, when calculating the J–V characteristic, the bias voltage between the N electrode and the CDWS is referenced to the normal metal: $V \equiv V_{\rm CDWS} - V_N$.

The positive polarity corresponds to probing quasiparticles above the energy gaps. The quasiparticle current $J(V)$ can be presented as a sum of different components J_i, which have the same structure

$$J_i \propto \frac{1}{R}\mathrm{Re}\int_{-\infty}^{\infty} d\omega' \int_{-\infty}^{\infty} d\omega \frac{\mathrm{Im}\, G_i^{\rm CDWS}(\omega')G^N(\omega)}{\omega' - \omega + eV + i0} \quad (4)$$

and correspond to different combinations of the temporal Green's functions. Here, R is the normal-state tunnel resistance of the junction and $e > 0$ is the elementary charge. The function $G^N(\omega)$ has a trivial form. However, instead of the single function $G^{\rm BCS}(\omega)$, describing a superconductor within the Bardeen–Cooper–Schrieffer (BCS) model, three functions $G_i^{\rm CDWS}(\omega)$ are introduced. These functions can be obtained from the following temperature Green's functions for a CDWS [5]:

$$\mathcal{G}_n(\mathbf{p}, \omega_m) = -\frac{i\omega_m + \xi_3(\mathbf{p})}{\omega_m^2 + \xi_3^2(\mathbf{p}) + \Delta^2}, \quad (5)$$

$$\mathcal{G}_d(\mathbf{p}, \omega_m) = -\frac{i\omega_m + \xi_1(\mathbf{p})}{\omega_m^2 + \xi_1^2(\mathbf{p}) + \Delta^2}, \quad (6)$$

$$\mathcal{G}_c(\mathbf{p}, \omega_m) = -\frac{\tilde{\Sigma}}{\omega_m^2 + \xi_1^2(\mathbf{p}) + \Delta^2}. \quad (7)$$

Here, $\omega_m = (2m + 1)\pi k_B T$; $m = 0, \pm1, \pm2, \ldots$; T is the temperature; and k_B is the Boltzmann constant. The quantities Δ and Σ are derived from the self-consistent set of Dyson–Gor'kov integral equations [38]. In this set, the bare parameters are the magnitudes of the gaps Δ_0 and Σ_0 at $T = 0$ in the absence of competing pairing. The quantities Δ_0 and Σ_0 are related to the corresponding coupling constants.

The total tunnel current $J(V)$ and the components $J_i(V)$ calculated from Eq. (4) are given by

$$J(V) = \sum_{i = n, d, c} J_i(V), \quad (8)$$

where

$$J_n = \frac{(1-\mu)}{4eR}\int_{-\infty}^{\infty} d\omega K(\omega, V, T)|\omega| f(\omega, \Delta), \quad (9)$$

$$J_d = \frac{\mu}{4eR}\int_{-\infty}^{\infty} d\omega K(\omega, V, T)|\omega| f(\omega, D), \quad (10)$$

$$J_c = \frac{\mu\Sigma\cos\varphi}{4eR}\int_{-\infty}^{\infty} d\omega K(\omega, V, T)\,\mathrm{sgn}(\omega) f(\omega, D). \quad (11)$$

Here,

$$K(\omega, V, T) = \tanh\frac{\omega}{2T} - \tanh\frac{\omega - eV}{2T}, \quad (12)$$

$$f(\omega, x) = \frac{\theta(|\omega| - x)}{\sqrt{\omega^2 - x^2}}. \quad (13)$$

The dynamic conductance $G_S(V) \equiv (dJ/dV)_S$ obtained from Eqs. (8)–(13) has square-root singularities at $eV = \pm\Delta$ and $\pm D$. We note that the amplitudes of the singularities at $eV = \pm D$ and the ratio of these amplitudes for the different branches of the J–V curve depend on the polarity of V and the phase φ. This is due to the superposition of the d and n current components, which satisfy the usual symmetry relations $J_i(V) = -J_i(-V)$, and the c component, which obeys a different relation $J_c(V) = J_c(-V)$ [39]. For this reason, the singularities of

J_d and J_c at $|eV| = D$ amplify each other on one branch of the J–V curve and compensate each other to a large extent on the other branch. Whether the singularities amplify or compensate each other on a given branch depends on the CDW phase φ. We note that the singularities of $G_S(V)$ at $eV = \pm D$ depend on both of the renormalized interaction constants for the electron–hole and Cooper pairing [40]. For cuprates, however, this approach is fairly rough, because it does not take into account the actual inhomogeneous spatial distribution of both OPs. For example, STM measurements performed on $Bi_{2-x}Pb_xSr_2CuO_y$ show that samples are broken into regions with Δ values ranging from 13 to 30 meV over a tested area 12.5 × 12.5 nm in size [12]. At the same time, the $G_S(V)$ spectrum in certain regions has a pseudogap character with $\Pi \le 30$ meV. It should be noted that the histogram plotted in [12] makes no distinction between the gaps Δ and Π. A similar situation is observed for nearly optimally doped BSCCO samples [13]; specifically, the STM spectra reveal spots 30 Å in size with small (25–30 meV) and large (50–75 meV) energy gaps. It is possible to observe such inhomogeneities owing to the short coherence length in the superconductor, $\xi_0 \approx 15$–20 Å. Because of the proximity effect, the observed spectra are somewhat averaged; so, the small and large gaps cannot be identified with Δ and Π, or, in our interpretation, with Δ and Σ.

Under certain conditions, for example, in the case of interplane tunneling along the crystallographic c axis in mesas consisting of 10–100 natural identical junctions (which are, obviously, symmetric SIS structures), the smooth pseudogap maxima turn into sharp peaks. Such a sharp separation of Δ and Π features was observed in BSCCO [14, 41].

3. CALCULATION RESULTS

In order to model the dynamic conductance of an inhomogeneous BSCCO, we perform averaging of the J–V characteristic over the gap parameters and μ. In order to determine the role played by the model parameters in the origin of the phenomena in question, we averaged the $G_S(V)$ dependences assuming each time that only one of the parameters has some spread; i. e., we assumed that dispersions of different parameters are independent of one another (cf. the similar approach in [42]). The distribution function of a parameter x is chosen to be the normalized function

$$W(x) = \frac{15}{16\sigma^5}[(x-x_0)^2 - \sigma^2]^2 \qquad (14)$$

within the range $|x - x_0| \le \sigma$ and to be zero beyond this range. This model distribution is the simplest function described by only two parameters, x_0 and σ, is defined on a finite interval, has a maximum at x_0, and vanishes smoothly outside this interval together with its derivative. The function $W(x)$ is smoother than the Gaussian used in [43] to study inhomogeneities of the superconducting OP in cuprates without allowance for a pseudogap. Strictly speaking, the form of the weight function $W(x)$ should be derived from microscopic theory. However, since we use a phenomenological approach, the form of $W(x)$ is one of the parameters of the problem. Nevertheless, it is obvious that the substitution of function (14) by any other function localized near x_0 can lead only to a numerical difference of about several percent in the final results, leaving the main conclusion of this work unchanged.

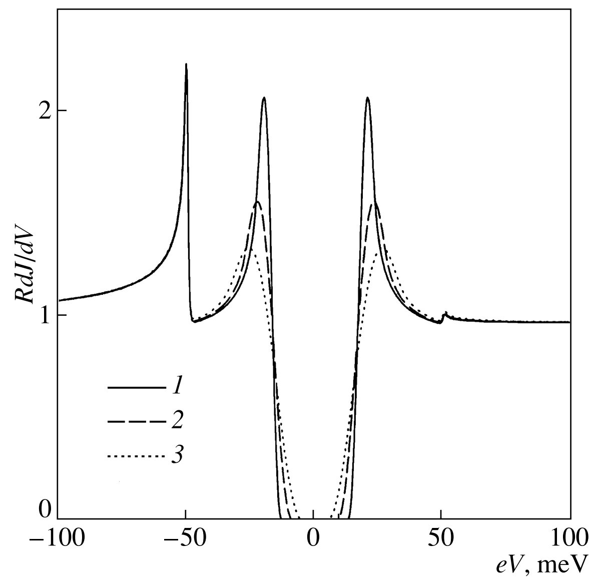

Fig. 2. Dimensionless conductance $RdJ/dV = RG(V)$ of the junction between a normal metal and a superconductor with a CDW (mean bare superconducting gap $\Delta_0 = 20$ meV, bare CDW gap $\Sigma_0 = 50$ meV, the dielectric FS gapping degree $\mu = 0.1$) as a function of the bias energy eV averaged over a magnitude distribution of Δ_0 with dispersion $\delta\Delta_0$ equal to (*1*) 5, (*2*) 10, and (*3*) 15 meV. $T = 4.2$ K.

Figure 2 shows the $G_S(V)$ dependence for the case where the averaged quantity is the bare superconducting gap Δ_0. The average values of Δ_0 and Σ_0 are chosen in accordance with the experimental data for BSCCO [17] (62-K curve in Fig. 1). Our calculations show that the DH structure should be observed on the negative branch of the J–V curve for φ = π.

The CDWS states with φ = 0 and π are thermodynamically equivalent. If the occurrences of these states are equally probable, the DH structure also have to be equally frequently observed either on the positive or negative branch of the J–V curve. We did not studied the statistics. However, if experimentally the DH structure appears predominantly on one branch [25], then this fact should be related to special features of the CDW behavior near the sample surface; studying these features at the microscopic level is beyond the scope of this paper. Therefore, we limit ourselves to the value φ = π in accordance to the results of typical experiments [17, 25]. In this case, the $G_S(V)$ dependence is

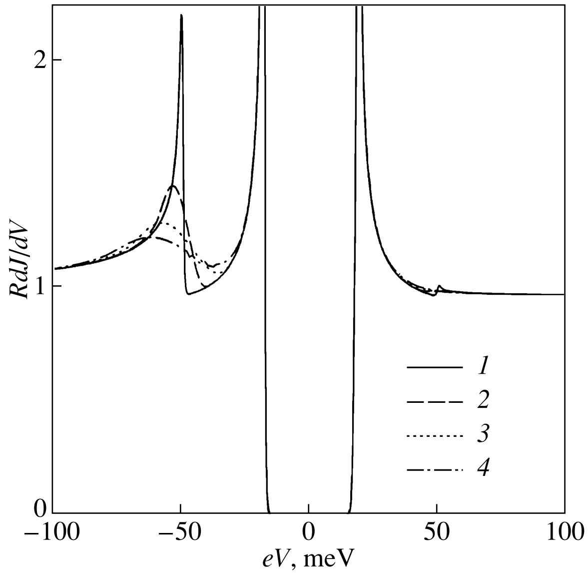

Fig. 3. Same as in Fig. 2 but the average is performed over a magnitude distribution of the bare CDW gap with dispersion $\delta\Sigma_0$ equal to (*1*) 0, (*2*) 10, (*3*) 20, and (*4*) 29 meV. All other parameters are the same as in Fig. 2.

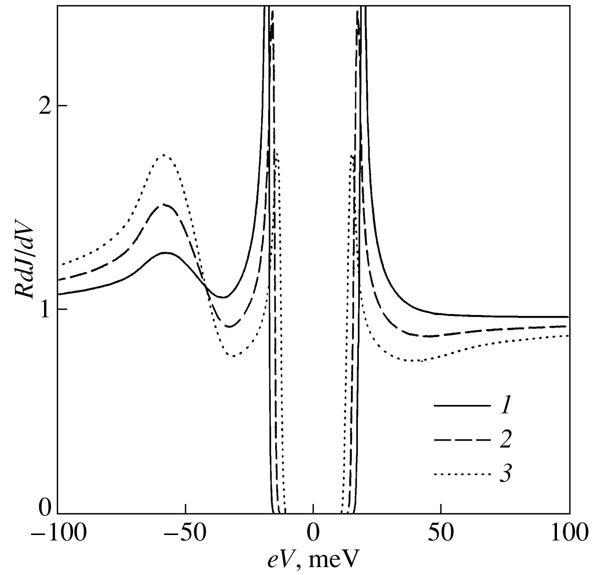

Fig. 4. Same as in Fig. 3 but for $\delta\Sigma_0$ = 20 meV and various values of μ: (*1*) 0.1, (*2*) 0.2, and (*3*) 0.3. All other parameters are the same as in Fig. 2.

well described inside the gap. In addition to the superconducting peaks near the edges of the gap Δ, there are specific features whose amplitude is determined by the dielectric gap. These features are also affected by averaging over Δ_0, but to a considerably smaller degree. Near $|eV| \approx D$, the function $G_S(V)$ is substantially asymmetric, in accordance with the experimental data, but even the strong averaging over Δ_0 we employed cannot smooth out the square-root singularity at $eV > 0$ to a hump.

For $\varphi = 0$, we would get a picture that is a mirror image with respect to the *OY* axis [44]. However, for $\varphi = \pi/2$, component (11), which is directly related to the electron–hole pairing, becomes zero; so, the total *J*–*V* curve becomes symmetric and the DH features are identical for both polarities of the voltage applied to the junction. This situation would correspond to additional averaging of the tunnel current in the case where the CDW phase at different points of the tunnel junction has a random scatter. This, in particular, can explain the almost symmetric *J*–*V* curve with DH features observed for some asymmetric SIN junctions [29].

The calculated $G_S(V)$ dependences averaged over Σ_0 are shown in Fig. 3. These curves excellently fit the experimental data for BSCCO near the DH region [17]. Small deviations of $G_S(V)$ from G_N are also observed for $eV < 0$. We note that the structure of the $G_S(V)$ curve at $|eV| \leq \Delta$ is almost unaffected by this averaging.

Figure 4 shows the *V* dependences of the conductance averaged over Σ_0 for various values of the dielectric gapping degree μ. It is seen that, in order to achieve a good fit to the experimental data, it is necessary to assume that only a part of FS of about 10% satisfies the congruence condition and is distorted by the gap associated with the CDW. For comparison, we note that, in the CDW metal $NbSe_3$, we have $\mu \approx 0.2$ [45] and in Cr–Re alloys, where a spin-density wave arises, $\mu \approx 0.1$ [46].

Thus, the proposed theory produces results that qualitatively describe the origin of the asymmetric DH structure of the *J*–*V* curves of asymmetric tunnel SIN junctions. We note that, for an actual inhomogeneous CDWS electrode, at least three parameters (Δ_0, Σ_0, μ) can vary simultaneously over the bulk of the sample. Our results are obtained under the assumption that only one of the parameters is nonuniform. Therefore, a close quantitative fit of the calculations to the experimental data may hardly be expected. Moreover, the experimental data (Fig. 1), first, undoubtedly include a background contribution of unknown origin, which our theory certainly does not take into account and, second, the data are given in the normalized form and the normalization constant is not stated. Nevertheless, the inclusion of inhomogeneities of each of the model parameters changes the shape of the *J*–*V* curve from the “ideal” one corresponding to fixed values of the parameters (Fig. 3, solid curve) toward the *J*–*V* profiles actually observed in experiment.

Sometimes, it is contended that the asymmetry of tunnel *J*–*V* curves due to the DH structure is typical mainly of heavily doped high-temperature superconductors. However, as is seen in Fig. 1, such asymmetry can also arise for underdoped superconductors (see, e.g., [47]). From the point of view of the theory developed here, it is likely that the DH structure is observed less often for underdoped superconductors because these are more homogeneous. To support this conclusion, we can mention the *J–V* curves of the tunnel junctions based on $YBa_2Cu_3O_{6+y}$, where there is no DH structure; the distribution of holes in the bulk of $YBa_2Cu_3O_{6+y}$ is much more uniform than that in BSCCO [48].

On the other hand, the asymmetry of the *J–V* curve due to the presence of a DH structure can actually be more typical of overdoped oxides like BSCCO because of the convergence of the pseudogap singularity (CDW singularity, in our interpretation) and the superconducting singularity near the superconducting dome in the *T–x* phase diagram [1].

4. CONCLUSIONS

Thus, using a model where the DH features are caused by the occurrence of a CDW and performing average over the width distribution of the insulating gap Σ, we have described the tunnel spectroscopy data quantitatively. At the same time, the most widespread alternative explanation [23] based on the existence of a narrow boson mode of unknown nature with an energy Ω leaves the origin of the asymmetric form of the *J–V* curves unclear. Moreover, when the oxygen doping of BSCCO is varied in a wide range, the variations of Δ and the DH position are not related to each other by any simple relation [49]. However, according to the "bosonic" approach, the DH structure have to be located at $eV = \Delta + \Omega$ for SIN junctions and at $eV = 2\Delta + \Omega$ for SIS junctions.

Within our approach, the absence of proportionality between the position of the DH structure and the gap feature position Δ with variations in the oxygen doping (though these quantities are correlated) is because the feature position D depends on the T_d shift in a twofold nonlinear manner, namely, via Σ and Δ, with the latter being dependent on Σ as well [38]. Our calculations indicate that the conclusion [18] that the experimentally observed deep dip cannot be described under the assumption that the pseudogap causing this dip is nonsuperconducting is incorrect.

5. ACKNOWLEDGMENTS

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