METROLOGY AND MEASUREMENT SYSTEMS
VOL. XV, NUMBER 2 (2008)

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CHARGE-DENSITY-WAV FEATURES IN TUNNEL SPECTRA OF HIGH-T SUPERCONDUCTORS

Tunnel conductance $G(V)$ was calculated for junctions between a normal metal and a spatially inhomogeneous superconductor with a dielectric gap on the nested sections of the Fermi surface or between two such superconductors. The dielectric gapping was considered to be a consequence of the charge density wave (CDW) appearance. Spatial averaging was carried out over domains with randomly varying parameters of the CDW superconductor (CDWS). The calculated $G(V)$s demonstrate a smooth transformation from patterns with a pronounced dip-hump structure (DHS) at low temperature, T, into those with a pseudogap depletion of the electron density of states at higher T within the range of actual critical temperatures of the CDWS domains. Thus, it is shown that both the DHS and the pseudogap have the same origin. This circumstance provides a new insight into the problem and explains the peculiar features of $G(V)$ for $Bi_2Sr_2CaCu_2O_{8+\delta}$ and related high-T_c cuprates. At the same time, the approach, being quite general, can be applied to other CDWSs which belong to various other classes of materials.

Keywords: superconductivity, pseudogap, charge-density wave, non-homogeneity, tunneling, dip-hump structure

1. INTRODUCTION

The mechanism of superconductivity in high-T cuprates remains still unknown, although it has been discovered more than 20 years ago [1]. Similar lack of knowledge concerns the symmetry of the superconducting order parameter in various high-T oxides [2, 3]. Finally, we do not know enough about the normal state of these nonstoichiometric compounds [4]. What is known for sure is that genuine manifestations of superconductivity are accompanied by the so-called pseudogap ones [5], the origin of the latter being the subject of the investigation in this paper.

The pseudogap phenomenon is observed above the superconducting critical temperature T_c and consists in the electron density-of-states (DOS) depletion, revealed by tunnel, point-contact or photoemission spectroscopies. On the other hand, the pseudogap was shown to exist below T_c as well, masked by a huge superconducting gapping of the electron spectrum [6]. However, at low $T \ll T_c$, the voltage, V, dependences of the tunnel conductance $G = dJ/dV$, where J is the quasiparticle current, reveal conspicuous features – the so-called dip-hump structures (DHSs) [6]. The latter are weaker than the superconducting gap-edge coherent peaks but quite reproducible. For non-symmetric (*ns*) high-T_c oxide/insulator/normal metal (S-I-N) junctions, DHSs are sometimes observed at one V polarity and sometimes at both. It is quite natural that DHSs emerge simultaneously at both polarities in the case of symmetric (*s*) S-I-S junctions.

Our main message is that both the pseudogap and DHS features of the $G(V)$ are consequences of the charge-density-wave (CDW) existence in cuprates. Pseudogap features (i.e. high-T manifestations of CDWs) are substantially quenched by Cooper pairing and thermal smearing, whereas their DHS counterparts are blurred by spatial inhomogeneity of the CDW (dielectric) order parameter. The scatter of dielectric order parameter has been studied recently in great detail [7, 8].

2. THEORY

We consider a CDW superconductor (CDWS) in the framework of the Bilbro-McMillan theory, where *s*-wave superconductivity and CDWs coexist [9, 10]. This theory assumes nesting conditions to be fulfilled only for certain ($i = 1, 2$) Fermi surface (FS) sections (d), which become dielectrically gapped below some temperature $T_d > T_c$ and can therefore be associated with a dielectric order parameter $\Sigma(T)$, while the rest of the FS ($i = 3$) remains ungapped (n) down to T_c, so that the CDW gapping is only partial. The degree of such a FS separation is described by a certain parameter ($0 < \mu < 1$). The isotropic superconducting order parameter $\Delta(T)$ is assumed to exist over the whole FS [9, 10]. Superconductivity and CDWs turn out to be detrimental to each other. The actual critical parameters of CDWSs are governed by the dielectric and Cooper pairing strength, which can be parameterized as the zero-T values of each order parameter in the absence of its rival: Δ_0^* and Σ_0^*.

As a consequence, an energy gap $\Delta(T)$ appears on the n FS section, whereas a combined gap $D(T) = [\Delta^2(T) + \Sigma^2(T)]^{1/2}$ arises on the d-ones. We emphasize that the phase φ of the dielectric order parameter does not affect the thermodynamic properties of CDWSs [10] but influences $G(V)$s for junctions with a CDWS as an electrode [11]. The value of φ can be pinned by various mechanisms in both excitonic and

Peierls insulators, so that φ acquires a value of either 0 or π in the first case, or is arbitrary in the unpinned state of Peierls insulator. If the CDWS is inhomogeneous, which is the case for $Bi_2Sr_2CaCu_2O_{8+\delta}$ (BSCCO) and other oxides [12], the φ values may be non-correlated over the junction area. Then, the contributions of elementary tunnel currents may compensate one another to some extent, and this configuration can be phenomenologically described by introducing a certain effective phase $\varphi_{\rm eff}$ of the dielectric order parameter. If the spread of the phase φ is random, the most probable value for $\cos(\varphi_{\rm eff})$ is zero, and the CVC for a non-symmetric junction involving CDWS becomes symmetric.

The microscopic nature of random inhomogeneities in BSCCO and other hole--doped cuprates still remains obscure, although some correlations between various quantities have been noticed [12].

3. CALCULATION OF THE TUNNEL CONDUCTANCE

Using the previously developed approach [10], we calculated $G(V)$ for two experimental set-ups mentioned above (S-I-N and S-I-S), where the notation S means a CDWS. Our calculations in the framework of the Green's function method follow the classical approach [13].

The calculations take into account the non-homogeneous background. The value of the FS gapping degree μ is responsible for the amplitude of the DHS. The dispersion of the parameter Σ_0^* leads to D-peak smearing (the Δ-peak also becomes smeared, but to a much lesser extent). The dispersion of the parameter Δ_0^* results in the smearing of the Δ-peak only. But, since the amplitude of the Δ-peak in the case of the S-I-N junction is large, this smearing is almost unnoticeable. Therefore, in this case, it was sufficient for our purpose to average only over Σ rather than simultaneously over all CDWS parameters, although the variation of any individual parameter made the resulting theoretical CVCs more similar to experimental ones.

The parameter Σ_0^* was regarded as distributed within the interval $[\Sigma_0^*-\delta\Sigma_0^*, \Sigma_0^*+\delta\Sigma_\delta^*]$. The profile of the weight function $W(x)$ was considered to be a bell-shaped fourth-order polynomial within this interval and equal to zero beyond it. The specific form of $W(x)$ was shown to be not crucial for final results and conclusions. Our approach is also applicable to superconductors with d-wave symmetry, which is usually considered true for at least hole-doped cuprates. The technical distinction lies in the dependence of the superconducting order parameter on the angle Θ in the Cu-O plane, which leads to additional mathematical complications and a V-shaped $G(V)$ in the vicinity of the point $V = 0$, although the physical picture remains essentially the same.

In the S-I-S case, both key parameters, Δ_0^* and Σ_0^*, were varied within the corresponding intervals.

4. RESULTS AND DISCUSSION

The calculations of $G(V)$ allow us to track the details of the DHS transformation into the pseudogap DOS depletion for junctions, involving CDWS. An example of such a transformation is displayed in Fig. 1 for CDWS-I-N junctions with $\varphi = \pi$ (panel *a*) and $\pi/2$ (panel *b*). The CDWS parameters are $\Delta_0^* = 20$ meV, $\Sigma_0^* = 50$ meV, $\mu = 0.1$, and the limit of Σ_0^*-variation is $\delta\Sigma_0^* = \pm 20$ meV. For this parameter set, the "actual" $T_c^{'}$s of CDWS domains lie within the interval 114-126 K, and $T_d^{'}$s are in the range 197-461 K. The asymmetric curves displayed in panel *a* are similar to the measured $G_{ns}(V)$ dependences for over-and underdoped BSCCO compositions obtained by scanning-tunnel-microscopy (STM) [7].

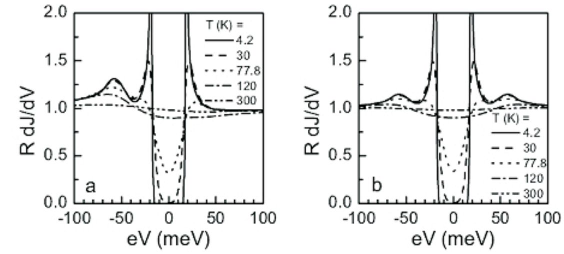

Fig. 1. $RG(V)$-dependences for tunnel junctions between an inhomogeneous CDWS and a normal metal for various temperatures $T.e > 0$ is the elementary charge, G is the conductance, V is the voltage, and R is the junction resistance. The dielectric order parameter phase is $\varphi = \pi$ (panel *a*) and $\varphi = \pi/2$ (panel *b*); the other CDWS parameters are $\Delta_0^* = 20$ meV, $\Sigma_0^* = 50$ meV, $\mu = 0.1$, $\delta\Sigma_0^* = \pm 20$ meV. The temperature $T = 4.2$ (solid), 30 (dashed), 77.8 (dash-dotted), 120 (dash-double dotted), and 300 K (short-dashed curve).

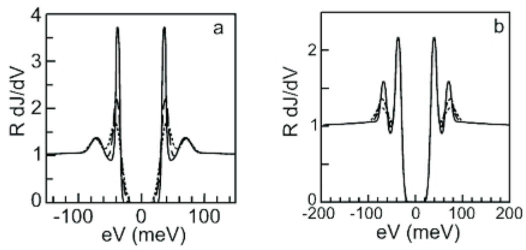

Fig. 2. he same as in Fig. 1 but for symmetric junctions between similar CDWSs. Here $\mu = 0.1$, $\Sigma_0^* = 50$ meV, $\Delta_0^* = 20$ meV, $T = 4.2$ K. Panel *a*: $\delta\Sigma_0^* = \pm 20$ mev; $\delta\Delta_0^* = \pm 5$ (solid), ± 10 (dashed), and ± 15 meV (short-dashed curve). Panel *b*: $\delta\Delta_0^* = \pm 10$ meV; $\delta\Sigma_0^* = \pm 10$ (solid), ± 20 (dashed), and ± 30 meV (short-dashed curve).

Similar CDW-related features should be observed in $G(V)$ measured for CDWS-I--CDWS junctions. The $G_s(V)$ dependences for this case with the same sets of parameters as in Fig. 1 are shown in Fig. 2, but here the dispersion of both order parameters is made allowance for. Panel *a* illustrates the influence of the $\delta\Delta_0^*$-scatter at a fixed $\delta\Sigma_0^*$ on the $G_s(V)$ profiles, while panel *b* analyzes the influence of the $\delta\Sigma_0^*$-scatter at a fixed $\delta\Delta_0^*$. In both cases, theoretical curves are very similar to experimental patterns.

The temperature evolution of the $G_s(V)$ dependence for a symmetric junction, where only the parameter Σ_0^* is scattered, is depicted in Fig. 3. Making allowance for the Δ_0^*-scatter is not necessary here, because the temperature-induced smearing effectively hides the spread altogether. As is readily seen, the transformation of the symmetric DHS pattern into the pseudogap-like picture is similar to that for the non-symmetric junction. This simplicity is caused by the smallness of the parameter $\mu = 0.1$, so that the features at $eV = \pm 2D$, which are proportional to μ^2, are inconspicuous on a chosen scale. At the same time, there are prominent square-root singularities at $eV = \pm(D+\Delta)$.

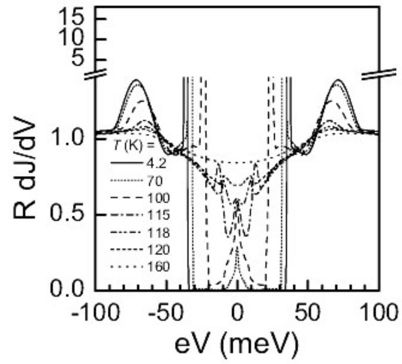

Fig. 3. The same as in Fig. 2 for $\Delta_0^* = 20$ meV, $\Sigma_0^* = 50$ meV, $\mu = 0.1$, $\delta\Sigma_0^* = \pm 20$ meV and various T.

The appearance of the T-driven zero-bias peaks is a salient feature of certain curves displayed in Fig. 3. It is well known [13], that, in the case of symmetric S-I-S junctions, this peak is caused by the tunneling of thermally excited quasiparticles onto empty states with an enhanced DOS, which are located above and below equal superconducting gaps in both electrodes. One should be careful not to confuse this peak with the DC Josephson peak restricted to $V = 0$, which is often seen for symmetric high-T junctions. The distinction consists in the growth of the quasiparticle zero-bias maximum with T up to a certain temperature, followed by its drastic reduction. On the other hand, the Josephson peak decreases monotonously as $T \to T_c$.

The conventional zero-bias peaks in $G_s(V)$ for junctions, involving electrodes with s-wave-like superconducting order parameters and studied here, have nothing to do with similarly looking features of tunnel $G_{ns}(V)$ for high-T_c oxides revealed by STM [14]. The latter points at the existence of bound states at the interface between a normal probe and a d-wave superconductor. In the latter case, the $G(V)$-peak in the superconducting state disappears with growing T.

Our theoretical approach can be directly applied to explain experimental data. To prove our considerations, we have made an experimental research at T = 4.2 K using break-junctions made of BSCCO single crystals. The measurements were carried out *in situ*, so that clean and fresh interfaces were studied. The conductance $G_s(V)$ was obtained using the four-probe, AC modulation technique. Samples 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. The experimental results are shown in Fig. 4. One can see well-developed DHSs beyond the coherent superconducting peaks. We simulated this dependence by a theoretical curve for a junction between identical CDWSs (solid curve), where both dispersions $\delta\Delta_0^*$ and $\delta\Sigma_0^*$ were allowed for. The 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 intra-gap region, which is the consequence of the adopted isotropic *s*-wave model.

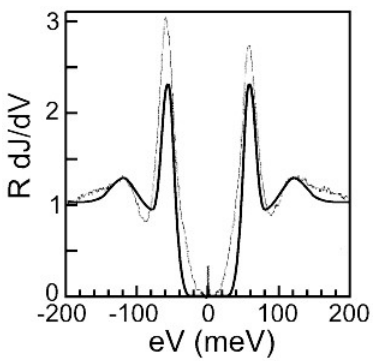

Fig. 4. $RG(V)$-dependences measured (thin) and calculated (solid curve) for a $Bi_2Sr_2CaCu_2O_{8+\delta}$ (BSCCO) break junction at T = 4.2 K. The fitting CDWS parameters are Δ_0^* = 30 meV, $\delta\Delta_0^*$ = ±15 meV, Σ_0^* = 90 meV, $\delta\Sigma_0^*$ = ± 35 meV, μ = 0.08.

We have experimentally found similar pseudogap features of $G(V)$ for the related cuprate $YBa_2Cu_3O_{7-\delta}$. The results will be published elsewhere.

5. CONCLUSIONS

We have shown that the CDW manifestations against the non-homogeneous background can explain both subtle DHS structures in the tunnel spectra for high-T oxides and large pseudogap features observed both below and above T_c. The DHS is smoothly transformed into the pseudogap-like DOS depletion as T grows. Hence, DHSs and pseudogaps should be considered as manifestations of the same CDW (electron-hole pairing) phenomenon.

It is pertinent to note that the phenomena described above should be observed for not only oxide perovskites but other CDW superconductors as well. In particular, we mean a very interesting layered CDW marginally insulating compound $TiSe_2$ intercalated by Cu: $Cu_{\times x}TiSe_2$ [15]. Here superconductivity appears if the compound is doped to $x \approx 0.4$, whereas CDWs are resistant to charge-carrier mitigating influence up to $x \approx 0.6$.

TE acknowledges the Grant-in Aid for Scientific Research (No. 19540370) given by the Japan Society for the Promotion of Science. AMG highly appreciates FY2007 Fellowship No. S-07042 granted by the Japan Society for the Promotion of Science. AMG and AIV are grateful to Kasa im. Józefa Mianowskiego, Polski Koncern Naftowy ORLEN, and Fundacja Zigmunta Zalieskigo for the financial support of their visits to Warsaw. MSL was supported by the Polski KBN grant No. 1P03B01827.

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