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ENERGY GAP ANISOTROPY AND TUNNELING SPECTROSCOPY OF HIGH-TEMPERATURE SUPERCONDUCTORS

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Tunneling characteristics of high- $T_{\rm c}$ superconductor junctions are strongly influenced by surface degradation effects. A simple theoretical approach to the problem is developed for an arbitrary normal region near the oxide interface. It is shown that the zero-bias conductance value of a normal-metal—superconductor contact together with the low-frequency, near-zero-voltage shot-noise spectrum can serve as a diagnostic tool to probe directly the gap symmetry of a superconductor. On the base of the model, some criteria to distinguish between s- and d-wave pairing states are proposed and recent experimental findings for high-temperature superconductor contacts are critically analyzed.

1. Introduction

Tunneling spectra of high-temperature superconductors (HTSC) usually exhibit highly anomalous conductance features that have not been frequently observed in the corresponding curves for conventional superconducting metals. Up to now, it is not clear whether these features are related to the intrinsic characteristics of the oxides, or they appear as a result of specific electrical properties of non-ideal HTSC interfaces. In particular, it concerns the inner-gap conductance peaks that have been repeatedly observed in HTSC-based junctions [1,2] and received a great interest since it was recognized that their appearance in the HTSC ab-plane tunneling spectra can be interpreted as an impact of the anisotropic d-wave orbital symmetry of the order parameter [3]. Now the main question concerning zero-bias conductance peaks (ZBCP) is if they can be understood within the ordinary s-wave pairing symmetry, or the only possible explanation is that related to the d-wave scenario. As it will be shown below, the anomalies can appear in the first case too if to take into account the complicated electrical properties of HTSC surfaces. In many cases they are covered by a thin non-superconducting (N') region greatly influencing their contact characteristics [4]. Mainly, it arises due to degradation processes in the upper atomic layers forming an oxygen depletion region on the cuprate surface [5]. In this paper we develop a simple theoretical approach to the ballistic charge transport in the heterostructure formed by a normal-metal injector and a superconducting bulk covered by a thin non-superconducting layer. The model captures the essential physics of the contacts and follows the main lines of the previous publications on the same subject [6-8] extending them to the case of an anisotropic order parameter and the magnetic-field effect. The main goal of this work is to obtain some general results that are independent on the nature of the transitional layer and to elaborate simple criteria that would be useful to distinguish between sand d-wave pairing states.

2. Formalism

Let us consider a superconducting heterogeneous structure shown in Fig. 1. An elastic-scattering nonsuperconducting N' part of the system is connected to a normal-metal (N) reservoir. The superconductor (S) with the pair potential depending on the direction of the traveling quasiparticle is connected to a superconducting reservoir. We assume the usual step-function approximation for the superconducting order parameter [9,10] and ignore the self-consistency of its spatial variation. The Fermi wave numbers k_F and other electronic parameters will be equal in the normal and superconducting regions of the mesoscopic system. The applied voltage V shifts the chemical potentials in both reservoirs and causes the current I in response to V. For simplicity, we shall focus solely on the near-zero-voltage, zero-temperature, two-dimensional conductance G(V) = dI/dV. For voltages corresponding to energies below the minimal value of the superconducting energy gap it is given by the well-known Landauer-type formula [11,12]:

$$G(V) = \frac{4e^2}{h} \sum_{n=1}^{M} \left| R_n^{he}(eV) \right|^2, \tag{2.1}$$

where $R_n^{he}(\varepsilon)$ is the scattering amplitude for an electron in the *n*-th mode with an excitation energy ε (ε is measured with respect to the Fermi energy) incident from left in the normal region and reflected back as a hole; M is the number of the propagating modes that will be characterized further by an initial wave vector \mathbf{k}_e ; e is the elementary charge. The amplitude $R_n^{he}(\varepsilon)$ can be expressed entirely in terms of scattering and transmission characteristics of an N' region, as well as those of the N'/S interface. It has to be emphasized that in our model these parts of the system are separated spatially (see Fig. 1). For oxide superconductors the corresponding distance of the order of the superconducting coherence length $\xi(\mathbf{k})$ is very small in comparison with the width of the degraded layer and its effect may be ignored.

Consider now in detail the scattering characteristics mentioned above. An electron with an

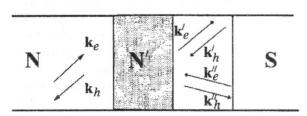


Fig. 1. Sketch of the two-dimensional heterostructure considered

injected wave vector \mathbf{k}_e transfers the N' layer (the corresponding amplitude is equal to $t_e(\mathbf{k}_e, \epsilon)$) without any energy losses and reaches the N'/S interface with a wave vector \mathbf{k}_e' and the same energy ϵ . Then it retroreflects as a hole (see Fig. 1) with a scattering amplitude [10]

$$r^{he}(\mathbf{k}'_{e}, \varepsilon) = \exp(-i\arccos(\varepsilon / |\Delta(\mathbf{k}'_{e})|) - i\varphi(\mathbf{k}'_{e}) + i\psi(\mathbf{k}'_{e})). \tag{2.2}$$

Here $\Delta(\mathbf{k}'_e)$ and $\varphi(\mathbf{k}'_e)$ are direction-dependent modulus and phase of the order parameter, respectively; $\psi(\mathbf{k}'_e)$ accounts the effect of a surface current in a superconductor. Without a surface current $\psi(\mathbf{k}'_e) \equiv 0$ but it is not so for a stationary magnetic field **B** applied perpendicular to the plane of Fig. 1. For the field penetration depth λ much greater than $\xi(\mathbf{k})$, as in the HTSC compounds, the width of the layer with a depressed pair potential is of the order of $\xi(\mathbf{k}'_e)$ in the direction considered. Inside the layer the vector potential **A** that can be chosen perpendicular to the field direction is constant and equals to $B\lambda$. Then the additional magnetic-

field dependent part of the phase shift occurring by a charge after its scattering from the superconductor is given by the following relation

$$\psi^{(B)} = \int d\mathbf{s} \left[\pm e\mathbf{A}/\hbar \right] = \pm 2\pi B/B_0(\mathbf{k}_e')\cos\alpha , \qquad (2.3)$$

where $B_0(\mathbf{k}_e') = \Phi_0/(\lambda \xi(\mathbf{k}_e'))$, $\Phi_0 = h/(2e)$, α is the angle between the \mathbf{k}_e' and \mathbf{A} vectors, the sign of the phase shift $\psi^{(B)}$ is defined by the field orientation and does not depend on the charge sign.

After the Andreev-scattering process a hole with a wave vector \mathbf{k}'_h and energy ε transfers through the non-superconducting transitional region with an amplitude $t^h(\mathbf{k}'_h, \varepsilon)$ or scatters from it with an amplitude $r^h(\mathbf{k}'_h, \varepsilon)$. In the last case it experiences the backscattering from the N'/S interface into an electron state with a wave vector \mathbf{k}''_e and energy ε that for ε near zero scatters back into an electron with a wave number \mathbf{k}'_e . For a scattering event when a hole is retroreflected as an electron we obtain an equation similar to Eq. (2.2)

$$r^{eh}(\mathbf{k}_{h}^{"}, \varepsilon) = \exp(-i\arccos(\varepsilon/|\Delta(\mathbf{k}_{h}^{"})|) + i\varphi(\mathbf{k}_{h}^{"}) + i\psi(\mathbf{k}_{h}^{"})). \tag{2.4}$$

In principle, we have a cascade of processes resulting in a hole going back with the wave vector \mathbf{k}_h . It consists of Andreev-like scattering events when an electron is retroreflected as a hole or a hole is scattered into an electron state with the same mode index (an outgoing particle traces back along the path of the incoming charge) and reflections from the N layer when an electron (hole) is scattered only in electron (hole) states. Summing the contributions, we arrive at

$$R^{he}(\mathbf{k}_{e}, \varepsilon) = \frac{t^{h}(\mathbf{k}'_{h}, \varepsilon)r^{he}(\mathbf{k}'_{e}, \varepsilon)t^{e}(\mathbf{k}_{e}, \varepsilon)}{1 - r^{he}(\mathbf{k}'_{e}, \varepsilon)r^{e}(\mathbf{k}''_{e}, \varepsilon)r^{eh}(\mathbf{k}''_{h}, \varepsilon)r^{h}(\mathbf{k}'_{h}, \varepsilon)}.$$
(2.5)

Here the amplitudes $t^{e(h)}$ and $r^{e(h)}$ include all phase shifts accumulated during electron (hole) traveling through the normal transitional region. For a given mode with an initial wave vector \mathbf{k}_e we obtain

$$G(\mathbf{k}_{e}, V) = \frac{4e^{2}}{h} \frac{\left|t^{e}(\mathbf{k}_{e}, eV)\right|^{2} \left|t^{h}(\mathbf{k}'_{h}, eV)\right|^{2}}{1 + \left|r^{e}(\mathbf{k}''_{e}, eV)\right|^{2} \left|r^{h}(\mathbf{k}'_{h}, eV)\right|^{2} - 2\operatorname{Re}\left\{e^{i\phi}r^{e}(\mathbf{k}''_{e}, eV)r^{h}(\mathbf{k}'_{h}, eV)\right\}}$$
(2.6)

with

$$\phi = -\arccos(\varepsilon / \left| \Delta(\mathbf{k}_{h}^{"}) \right|) - \arccos(\varepsilon / \left| \Delta(\mathbf{k}_{e}^{'}) \right|) + \phi(\mathbf{k}_{h}^{"}) - \phi(\mathbf{k}_{e}^{'}) + \psi(\mathbf{k}_{h}^{"}) + \psi(\mathbf{k}_{e}^{"}). \tag{2.7}$$

The corresponding normal-state conductance depends only on the transmission properties of the interlayer between two reservoirs and is equal to

$$g(\mathbf{k}_e, V) = \frac{2e^2}{h} |t^e(\mathbf{k}_e, eV)|^2$$
 (2.8)

Let us analyze the formula (2.6). The nominator consists of the product of two transmission amplitudes. In the presence of time-reversal symmetry, i.e., in zero magnetic field, electrons and holes at the Fermi energy can be considered as each other's time-reversed particles with opposite energy signs and thus $\left|t^h(\mathbf{k}'_h, \varepsilon)\right|^2 = \left|t^e(\mathbf{k}_e, -\varepsilon)\right|^2$. Because of it in the case of an energy-dependent interlayer transmissivity a ZBCP appears independently on the superconducting

pairing state. It seems to be just a reason why such anomaly has been detected in the tunneling characteristics of ordinary s-wave superconductors. Another source of a ZBCP is the denominator of Eq. (2.6) that defines the energies of the quasi-bound states formed by scattering processes from the N' layer and the N'/S interface. Their positions in energy depend on the phase difference $\varphi(\mathbf{k}''_h) - \varphi(\mathbf{k}'_e)$. If we are dealing with an isotropic s-wave superconductor where the effective pair potential does not change with the wave vector direction, i.e., $\varphi(\mathbf{k}''_h) = \varphi(\mathbf{k}'_e)$, then in the absence of a magnetic field φ is equal to $-\pi$ at $\varepsilon = 0$. It means that the denominator is maximal at zero voltage and hence without an impact of the nominator we obtain a dip in the conductance spectrum at V = 0. Taking into account that at the Fermi energy electron and hole excitations coincide we find the following expression

$$G_s(\mathbf{k}_e, 0) = \frac{4e^2}{h} \frac{\left| t^e(k_F, 0) \right|^4}{\left(1 + \left| r^e(k_F, 0) \right|^2 \right)^2} = \frac{4e^2}{h} \frac{\left| t^e(k_F, 0) \right|^4}{\left(2 - \left| t^e(k_F, 0) \right|^2 \right)^2} \,. \tag{2.9}$$

From Eqs. (2.9) and (2.8) it follows that for any ballistic normal-superconducting junction the ratio of conductance values in the normal and superconducting states (it is known as the normalized conductance) at zero voltage bias cannot exceed the factor of two that is reached only for an ideal situation when $\left|t^e(k_F,0)\right|^2=1$.

For anisotropic superconductors this result changes dramatically. Let us illustrate it for a $d_{x^2-y^2}$ -wave superconductor with $\Delta(\mathbf{k}) = \Delta_d \cos(2\Theta_{\mathbf{k}})$ (the angle $\Theta_{\mathbf{k}}$ is measured relative to the crystalline axis along which the *d*-wave order parameter reaches maximum). In this case we have a situation when the order parameter can be of the opposite sign for \mathbf{k}_h'' and \mathbf{k}_e' directions. Without magnetic fields for such a mode we obtain $\phi(\mathbf{k}_h'') - \phi(\mathbf{k}_e') = \pi$. From Eq. (2.6) for an specular-scattering interface between a normal injector and a *d*-wave superconductor we arrive at

$$G_d(\mathbf{k}_e, 0) = \frac{4e^2}{h} \frac{\left| t^e(k_e, 0) \right|^4}{\left(1 - \left| r^e(k_e, 0) \right|^2 \right)^2} = \frac{4e^2}{h} . \tag{2.10}$$

The formula looks like an expression for a normal metal – s-wave superconductor junction with a clean interface and appears as a result of the constructive interference for scattering quasiparticles. The last statement concerns only the conductance in the superconducting case. If to transfer a d-wave superconductor into the normal state we obtain the same result (2.8) as for the s-wave symmetry. It means that for small transparencies of the N' interlayer the mode contribution into the normalized zero-bias conductance value may be huge. As a result, the whole normalized conductance spectrum defined by summation over all modes can exhibit a giant ZBCP. The fundamental difference in the ϕ value reveals itself also in the magnetic-field dependence. If the magnetic field penetration depth is much greater than the typical width of the normal interlayer (as in the HTSC compounds), the main impact of the field arises from Eq. (2.3) and its effect on the charge traveling inside the N' region may be ignored. For low fields we obtain an increase of the zero-bias conductance value for an s-wave superconductor and a decreasing function of B in the case of a d-wave superconductor.

Above we have been dealing with the average current $I = \langle I(t) \rangle$. In the presence of the charge transport an electrical shot noise (time-dependent fluctuations of the current around I) arises due to the discreteness of the charge carriers. Its measurement can provide an additional information about the nature of the phase-coherent transport in a heterostructure [13]. The usu-

ally used characteristic of this process is the Fourier transform of the current-current correlator $S(\omega) = \int dt \exp(i\omega t) \langle \Delta I(t) \Delta I(0) \rangle$, where $\langle \Delta I(t) \rangle = I(t) - \langle I(t) \rangle$ is the current fluctuation away from its average. In the low-frequency limit the correlation spectrum can be expressed in terms of the $R_n^{he}(\varepsilon)$ scattering amplitudes [14]. At T=0 and for low-voltage biases, this quantity for a normal-metal - superconductor junction is equal to

$$S_{V}(0) = \frac{8e^{3}|V|}{h} \sum_{n=1}^{M} \left| R_{n}^{he}(eV) \right|^{2} (1 - \left| R_{n}^{he}(eV) \right|^{2}). \tag{2.11}$$

In ordinary s-wave superconductors with uncorrelated electron transmission the shot noise is twice the Poisson value for the corresponding normal junction that is known to be equal to 2e|I|. But it is only the maximal noise power that can be reduced as a consequence of noiseless open scattering channels [14]. In a d-wave superconductor every n-th channel producing a giant contribution to the zero-bias conductance corresponds to $\left|R_n^{he}(eV)\right|^2 = 1$ and thus is completely noiseless. It means that in this case the shot noise has to be strongly suppressed and the effect will crucially depend on the junction orientation.

3. Challenges

Our results show that an appearance of a ZBCP itself is insufficient for proving the unconventional nature of the pair potential symmetry in HTSC because an enhancement of the differential conductance in junctions formed by a normal-metal injector and a superconducting oxide could be in principle explained within the ordinary pairing scenario if to consider a realistic model with a normal interlayer between normal and s-wave superconducting bulks. To make a final conclusion about the order parameter symmetry, we need more sophisticated criteria. Below we propose such criteria easily verified experimentally without any detailed comparison with the curves theoretically predicted:

- (i) the amplitude of the ZBCP. As it was emphasized above, the normalized conductance at V=0 for an s-wave superconductor cannot exceed the factor of two. A narrow ZBCP with a greater height can serve as a first indication of the d-wave scenario in a superconductor studied.
- (ii) the angular dependence of the ZBCP. The next test relates to the drastic effect of the junction orientation on the ZBCP for a *d*-wave situation. First of all, a maximum meeting the first criterion must be observed only for *ab*-tunneling curves and, if so, its value must strongly depend on the injection direction with the most prominent anomaly corresponding to the maximal value of the traveling modes where the electron and hole states involving in the scattering process experience phase-reversed pair potentials. This test can be realized, e.g., in STM spectroscopic measurements.
- (iii) the ZBCP dependence on the interface transmissivity. For a d-wave orbital symmetry the maximal zero-bias value must not be greatly influenced by modification of the N' layer scattering properties. On the contrary, in the s-wave case the conductance spectrum strongly depends on its transmissivity. The best way to realize this test is to change the tip-specimen distance in STM experiments.
- (iv) the magnetic field effect on the ZBCP. For low fields a ZBCP has to increase for an s-wave superconductor and to decrease in the d-wave state.
- (v) the zero-voltage shot-noise power. For d-wave superconductors the shot-noise power spectrum has to be highly anisotropic in comparison with the s-wave case and greatly (or even completely) suppressed for a definite junction orientation corresponding to a maximal ZBCP.

Now we want to transfer to recent experimental results and compare them with the criteria proposed. Because shot-noise measurements on the HTSC-based junctions are unknown to us, we shall discuss only the corresponding transport properties. The main experimental data (even those invoked to prove the unusual orbital symmetry of the cuprate order parameter) do not meet the requirements formulated above and thus, in principle, could be interpreted within the standard theory. But at the same time we have found some results that can be understood only within the d-wave pairing hypothesis. First of all, it concerns the value of the zero-bias peak in the normalized conductance that was detected to be about 8 in STM experiments for the (110) crystal face of YBCO [15] and about 3 for an Ag/BSCCO junction [16]. A ZBCP dependence on the junction orientation measured in the paper [15] agrees with the second criterion. The findings of the work [17] well correspond to the third one. For the most prominent zero-bias peak value in the STM investigations of a LSCO single crystal the authors found no effect of the tip-sample distance changed in a wide range. There are some observations of the magnetic field impact on the ZBCP [18,19]. Although in these papers ZBCP amplitudes have not been greater than the value of two, their behavior agrees with our results. The anomalies were suppressed by magnetic field application in contrast with the data for a conventional superonductor as, for example, it was obtained in the paper [20].

To conclude we emphasize that some experimental findings for HTSC oxides cannot be definitely interpreted in terms of the conventional pairing theory and have to be regarded as arguments for an unusual symmetry of the order parameter in superconducting cuprates. More refined experiments are needed to clear up the controversial situation.

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