SURFACE ELECTRON SCATTERING IN d-WAVE SUPERCONDUCTORS

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Theoretical model of a rough surface in a d-wave superconductor is studied for the general case of arbitrary strength of electron scattering by an impurity layer covering the surface. Boundary conditions for quasiclassical Eilenberger equations are derived at the interface between the impurity layer and the d-wave superconductor. The model is applied to the selfconsisrent calculation of the surface density of states and the critical current in d-wave Josephson junctions.

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Understanding the transport properties of surfaces and interfaces in high temperature superconductors (HTS) is important for correct interpretation of the experimental data and for applications of these materials. Up to now surface peculiarities in d-wave superconductors were extensively discussed in the framework of theoretical models based on quasiparticle reflection from specular interfaces [1–4]. The influence of surface roughness in this approach was studied by the Ovchinnikov method [5], namely, by introducing a thin impurity layer covering the surface [3–6]. The degree of roughness is then measured by the ratio of the layer thickness d to the quasiparticle mean free path in the layer ℓ. This approach was used to study the smearing of Andreev surface bound states by weak disorder $(d \ll \ell)$.

The regime of strong surface roughness, $d \gg \ell$, was discussed in [7]. In this case the parameter-free boundary conditions were derived at the interface between the superconductor and the disordered layer. Similar conditions were also derived earlier in [8] at rough walls in superfluid ^{3}He-B. As was shown in [7], an isotropic order parameter is nucleated in the disordered layer even in the absence of the bulk subdominant pairing interaction in the s-wave channel. This leads to the formation of the gapless s-state at the interface. This phenomenon was called an anomalous proximity effect between a d-wave superconductor and a disordered layer.

In the present paper we consider the anomalous proximity effect between a d-wave superconductor and a surface impurity layer of thickness $d \ll \min\{\sqrt{\xi_0 \ell},\ \xi_0\}$ in the general case of an arbitrary electronic mean free path ℓ.

We consider the interface oriented normally to the crystallographic ab plane and assume elastic Born scattering. The normal and anomalous quasiclassical propagators, g and f, depend on the coordinate x in the direction of the surface normal and on the angle θ between the surface normal and quasiparticle trajectory and obey the quasiclassical Eilenberger equations [9]. Using the substitutions [10]

$$f = \frac{2a}{1+ab}, \quad f^+ = \frac{2b}{1+ab}, \quad g = \frac{1-ab}{1+ab}, \tag{1}$$

we rewrite these equations in terms of the scalar differential equations of the Ricatti type

$$v \cos \theta \frac{db(x)}{dx} - \left[2\omega_n + \frac{1}{\tau} \langle g \rangle + b(x)(\Delta(x) + \frac{1}{2\tau} \langle f^+ \rangle) \right] b(x) = -\Delta(x) - \frac{1}{2\tau} \langle f^+ \rangle, \quad (2)$$

$$v \cos \theta \frac{da(x)}{dx} + \left[2\omega_n + \frac{1}{\tau} \langle g \rangle + a(x)(\Delta(x) + \frac{1}{2\tau} \langle f \rangle) \right] a(x) = \Delta(x) + \frac{1}{2\tau} \langle f \rangle. \quad (3)$$

The pair potential Δ should be found from the selfconsistency equation

$$\Delta \ln \frac{T}{T_c} + 2\pi T \sum_{\omega > 0} \left(\frac{\Delta}{\omega} - \langle \lambda(\theta, \theta') f \rangle \right) = 0. \quad (4)$$

Here $\omega_n = \pi T(2n+1)$ are the Matsubara frequencies, v is the Fermi velocity, $\tau = \ell/v$. Assuming a cylindrical Fermi surface, angle averages are defined as $\langle ... \rangle = (1/2\pi) \int_0^{2\pi} (...) d\theta$.

We consider pure d-wave interaction in the bulk with the coupling constant [11]

$$\lambda(\theta, \theta') \equiv \lambda_d(\theta, \theta') = 2\lambda \cos(2(\theta - \alpha)) \cos(2(\theta' - \alpha)),$$

where α is the misorientation angle between the crystallographic a axis and the surface normal. In this case the bulk anomalous propagator has the d-wave symmetry

$$b(+\infty, \theta) = a(+\infty, \pi + \theta) = \frac{\sqrt{2}\Delta_\infty \cos(2(\theta - \alpha))}{\omega + \sqrt{\omega^2 + 2\Delta_\infty^2 \cos^2(2(\theta - \alpha))}}. \quad (5)$$

As will be shown below, this symmetry is violated near the interface.

Equations (2)-(4) must be supplemented with the boundary conditions connecting functions $b(0, \theta)$ and $a(0, \theta)$ which describe respectively the electrons incident and reflected from the interface. This can be done by matching the solutions in the impurity layer $(-d < x < 0)$ and in the clean d-wave region $(0 < x)$.

Since the thickness of the impurity layer $d \ll \xi_{eff} = \min \{ \sqrt{\xi_0 \ell}, \xi_0 \}$, we can neglect the terms proportional to ω and Δ in (2) and (3) and consider $\langle f \rangle$ and $\langle g \rangle$ as spatially-independent constants, which must be determined selfconsistently. Making use of the boundary condition [12] at the totally reflecting free specular interface $(x = -d)$

$$b(-d, -\theta) = a(-d, \theta), \quad (6)$$

we find the solution of the equations (2), (3) at $-d \leq x \leq 0$ in the form

$$\frac{Fb(x, -\theta) + G - 1}{Fb(x, -\theta) + G + 1} = \frac{Fb(0, -\theta) + G - 1}{Fb(0, -\theta) + G + 1} \exp \{kx\}, \quad (7)$$

$$\frac{Fa(x, \theta) + G - 1}{Fa(x, \theta) + G + 1} = \exp \{-k(d + x)\} \frac{Fb(-d, -\theta) + G - 1}{Fb(-d, -\theta) + G + 1}, \quad (8)$$

$$k = \frac{\sqrt{\langle g \rangle^2 + \langle f \rangle^2}}{\ell \cos(\theta)}, \quad F = \frac{\langle f \rangle}{\sqrt{\langle g \rangle^2 + \langle f \rangle^2}}, \quad G = \frac{\langle g \rangle}{\sqrt{\langle g \rangle^2 + \langle f \rangle^2}}.$$

From (7), (8) after a simple algebra we arrived at the boundary condition at the interface between the clean d-wave superconductor and disordered layer

$$a(0,\theta) = b(0,-\theta)\frac{(1 - G\tanh(kd))}{(Fb(0,-\theta)+G)\tanh(kd)+1} + F\frac{\tanh(kd)}{(Fb(0,-\theta)+G)\tanh(kd)+1}. \quad (9)$$

Eq. (9) describes the fact that the amplitude of anomalous Green's function along outgoing trajectories, $a(0,\theta)$, consists of two parts. The first, specular part, is proportional to $b(0,-\theta)$ and describes the correlation between with the incoming $-\theta$ and reflected θ trajectories. The second, diffusive part, is proportional to F and describes an average contribution of all the incident trajectories to the outgoing one in the $\theta-$direction.

In the limit of weak disorder $(d \ll \ell)$ the boundary condition (9) reduces to the specular one (6). At finite d there is a cone of angles $\arccos d/\ell \leq \theta \leq \pi/2$ in which the scattering from the interface is rather diffusive than specular. The larger is d the smaller is the correlation between incoming and outgoing trajectories.

In the limit of strong disorder $(d \gg \ell)$ the solutions (7), (8) transform to those of Usadel equations obtained in [7] and it follows from (9) that

$$a(0) = \frac{\langle f(0,\theta)\rangle}{1 + \langle g(0,\theta)\rangle}. \quad (10)$$

This is exactly the condition used previously in [7] for the analysis of strongly disordered d-wave interfaces. According to this condition the incoming and outgoing trajectories at the rough interface with strong disorder are completely uncorrelated as a result of the scattering from the impurity layer.

It is straightforward to find selfconsistent solutions of the set of equations (2)-(5), (9). First, we have numerically integrated the equation (2) for $b(x)$ with the initial condition (5) along the trajectory from $x = +\infty$ (bulk) to $x = 0$ (interface). Then the eq. (3) for $a(x)$ was integrated from $x = 0$ to $x = +\infty$ with the initial condition (9). The angle averages $\langle f(0)\rangle$ and $\langle g(0)\rangle$ and the pair potential $\Delta(x)$ were calculated iteratively.

We have applied this model for calculation of the low-temperature conductance of NID tunnel junction, which is expressed through the surface density of states $N(0,\theta)$

$$R_N dI/dV = \frac{\int_{-\pi/2}^{\pi/2} N(0,\theta)D(\theta)\cos\theta d\theta}{\int_{-\pi/2}^{\pi/2} D(\theta)\cos\theta d\theta}, \quad (11)$$

where R_N is the normal state junction resistance and $D(\theta)$ is the barrier transmission coefficient. The angle-resolved surface density of states is given by $N(0,\theta;\varepsilon) = \text{Re}(g(0,\theta;\omega = -i\varepsilon))$.

Fig.1 shows the results of calculations for $\alpha = 20^0$ and various values of the surface scattering parameter d/ℓ. We have chosen δ-shaped potential barrier with the angular dependence of transmission $D(\theta) = D(0)\cos^2\theta$. Zero-bias anomaly (ZBA), which is the manifestation of the sign reversal of the d-wave pair potential, is strongly broadened with increase of d/ℓ. In the limit of weak disorder $d/\ell \ll 1$ the results exactly correspond to those of Ref.[3].

With the increase of d/ℓ ZBA is smeared out completely, while the signatures of finite-energy Andreev bound states are still present. The latter are due to quasiparticles trapped in the surface region with the reduced pair potential $\Delta(x)$. As is seen from Fig.1, the angle-averaged density of states in the disordered layer is gapless and has a number
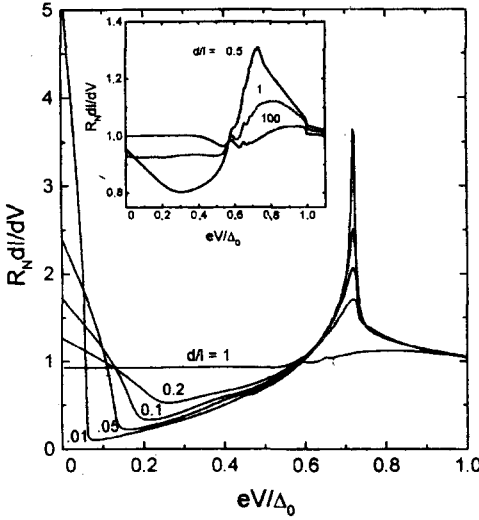
Fig.1.Smearing of ZBA in the low-temperature conductance of NID junction. Inset demonstrates the oscillations for large d/ℓ due to the finite-energy Andreev bound states
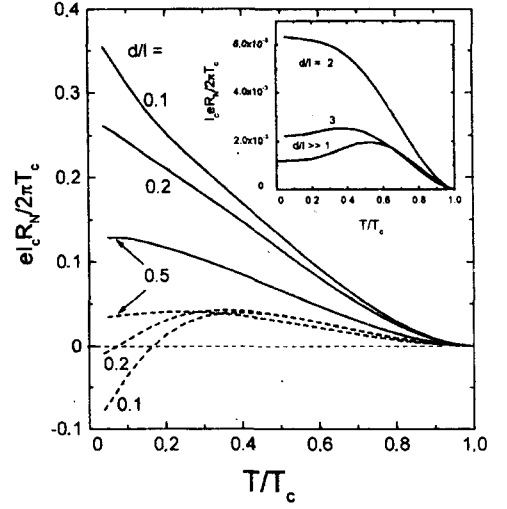
Fig.2. Influence of surface roughness on the temperature dependence of the critical current in the DID tunnel junction. Dashed lines: symmetrical junction $\alpha_1 = \alpha_2 = 20^0$. Dotted lines: mirror junction $\alpha_1 = -\alpha_2 = 20^0$. Inset: nonmonotonous behavior of I_c for $d/\ell \gg 1$

of peaks at the energy below the bulk pair potential. Note that for large values of d/ℓ there are several (weak) peaks corresponding to more than one bound state, in contrast to the case of specular interface when only a single bound state exists at finite energy [3]. This is because the average trajectory length of trapped quasiparticles, which determines the number of resonances, is larger than ξ_0 in the diffusive case. Mathematically this fact is described by the boundary condition Eq.9.

Next we apply the model to the study the influence of surface roughness on the Josephson supercurrent in a tunnel junction based on d-wave superconductors (DID junction). The critical current is given by the expression [12, 13]

$$eR_N I_c = \frac{\pi T \sum_{\omega>0} \int_{-\pi/2}^{\pi/2} [f_{1s}(\theta) f_{2s}(\theta) - f_{1a}(\theta) f_{2a}(\theta)] D(\theta) \cos\theta d\theta}{\int_{-\pi/2}^{\pi/2} D(\theta) \cos\theta d\theta}. \qquad (12)$$

Here $f_{1,2s(a)} = (f_{1,2} \pm f_{1,2}^+)/2$ and where $f_{1,2}$ are the surface Green's functions of the left (right) electrode.

The critical current was calculated numerically using the solutions for $f_{1,2}$ and assuming $D(\theta) = D(0) \cos^2\theta$. We consider two cases: 1) symmetric junction with the misorientation angles $\alpha_1 = \alpha_2 = 20^0$, 2) antisymmetric (mirror) junction with $\alpha_1 = -\alpha_2 = 20^0$. The results of calculations are shown in Fig.2. In complete agreement with the results of Ref. [13 − 16] the mirror junction exhibits a nonmonotonous $I_c(T)$-dependence due to the anomaly $f_{1,2a} \sim 1/\omega_n$ at low frequencies related to the midgap surface bound state. Like ZBA in conductance, this anomaly is smeared out with the increase of the surface scattering parameter d/ℓ.

In the strong scattering regime $d/\ell \gg 1$ the $I_c R_N$ product of the DID junction becomes small and saturates at the level $eI_c^{SIS}R_N/2\pi T_c \sim 10^{-3}$ (the corresponding number for a conventional SIS junction is $eI_c^{SIS}R_N/2\pi T_c \simeq 0.44$). The anomalous contribution $f_{1a}f_{2a}$ vanishes in this case and I_c for the symmetric and mirror junctions coincide. However, as shown in inset in Fig.2, $I_c(T)$ becomes nonmonotonous with an increase of d/ℓ. The reason is the destructive interference within the impurity layer: the phases of Eilenberger functions on the incoming trajectories alternate due to the d-wave angular structure. As a result, the angle average $\langle f_{1,2} \rangle$ vanishes at $\omega_n \ll \pi T_c$, reaches a maximum at $\omega_n \sim \pi T_c$ and falls down as ω_n^{-2} at $\omega_n \gg \pi T_c$. It is the property $f_{1,2s} \to 0$ at small ω_n which is the reason of decreasing $I_c(T)$ at low T. Variation of the misorientation angle α for $d/\ell \gg 1$ does not change the $I_c(T)$ behavior, while $I_c R_N$ product at $T = 0$ scales as $\cos^2(2\alpha)$.

In conclusion, we have derived the boundary conditions for the Eilenberger functions at the rough surface of a d-wave superconductor and applied them to the study of the crossover from specular to diffusive surface scattering. The low-temperature conductance of NID tunnel junction and the Josephson supercurrent in DID tunnel junction are calculated for arbitrary degree of surface roughness. It is shown that the width of the anomalies in the conductance and in the critical current is controlled by a single scattering parameter d/ℓ.

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