Effect of surface pair breaking, entirely neglected by M. Samanta and S. Datta [ Phys.Rev. B 57, 10972 (1998) ], is quite important in considering surface (or interface ) quasiparticle bound states and associated characteristics of junctions involving unconventional superconductors. The whole class of bound states with nonzero energy is simply omitted within the framework of the approach, using uniform spatial profile of the order parameter up to the interface. The consideration of these bound states (as well as midgap states) to current-voltage characteristics of the SIS’ tunnel junctions were studied for the first time in our earlier article. Dependence of midgap state contribution to the Josephson critical current upon crystal to interface orientations is shown as well to be fairly sensitive to the effect of surface pair breaking.

In a recent article [1], M. Samanta and S. Datta considered theoretically electrical transport of junctions involving unconventional superconductors. In particular, they discussed contributions to junction properties from midgap surface states, that arise in d-wave superconductors due to sign change of the order parameter. They pointed out that the effect of midgap states is most prominent for weakly coupled junctions (tunneling limit), concentrating in this respect mainly on the first order theory in transmission coefficient. In evaluating electric current across the junction the authors [1] neglected from the very beginning all the effects of surface pair breaking, considering order parameters from both sides of the junction to be equal to their bulk values up to the junction barrier plane. In this Comment we demonstrate that the approximations [1] lead to incorrect results for unconventional superconductors, since effects of surface pair breaking is of crucial importance for the I-V characteristics of tunnel junctions, especially due to the appearence of surface quasiparticle states with nonzero energy. Also we point out that correct theory for current-voltage characteristics of tunnel junctions involving anisotropically paired superconductors was developed for the first time in [2].

In contrast to s-wave isotropic superconductors, d-wave superconductors are known to be quite sensitive to any inhomogeneities (impurities, surfaces, interfaces). In particular, for many of crystal to surface orientations the order parameter turns out to be essentially suppressed on the tunnel barrier plane. Several important experimental methods used for studying the anisotropic structure of the order parameter, for example, tunneling measurements are, in turn, fairly sensitive to the superconducting properties close to the surface of the sample. The effects of anisotropic pairing on the tunneling density of states (the local quasiparticle spectrum at the surface), the Josephson and quasiparticle current of SIS’ and SIN tunnel junctions were theoretically studied by taking account of surface pair breaking and quasiparticle surface bound states in [3–5].

Our main assertion is that the whole class of surface quasiparticle states is omitted in [1] due to the disregard the surface pair breaking there. Spatial profile of the order parameter suppressed near the surface, can be considered as effective potential well for quasiparticles, which suffer Andreev reflection towards the surface in this case. Andreev reflection processes along with the conventional reflection from the surface, can result in forming quasiparticle bound states (Andreev bound states) localized near the surface within the characteristic length roughly of order of the superconducting coherence length. Quasiparticle surface bound states with nonzero energy are present in the case of surface pair breaking and do not exist for a uniform spatial profile of the order parameter. Only mid-gap surface states, having supersymmetric origin, still exist for that uniform model profile. Thus, for the order parameter, which is independent of the spatial coordinate up to the surface or interface, one can find in the tunneling limit only peak at zero energy in the local density of states, while all nonzero peaks taking place in the presence of surface pair breaking turn out to disappear in the model.

Bound states with nonzero energy result in the anomalies of current-voltage characteristics in the presence of externally applied voltage, described in [6,7] and entirely omitted in [1]. Positions and characteristics of those anomalies turn out to be associated with positions and types of extremal points of momentum dependence (dispersion) of bound state energies. Possible characteristic points on the I-V curves for SIS’ and SIN tunnel junctions are described in [6,7], by using Eilenberger’s equations for the quasiclassical Green’s functions combined with corresponding boundary conditions and the microscopic expression for the tunnel current.

Midgap states are dispersionless bound states, so that
their contributions to junction characteristics can differ from the ones with nonzero energy. In particular, if midgap states take place only from one side of a SIS’ tunnel junction, they contribute to the specific features of quasiparticle current (and not to ac Josephson effect) at the voltage values, determined by anomalies of the local density of states on the other bank of the junction. For example, in the case of an isotropic s-wave superconductor on the other bank, with an order parameter $\Delta$, quasiparticle current has peaks at voltage values $eV = \pm \Delta$. The peaks have inverse square-root “divergent” behavior in the vicinity of $|eV| = |\Delta|$:

$$I_{qp} \propto \Theta(|eV| - |\Delta|)/\sqrt{|eV|^2 - |\Delta|^2}.$$  

This particular result, obtained for the first time in [4], was rederived in [1] in disregarding the surface pair breaking. There are various reasons for the modification of this inverse square root singularity, at least sufficiently close to the point $|eV| = |\Delta|$, in particular, due to the surface roughness and bulk impurities. We do not discuss in the Comment this kind of effects, determining the height of the peaks, since it is not discussed at all in [1]. We note that even in the absence of any surface pair breaking there are some additional peaks and jumps of the conductance of SIS’ junction, involving anisotropically paired superconductors. Positions of the specific features of the conductance are determined by the extremal points of the sum of order parameters from both sides of the junction (and for the difference as well, although not for sufficiently low temperatures), taken for incoming and transmitted quasiparticle momenta [2]. These specific features are omitted in [1] as well.

As it is known, for SIN tunnel junction of high quality involving a d-wave superconductor, the zero-bias anomaly of the conductance takes place due to the midgap states. Let the normal metal suffer the superconducting transition at lower temperature into a s-wave isotropic superconducting state. Then, according to the result of Ref. 2, just stated above, the zero-bias conductance peak should split into two peaks lying at the applied voltage $eV = \pm \Delta(T)$. This splitting increases along with $\Delta(T)$ with further decrease of temperature. The behavior of I-V curves of this type for the tunnel junction between $Bi_2Sr_2CaCu_2O_8$ (hight-$T_c$ superconductor) and $Pb$ (s-wave superconductor) was recently observed experimentally in [4]. There are several experimental results, which could be interpreted as due to zero energy bound states [1,4]. At the same time no anomaly in the Josephson critical current due to midgap states is observed to our knowledge. Manifestations of bound states with nonzero energies are not noticed experimentally up to now as well. Possibly, this is due to reasons resulting in broadening of Andreev bound states (e.g. due to interface roughness [4]).

In the presence of midgap states from both sides of tunnel junction, they cause the specific changes both in the quasiparticle current and in ac Josephson effect [4]. The effect of finite transmission of the barrier plane beyond the tunneling limit may result in the shift of midgap states to nonzero values of energy (though for particular case of “mirror” tunnel junctions and no phase difference between superconductors there is no shift for the midgap states due to this reason). These “former midgap states” take place for the uniform model as well, in contrast to other interface bound states.

Disregarding the surface pair breaking is the common feature of many articles, which consider surface (interface) bound states in d-wave superconductors both in studying current-voltage characteristics [11,20] and dc Josephson effect [21,24]. It is worth noting, that the effect of surface pair breaking can be of importance not only for studying the current-voltage characteristics but in considering the Josephson critical current as well. In particular, in the presence of essential suppression of the order parameter at the surface there are deviations of temperature dependence of the Josephson critical current $I_c$ from conventional Ambegaokar-Baratoff behavior both near $T_c$ [3] and at low temperatures [1]. For example, in the vicinity of $T_c$ the Josephson critical current turns out to be proportional to $(T_c - T)^3$ for sufficiently small surface values of the order parameters on both banks of the junction. It is proportional to $(T_c - T)^3/2$ if the order parameter vanishes only from one side of the tunnel barrier plane. Conventional Ambegaokar-Baratoff behavior $I_c \propto (T_c - T)$ holds near $T_c$ in the absence of any essential suppression of the order parameters at the interface.

Since the low-temperature anomaly of the Josephson critical current is associated with the effect of midgap states [3], the influence of surface pair breaking on the characteristics of midgap states should be discussed in this context. The occurrence of the zero-energy peak in the tunneling density of states is unaffected by the self-consistency of the order parameter. However, disregarding surface pair breaking can result in essential overestimating the weight of the peak and, as a consequence, the Josephson critical current. Moreover, since surface pair-breaking is sensitive to the crystal to surface orientation, disregarding its effect results in qualitative changes in dependences of the peak height and $I_c$ upon the misorientation angles of superconductors from both sides of the junction. To illustrate the above assertion we consider the midgap state contribution to the Josephson critical current between two identical d-wave superconductors, as a function of the crystal orientation of superconducting electrodes with respect to the specularly reflecting tunnel barrier plane. For the sake of simplicity we consider symmetric tunnel junction, when crystal axes have the same orientation in both electrodes.
fact that suppression of the order parameter near the tunnel barrier is essential for a wide range of crystalline orientations and sensitive to change of the orientation. The most significant deviation takes place for $\theta = 45^0$, when the order parameter is completely suppressed near the boundary. For this particular orientation disregarding the surface pair breaking results in overestimation of midgap states contribution to the Josephson critical current more than in three times. Similar difference can be seen in Fig. 2 in Ref. [23]. Our results demonstrate, in particular, the failure of the simple orientation dependence $I_c (\text{midgap}) \propto \sin(2\theta_1)\sin(2\theta_2)$, obtained in [20] on the basis of a uniform model order parameter and some additional approximations. One can show, however, that signs of $I_c (\text{midgap})$ and $\sin(2\theta_1)\sin(2\theta_2)$ coincide for the particular pairing potential considered.

The authors of Ref. [1] make also an accent on the fact that they do not use quasiclassical approximation in their theory. Extension of the theory beyond the quasiclassical approximation would be interesting both in the case of any new qualitative features of the phenomena in question, or due to noticeable quantitative corrections, containing powers of the parameter $a/\xi$, where $a$ is the atomic scale. However, no new qualitative features of nonquasiclassical nature are found in [3]. We believe, that taking account of the effect of surface pair breaking within the quasiclassical theory, is much more important from the qualitative point of view, while quantitatively disregarding this effect makes the extension of the approach beyond the quasiclassical approximation to be senseless.

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