Localized surface states in HTSC: alternative mechanism of zero-bias conductance peaks

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(March 22, 2022)

It is shown that the quasiparticle states localized in the vicinity of surface imperfections of atomic size can be responsible for the zero-bias tunneling conductance peaks in high-$T_c$ superconductors. The contribution from these states can be easily separated from other mechanisms using their qualitatively different response on an external magnetic field.

PACS numbers: 74.50.+r, 74.20.Rp, 74.72.-h, 73.20.Hb

One of the striking features of high-$T_c$ superconductors (HTSC) is the presence of zero-bias peaks in the voltage dependence of the tunneling conductance (ZBCP’s). These peaks, which have been observed in numerous experiments using low-temperature scanning tunneling microscopy (STM) technique, planar SIN junctions, and grain boundaries Josephson junctions, are generally considered as a clear signature of the unconventional pairing symmetry in cuprates. Thus it is important to understand what physical mechanisms can lead to the formation of ZBCP’s and how the contributions from different mechanisms can be separated in experiments.

The most popular model attributes the origin of ZBCP’s to the Andreev surface bound states (ABS’s), whose existence in unconventional superconductors is related to the fact that quasiparticles reflected from the interface see a change in the sign of the order parameter along their classical trajectories. The interplay of multiple Andreev and specular reflections then leads to the formation of zero-energy bound states in the vicinity of the interface. The theory predicts that the ABS contribution to ZBCP’s is strongly anisotropic reflecting the underlying symmetry of the order parameter and, in particular, is absent for those orientations of the interface for which the gap does not change its sign along the quasiparticle’s trajectory. This result, however, contradicts some of the experimental data, in which no significant dependence of the ZBCP magnitude on the interface orientation in $a$-$b$ plane has been found. On the other hand, the analysis of the behaviour of ABS’s in an external magnetic field shows that ZBCP’s should split symmetrically, the splitting being linear in $H$. The experimental situation, however, does not lend unambiguous support to this prediction. In particular, in Refs., a suppression and broadening of the in-plane ZBCP’s has been observed (see also Ref., where similar results for the $c$-axis tunneling were reported). The most plausible explanation of the presence of ZBCP’s for all surface orientations is that the surfaces of real samples are not perfectly flat at the atomic scale, so the incident quasiparticles are not reflected specularly, but rather get scattered in all directions resulting in the formation of ABS, albeit with a smaller spectral weight. However, the absence of ZBCP splitting in magnetic field cannot be explained in the framework of existing theories.

In this article, we propose a new mechanism for the formation of zero-bias anomalies in $d$-wave superconductors which does not rely on the existence of ABS’s. Briefly, our idea is that a significant contribution to ZBCP’s, at least for some in-plane surface orientations, can come from the states which are localized near atomic-scale surface imperfections, and thus are very different from ABS’s which propagate along the surface. In contrast to the previous approaches, we use an essentially non-quasiclassical way of modeling the surface roughness, namely, we assume that there are strong defects at the surface of a lattice superconductor, such as missing atoms. It is known that a single scalar impurity has a notable effect on the bulk $d$-wave superconducting state, creating an impurity bound state (IBS) in its vicinity, whose energy and width tend to zero in the limit of strong impurity potential. Experimentally, IBS’s manifest themselves in the existence of sharp zero-bias peaks in the voltage dependence of the differential tunneling conductance, which have been observed recently in beautiful STM experiments on BSCCO compounds. We will show that ZBCP’s in HTSC can be attributed to the formation of zero-energy IBS’s by strong surface defects, similar to those in the bulk. These states possess the two desirable features: (i) they exist for the “anti-node” surface orientations, and (ii), in contrast to the Andreev states which split in magnetic field, the IBS peaks remain centered around the zero energy, but get suppressed and broadened.

Let us consider a single missing atom or a strong repulsive point-like impurity at a (100) surface of a two-dimensional $d$-wave superconductor. (We consider this geometry because it is the simplest case with no ABS’s, see the discussion in the end of the article.) Because of the inherent non-locality of the order parameter in a superconductor with higher angular momentum pairing and the shortness of the coherence length in HTSC, which is typically of the order of $1nm$, it is convenient to use the lattice representation of the Hamiltonian:

$$\mathcal{H} = \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle} C^\dagger(\mathbf{r}) \mathcal{H}(\mathbf{r}, \mathbf{r}') C(\mathbf{r}'),$$  

(1)
where $C(r) = (c_1(r), c_1^+(r))^T$ are Nambu operators, and
\[ H = \begin{pmatrix} H_0 & \Delta \\ \Delta^* & -H'_0 \end{pmatrix}. \tag{2} \]
is the Bogoliubov-de Gennes (BdG) operator with $H_0(r, r') = -t(r, r') + U(r)\delta_{rr'} + \mu\delta_{rr'}$. The lattice
sites are labeled by $r$, and $(rr')$ means nearest neighbors. We choose the gauge in which the order parameter
is real, so the hopping matrix element has the form $t(r, r') = te^{ip_s(r-r')}$. The magnetic field is directed along
the $c$-axis, and the sample is in the Meissner state, so the screening supercurrent decays in the bulk and can
be assumed to be constant in the vicinity of the surface: $p_s = -(e/c)A(x = 0) = (e/c)HAb$, where $\lambda$ is the London
penetration depth. The impurity scattering is described by the scalar potential $U(r) = u_0\delta_0$ with $u \to \infty$
(the unitary limit), which describes a surface irregularity of atomic size. The mean-field order parameter $\Delta(r, r')$, corresponding to $d_{x^2-y^2}$ symmetry, is equal to $+\Delta_0$ for $r = r' \pm a$, and $-\Delta_0$ for $r = r' \pm b$, where $a, b$ are unit vectors of the square lattice (see Fig. 1). We do not cal-
culate the order parameter self-consistently, thus $\Delta_0$ is assumed to be constant. This assumption is valid only
for the (100) surface orientation, which follows from the boundary condition for the order parameter in the ab-
sence of an impurity [11]. The situation could be further
boundary condition for the order parameter in the ab-
finite strong repulsive impurity, which corresponds to
finites the impurity site was to be taken into account. Although
the numerical investigation of the self-consistency equations shows that such an effect does exist [12], we neglect it because it leads only to a renormalization of the effective
impurity strength towards the unitary limit [13].

The quantity measured in tunneling experiments is the
differential conductance, which is proportional to the local
density of states (DoS)
\[ N(r, \omega) = -\frac{1}{\pi} \text{Im} G^{R\dagger}_{11}(r, r; \omega), \tag{3} \]
where $G^R$ is the retarded Gor’kov-Nambu matrix Green’s function. In the presence of a point-like scalar static
impurity, $G^R = G^R_0 + G^R T G^R_0$, where $G^R_0$ is the Green’s function of a half-infinite clean superconductor, and the
T-matrix is given by $T(\omega) = u\tau_3 [1 - u g(\omega)\tau_3]^{-1}$. Here $g(\omega) = G^0_0(0, 0; \omega)$, and $\tau_3$ are the Pauli matrices. The
poles of the $T$-matrix correspond to the energies of the
impurity-induced quasiparticle bound states. A surface
vacancy (missing atom) prevents electrons from residing
at its site and thus can be thought of as an infi-
\[ N(r, \omega) = -\frac{1}{\pi} \text{Im} \left[ G^R_0(r, 0; \omega)g^{-1}(\omega)G^R_0(0, r; \omega) \right]_{11}. \tag{4} \]

The unperturbed Green’s function $G^R_0$ can be ex-
pressed in terms of the eigenfunctions $\Psi_{\alpha}(r)$ and
eigenvalues $E_\alpha$ of the BdG operator [3]: $G^R_0(r_1, r_2; \omega) =$
\[ \sum_{\alpha} \Psi_{\alpha}(r_1)\Psi_{\alpha}^\dagger(r_2)/(\omega_+ - E_\alpha), \]
where $\omega_+ = \omega + i0$. An essential ingredient of our theory which makes it different
from the previous work on IBS’s in the bulk, is the neces-
sity to impose some boundary conditions on the quasipar-
ticle wave functions at the superconductor-vacuum inter-
face. If the surface coincides with the $x = 0$ plane, then
the boundary conditions are $\Psi_{1,2}(x = -d, y, \omega) = 0, \quad$ where $d$ is the lattice constant. It is worth mentioning here that
if we used a continuum model, then the wave function
would be required to vanish right at the interface, i.e. at
$x = 0$. In this case, a point-like surface impurity would
not have any effect, so a more complicated approach to
dealing with surface roughness would be necessary [4].
In our theory, using the lattice model allows one to incor-
porate both the non-locality of the order parameter and
the surface roughness on the atomic scale in a simple and
natural way. The authors of Ref. [13] used a somewhat
similar approach in their numerical investigation of the self-consistent solution of the BdG equations. Our model
differs from that of Ref. [13] in several important aspects:
(i) we clarify the physical reason behind the appearance of
ZBCP’s, namely the formation of bound states, (ii) our
configuration of surface defects and the way of im-
posing the boundary conditions at the interface are dif-
ferent, and (iii) we study the magnetic field response of a
surface IBS, the problem which has not been addressed
before.

The quasiparticle wave functions are considerably
modified in the presence of a surface, and the Green’s
function satisfying the boundary conditions takes the
form
\[ G^R_0(r_1, r_2; \omega) = 4 \int_{-\pi/d}^{\pi/d} \frac{dk_x}{2\pi} \int_{-\pi/d}^{\pi/d} \frac{dk_y}{2\pi} G^R(k, \omega) \]
\[ \times \sin k_x(x_1 + d) \sin k_x(x_2 + d) e^{i(k_y(y_1 - y_2))}, \tag{5} \]
where
\[ G^R(k, \omega) = \frac{(\omega_+ - v_kD_s)\tau_0 + \xi_k\tau_3 + \Delta_k\tau_1}{(\omega_+ - v_kD_s)^2 - \xi_k^2 - \Delta_k^2}. \tag{6} \]
is the Green’s function of a bulk clean superconductor
affected by a “Doppler shift” in the quasiparticle energy,
\[ \xi_k = -2(\cos k_xd + \cos k_yd) - \mu \]
is the normal state excitation spectrum, $v_k = v_0k_0$ is the Fermi velocity, and $\Delta_0 = 2\Delta_0(\cos k_xd - \cos k_yd)$ is the momentum-
dependent superconducting gap. We use the values of the parameters typical for YBCO compound: $t = 185meV, \quad \mu = 0.51eV, \quad \Delta_0 = 15meV$.

The energies of the impurity-induced surface bound
states satisfy the equation $\det(g(\omega) = 0$, whose solutions
can be complex. We are interested in the case of strong
impurity scattering and small supercurrent, so that the
relevant energies are expected to be small compared to
the magnitude of the gap. At $\omega, \nu e_{FP} \ll \Delta_0$, the momentum
integrals are restricted to small vicinities of the two
gap nodes \((k_0, k_0)\) and \((k_0, -k_0)\), where \(\cos k_0d = -\mu/4t\), and \(v_F = 2\sqrt{2}d\sin k_0d\) is the Fermi velocity at the gap nodes. Introducing the notation \(z = \omega/\Delta_0\), we have 
\[
g(\omega) = (1/4t \Delta_0^2)F(z)\tau_0 \text{ at complex } \omega,
\]
with \(z_s = v_F p_s/\sqrt{2\Delta_0}\). Two logarithmic branch cuts are chosen to go down from \(z = \pm z_s\) parallel to the negative imaginary axis. The equation for the spectrum of bound states in the unitary limit takes the form \(F(z) = 0\). In the absence of supercurrent, \(F(z) \rightarrow F_0(z) = (2/\pi)z \ln z - iz\), and the above equation can be easily solved, the solution being \(z_0 = 0\). Both the real and imaginary parts of the bare IBS energy vanish, which means that there is a zero-energy bound state in the vicinity of a surface vacancy. The presence of this state gives rise to a sharp peak in the DoS, in full analogy to the situation in the bulk [9]. At nonzero magnetic field, the dominant energy scale in the unitary limit is provided by the Doppler shift \(v_F p_s\). It can be checked that the spectral equation with \(F(z)\) given by (7) has only one solution in the complex plane: 
\[
z_0 = -i\pi z_s/2 \ln z_s,
\]
so the IBS energy \(\omega_0 = z_0\Delta_0\) has the form
\[
\text{Re} \omega_0 = 0, \quad \text{Im} \omega_0 = -\frac{\pi v_F p_s}{2\sqrt{2}} \left|\ln \frac{v_F p_s}{\sqrt{2\Delta_0}}\right|^{-1}.
\]
From Eqs. (8) we see that IBS in the unitary limit is destroyed by supercurrent and replaced by a resonance peak centred around zero energy, whose width depends nonanalytically on \(H\), proportional to \(H(\ln H)^{-1}\). The physical reason for this is clear from Eq. (3): at \(p_s \neq 0\), the bulk DoS does not vanish at \(\omega = 0\), being proportional to \(v_F p_s\), which leads to a much stronger hybridization between IBS and the bulk states. It can be shown that at large but finite impurity strength, the surface IBS peak is shifted away from zero energy, the shift being proportional to \(H^2\). However, if \(v_F p_s\) is larger than the bare IBS energy \(\delta\), the results for the unitary limit are recovered. This behaviour is similar to what is expected for impurities in the bulk [10].

In order to visualize our results and facilitate the comparison with experiments, we compute numerically the surface DoS for a finite concentration of surface defects. It is easy to see that \(\delta N(0, \omega) \rightarrow 0\) at \(u \rightarrow \infty\). For this reason, in order to study the surface IBS, one should calculate either the local DoS, for example at one of the nearest neighbors of the impurity site, which can be probed by STM technique, or the total interface DoS measured in planar tunneling experiments. Here we concentrate on the latter case, which is obtained by putting \(r = (0, y)\) in Eq. (1) followed by the integration over \(y\). The resulting contribution to the total DoS from the surface IBS’s is
\[
\delta N(\omega, p_s) = n_i \text{Im } I(\omega)F^{-1}\left(\frac{\omega}{\Delta_0}\right),
\]
where \(n_i\) is the linear concentration of surface defects, \(I(\omega) = (4t \Delta_0^2/\pi) \int dy |G_0(y, \omega)G_0(-y, \omega)|_1\), and \(F(z)\) is given by Eq. (7). We assume a random distribution of defects and neglect the quantum interference effects, which gives rise to a prefactor \(n_i\) on the right-hand side of Eq. (8) (see the discussion below). At \((\omega, v_F p_s)/\Delta_0 \rightarrow 0\), \(F^{-1}(\omega)\) is singular, whereas \(I(\omega)\) is not and can be replaced by its value at \(\omega = p_s = 0\), which is real. We have plotted the results in Fig. 2. The plot confirms that there is a sharp zero-bias peak due to IBS’s in the in-plane tunneling conductance, and the magnetic field leads to the broadening of this peak near the zero bias, and the suppression of its magnitude. This behaviour is in a stark contrast to what is expected for the Andreev states. It should be mentioned that the numerical results of Ref. [7] show that the contribution of bound states at randomly distributed strong impurities to ZBCP’s in the c-axis planar tunneling is either negligible, or leads just to a finite conductance at zero bias. We have studied a different setup, namely the in-plane tunneling, and come to opposite conclusions, a possible explanation being that the surface disorder configuration in our system favors the appearance of a significant IBS contribution, because all the defects lie at the same line – the (100) interface.

We would like to emphasize here that the surface impurity states is not the only mechanism that can lead to the observation of ZBCP’s for a nominal (100) orientation [8]. It is the magnetic field response of ZBCP’s that should help determine which mechanism gives the dominant contribution. As said in the introduction, suppression and/or broadening of the in-plane ZBCP’s without any trace of splitting has been seen in some tunneling experiments (see e.g. Ref. [1] where the STM results for (100) YBCO films were reported), which qualitatively agrees with our predictions. However, the possibility of a quantitative comparison of the experimental data to our results strongly depends on the details of the sample preparation and the surface quality. The basic assumption of our model is that the microscopic surface roughness can be described in terms of strong potential scatterers of atomic size, which is likely to be the case for flat surfaces with missing atoms or steps. On the other hand, this assumption is definitely wrong if the characteristic size of the surface imperfections is larger than the coherence length \(\xi_0\). An ideal experimental test of our model should be performed on a high-quality (100) surface in a broad range of parallel magnetic fields.

In this article, we concentrated on the zero-energy IBS’s which are formed in the vicinity of (100) surfaces. For other surface orientations, the situation is complicated by the presence of ABS’s, which also have zero energy and should therefore experience a strong hybridization with IBS’s. The result of this interplay is not clear a
priori and requires a separate investigation, which is beyond the scope of the present study. Other factors which can potentially threaten our results in the presence of a finite concentration of defects are the multiple-scattering interference effects and the self-consistent order parameter variation $[18]$. Although their role certainly deserves further analysis, one can always assume that if the surface disorder concentration is sufficiently small, then the characteristic energy scales of our problem, such as the Doppler shift, can be made greater than those at which the “dangerous” effects mentioned above come into play.

In conclusion, we have proposed a new mechanism of the formation of zero-bias peaks in HTSC. We predict that the strong defects at an “anti-node” surface can lead to the creation of zero-energy localized states in their vicinities, whose properties significantly differ from those of the Andreev surface states. These localized states should manifest themselves by the presence of sharp zero-bias peaks in tunneling experiments, which get suppressed and broadened in an external magnetic field.

We would like to thank Patrick Fournier and John Wei for stimulating discussions. This work was supported by the Natural Sciences and Engineering Research Council of Canada.

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