Quasiparticle Bound States and Low-Temperature Peaks of the Conductance of NIS Junctions in d-Wave Superconductors

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Quasiparticle states bound to the boundary of anisotropically paired superconductors, their contributions to the density of states and to the conductance of NIS junctions are studied both analytically and numerically. For smooth surfaces and real order parameter we find some general results for the bound state energies. In particular, we show that under fairly general conditions quasiparticle states with nonzero energies exist for momentum directions within a narrow region around the surface normal. The energy dispersion of the bound states always has an extremum for the direction along the normal. Along with the zero-bias anomaly due to midgap states, we find, for quasi two-dimensional materials, additional low-temperature peaks in the conductance of NIS junctions for voltages determined by the extrema of the bound state energies. The influence of interface roughness on the conductance is investigated within the framework of Ovchinnikov's model. We show that nonzero-bias peaks at low temperatures may give information on the order parameter in the bulk, even though it is suppressed at the surface.

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I. INTRODUCTION

It is now widely recognized, that the anisotropy ratio of the order parameter on the Fermi surface for many of the high-$T_c$ superconductors is of the order of unity. By contrast, for conventional low-temperature superconductors the anisotropy ratio is known to be much smaller, so that they are almost isotropic $s$-wave superconductors. This fact itself, essentially irrespective of the specific type of the superconducting pairing, results in many new important consequences for the properties of HTSC, compared to isotropic $s$-wave superconductors. In particular, a highly anisotropic order parameter turns out to be quite sensitive to any kind of inhomogeneities in the material, including nonmagnetic impurities as well as interfaces.

For most surfaces the bulk behavior of an anisotropic order parameter can differ essentially from its behavior at the wall. Even smooth specularly reflecting walls are, in general, pair breaking, which results in a suppression of the order parameter near the boundary. This concerns both anisotropic superconductors and superfluids. At the same time, quasiparticle states bound to the boundary appear due to this suppression or/and due to the sign change of the anisotropic order parameter with momentum direction. Furthermore, in the region where the bulk order parameter is essentially suppressed, subdominant pairing channels with different symmetries may come into play and become stable near the wall.

Several important experimental methods used for studying the anisotropic structure of the order parameter, in particular tunneling measurements, are fairly sensitive to the superconducting properties close to the surface of the sample. The local quasiparticle spectrum at the surface which differs, in general, from the bulk density of states is of crucial importance for the I-V characteristics of tunnel junctions. Apart from the fact, that the gap anisotropy washes out those peaks in the tunneling current which would occur in the isotropic case, the presence of quasiparticle bound states or/and the order parameter of subdominant symmetry channels near the surface results in new characteristic features of the I-V curves in the vicinity of some specific points. One of the most striking features of NIS junctions with $d$-wave superconductors is the zero-bias anomaly of the conductance which is associated with surface midgap states. These states localized at the surface are a consequence of the sign change of the order parameter on the Fermi surface. A further consequence of those states is a low-temperature anomaly in the Josephson critical current. By contrast, some other important features of the Josephson effect do not depend on the quasiparticle spectrum at the surface, having a more universal character. Actually, they depend only on the phase difference of the order parameters in the bulk superconductors on both sides of the junction.

Below we develop an analytical investigation, including numerical calculations, of quasiparticle states bound to the boundary of anisotropically paired superconductors, their contributions to the density of states and to the conductance...
of NIS junctions with weak transparency. Our approach to the problems is based on the quasiclassical formulation of superconductivity. Both smooth specularly reflecting and diffusive interfaces are considered. The spatially dependent order parameter is supposed to be real. The analytical study of quasiparticle states with nonzero energies bound to a smooth wall is carried out for the first time, and some general results are obtained. In particular, we show that the energy of a bound state is closely connected with the phase of the complex residue of the anomalous propagator. Quasiparticle bound states with nonzero energies turn out to exist under fairly general conditions for momentum directions within a narrow region around the surface normal for which the energy dispersion always has an extremum.

While the presence of a zero-bias anomaly in the conductance does not depend upon details of the Fermi surface but only on the appearance of midgap states, low-temperature anomalies in the conductance due to nonzero-energy levels near the surface are absent for three dimensional systems. For quasi two-dimensional materials we find, that quasiparticle bound states with nonzero energies lead, at least at low enough temperatures, to peaks in the conductance for voltages determined by the extrema of the bound state energies. It is shown below, that for a smooth barrier plane the magnitudes of those peaks are proportional to the inverse square root of the temperature ($G(T \to 0) \propto 1/\sqrt{T}$) in contrast to zero-bias anomalies for which $G(T \to 0) \propto 1/T$.

In realistic systems, the peaks in the quasiparticle spectrum will be broadened. The shape and the height of these peaks are governed by the physical parameters of the junction like interface roughness (e.g., lattice constant mismatch) and transparency. We investigate the influence of interface roughness on the local density of states and on the conductance within the framework of Ovchinnikov’s model. In all our calculations the order parameter is determined self-consistently. In contrast to midgap states, nonself-consistent calculations, disregarding surface pair breaking, do not permit to find and describe quasiparticle bound states with nonzero energy and the corresponding peaks in the conductance at nonzero-bias voltage.

II. QUASICLASSICAL THEORY

A. Basic Equations

In general, strongly anisotropic superconductors react sensitively to surfaces and interfaces. For instance, the superconducting order parameter near the surface is reduced due to pair-breaking effects. The quasiclassical theory of superconductivity is the most efficient theory for investigating effects of surfaces and interfaces. We use Eilenberger’s equations for the quasiclassical retarded propagator $\hat{g}^R$ which for a clean singlet anisotropically paired superconductor reduce to the following $2 \times 2$ matrix form:

$$
\begin{bmatrix}
\varepsilon \tau_3 - \hat{\Delta}(p_f, R), \\
\hat{g}^R(p_f, R; \varepsilon)
\end{bmatrix} + i v_f \cdot \nabla_R \hat{g}^R(p_f, R; \varepsilon) = 0,
$$

$$
[\hat{g}^R(p_f, R; \varepsilon)]^2 = -\pi^2 \mathbb{1}.
$$

Here, $\varepsilon$ is the quasiparticle energy, $p_f$ the momentum on the Fermi surface, $v_f$ the Fermi velocity, and $\hat{\Delta}$ the order parameter matrix. Following standard notations we use a “hat” to indicate matrices in Nambu space. A convenient basis set of Nambu matrices is the unit matrix $\mathbb{1}$ and the three Pauli matrices $\tau_1, \tau_2, \tau_3$. The propagator $\hat{g}$ (here and in the following we drop the superscript $R$ for simplicity) and the order parameter matrix $\hat{\Delta}$ have the form

$$
\hat{g} = \begin{pmatrix}
f & g \\
g^* & -f
\end{pmatrix}
$$

and

$$
\hat{\Delta} = \begin{pmatrix}
0 & \Delta \\
-\Delta^* & 0
\end{pmatrix}.
$$

(3)

The gap function $\Delta(p_f, R)$ is related to the anomalous Green function $f$ and has to be determined self-consistently (see Ref. [3]). The diagonal part $g$ of the full matrix propagator $\hat{g}$ carries information on the superconducting density of states (DOS),

$$
\nu(p_f, R; \varepsilon) = -\frac{1}{\pi} \text{Im} [g(p_f, R; \varepsilon)].
$$

(4)

This quantity contains all the information we need for calculating the tunneling current across an NIS interface (see Eqs. (33)).
B. Interface Model

The boundary conditions at an ideal interface are given by Zaitsev’s relations (see Refs. 28,29), which reduce in the limit of zero-transparency to

\[ \hat{g}(p_f) = \hat{g}(p_f^r) , \]  

(5)

where the propagators are taken at the metal-insulator boundary. Equation (5) connects the propagator of an incoming quasiparticle with Fermi momentum \( p_f \) and the propagator of the reflected quasiparticle with Fermi momentum \( p_f^r \) at the interface. For specular reflection the momentum parallel to the interface is conserved, i.e., \( p_f^\parallel = p_f^r \parallel \). For a complete determination of the quasiclassical propagator we have to take into account that deep inside the superconductor the propagator approaches its bulk value.

In realistic systems the reflection of quasiparticles from surfaces and interfaces is expected to be diffuse, at least to some degree, due to imperfections at the boundary. For isotropic superconductors, elastic scattering of quasiparticles on walls has no effect on the density of states near the interface, and thus, on the tunneling current. The reason for this is that the order parameter for the reflected quasiparticles is the same for all directions. In anisotropic superconductors the value of the order parameter is no longer independent on direction. A quasiparticle on an outgoing trajectory will see an order parameter which is, in general, different from the one on its incoming trajectory. This leads to pair breaking even for a specularly reflecting wall, and, as a consequence, to a suppression of the order parameter near the boundary. For diffuse scattering of quasiparticles at the interface all outgoing trajectories are mixed. As a result, sharp structures in the density of states (e.g., bound states) which would occur for ideal interfaces are smeared out near rough interfaces. Thus, the effect of surfaces and interfaces is similar to the effect of static impurities which leave the order parameter of isotropic superconductors unaffected (“Anderson’s theorem”), but have destructive influence in anisotropic systems where superconductivity can even disappear when the impurity concentration exceeds a critical value.

We model a rough interface by coating an ideal interface (transparency \( D \)) on both sides by thin layers of strongly disordered metals which differ from the respective bulk materials only by their very short mean free paths (see Fig. 1). The roughness of the interface is measured by the phenomenological parameter \( \rho \) which is essentially the ratio of the thickness of the layers \( \delta \) and the mean free path \( \ell \), i.e., \( \rho = \delta/\ell \). The case \( \rho = 0 \) corresponds to an ideal interface, whereas \( \rho = \infty \) describes a diffuse interface. The transport of quasiparticles across the disordered layers is determined by the following transport equation:

\[ - \left[ \frac{\rho}{2\pi} \langle \hat{g}^l_r, \hat{g}^l_r \rangle + i \nabla_{\perp}^l \partial_\perp \hat{g}^l_r \right] = 0 . \]  

(6)

The superscripts \( l \) and \( r \) stand for the left and right sides of the interface. The dimensionless velocity \( \nabla_{\perp}^l \) is the perpendicular to the interface component of the quasiparticle velocity in the bulk material normalized by an averaged Fermi velocity, \( \nabla_{\perp}^l = v_{f\perp}^l / \sqrt{\langle (v_{f\perp}^l)^2 \rangle} \). The first term in Eq. (6) is Ovchinnikov’s anisotropic scattering self-energy for incoming and outgoing quasiparticles. At the ideal interface which separates the two layers the quasiclassical propagators are discontinuous and the jump is given by Zaitsev’s relations. The normal state resistance \( R_N \) of the interface turns out to be independent of the roughness and is given by

\[ R_N^{-1} = 2e^2A \int_{v_{f\perp}^l > 0} \frac{\partial^2 S^l}{(2\pi)^3 |v_{f\perp}^l| v_{f\perp}^l D(p_f^l)} , \]  

(7)

where \( A \) is the area of the interface. A detailed description of this interface model can be found in Ref. 14.

III. QUASIPARTICLE BOUND STATES AT SPECULARLY REFLECTING WALLS

In this section, we study in detail the appearance of quasiparticle bound states near specularly reflecting impenetrable surfaces. Bound states are localized within a few (or even many; see below) coherence lengths near the surface, and their energies lie below the bulk value of the (momentum dependent) gap. Their existence manifests in \( \delta \)-peaks in the momentum resolved density of states below the continuous spectrum. There are two types of bound states of different origin: a) zero-energy bound states or midgap states, which are a consequence of the change of sign of the order parameter along a quasiparticle trajectory which is reflected from the wall, and b) nonzero-energy bound
states which emerge due to the depletion of the order parameter associated with the interface. While zero-energy bound states are a robust phenomenon of quite general origin, less information is available for nonzero-energy bound states.

A. Analysis of Quasiparticle Bound States at Specular Walls

Let the quasiclassical propagator \( \hat{g} \) have a pole at \( \varepsilon = \varepsilon_B(p_f) \), where \( \varepsilon_B(p_f) \) is the energy of a bound state with Fermi momentum \( p_f \) (note that \( \varepsilon_B(p_f) = \varepsilon(p_f) \)). It is convenient to introduce the residue of the propagator \( \hat{g} \) by

\[
\hat{g}(p_f, R; \varepsilon_B(p_f)) = \lim_{\varepsilon \to \varepsilon_B(p_f)} [(\varepsilon - \varepsilon_B(p_f)) \hat{g}(p_f, R; \varepsilon)],
\]

which is finite and satisfies the same transport equation as \( \hat{g} \), but with a modified normalization condition,

\[
[\hat{g}(p_f, R; \varepsilon_B(p_f))]^2 = 0.
\]

The boundary conditions for \( \hat{g} \) coincide with \([1] \). But, in contrast to \( \hat{g} \) the new propagator \( \hat{\tilde{g}} \) vanishes in the bulk of the superconductor. Thus, the quantity \( \hat{g} \) describes just a quasiparticle state bound to the boundary plane.

For the sake of definiteness, the superconductor is supposed to occupy the half-space \( x > 0 \) with an impenetrable boundary. Furthermore, we assume that the gap function \( \Delta \) can be chosen real. Then one obtains from Eilenberger’s equations:

\[
\hat{f}^+(p_f, x; \varepsilon_B(p_f)) = -\hat{f}^*(p_f, x; \varepsilon_B(p_f)),
\]

\[
\hat{g}(p_f, x; \varepsilon_B(p_f)) = \hat{g}^*(p_f, x; \varepsilon_B(p_f)) = [\hat{f}(p_f, x; \varepsilon_B(p_f))].
\]

The last identity is a consequence of Eq. \([3] \). We introduce the phase of the complex anomalous Green function by

\[
\hat{f}(p_f, x; \varepsilon_B(p_f)) = -\hat{g}(p_f, x; \varepsilon_B(p_f)) \exp (i\varphi(p_f, x)),
\]

and obtain from \([1] \), \([3] \)

\[
\hat{g}(p_f, x; \varepsilon_B(p_f)) = \hat{g}(p_f, 0; \varepsilon_B(p_f)) \exp \left( -\frac{2}{v_{f,x}} \int_0^x \Delta(p_f, \tilde{x}) \sin (\varphi(p_f, \tilde{x})) \, d\tilde{x} \right),
\]

together with the following equation for the phase,

\[
-\frac{v_{f,x}}{2} \partial_x \varphi(p_f, x) + \varepsilon_B(p_f) - \Delta(p_f, x) \cos (\varphi(p_f, x)) = 0,
\]

and the boundary and asymptotic conditions,

\[
\varphi(p_f, 0) = \varphi(\underline{p}_f, 0) \quad \text{and} \quad v_{f,x} \Delta_\infty(p_f) \sin (\varphi_\infty(p_f)) > 0.
\]

If \( \varphi(p_f, x) \) is a solution of Eqs. \([13] \), \([14] \) with the energy \( \varepsilon_B(p_f) \), then \( \pi - \varphi(p_f, x) \) is a solution with the energy \( -\varepsilon_B(p_f) \).

Since \( \partial_x \varphi(p_f, x) \) vanishes in the bulk \( (x \to \infty) \), we immediately get from Eqs. \([13] \) and \([14] \) the relation between the bound state energy \( \varepsilon_B(p_f) \) and the phase in the bulk of the superconductor,

\[
\varepsilon_B(p_f) = \Delta_\infty(p_f) \cos (\varphi_\infty(p_f)) = \Delta_\infty(\underline{p}_f) \cos \left( \varphi_\infty(\underline{p}_f) \right).
\]

As a consequence, bound states might exist for a given momentum direction only below the band edges for the momenta \( p_f \) and \( \underline{p}_f \), i.e., for

\[
|\varepsilon_B(p_f)| \leq \min \left\{ |\Delta_\infty(p_f)|, |\Delta_\infty(\underline{p}_f)| \right\}.
\]

Under certain conditions it is possible to find explicit expressions for the bound state energy \( \varepsilon_B(p_f) \) and the phase \( \varphi_\infty(p_f) \) in terms of the spatial dependence of the order parameter near the surface. For this purpose we transform Eq. \([13] \) into the corresponding integral equation,
\[ \varphi(p_f, x) = \varphi(p_f, 0) + \frac{2 \Delta_{\infty}(p_f)}{v_{f,x}} \int_0^x \left( \cos(\varphi_{\infty}(p_f)) - \frac{\Delta(p_f, \tilde{x})}{\Delta_{\infty}(p_f)} \cos(\varphi(p_f, \tilde{x})) \right) d\tilde{x}. \] (17)

Furthermore, we suppose that the phase \( \varphi(p_f, x) \) deviates only weakly from its value at the surface everywhere within the superconductor (\(|\varphi(p_f, x) - \varphi(p_f, 0)| \ll 1\)). Then, as a first approximation, one can substitute on the right hand side of Eq. (17), \( \cos(\varphi(p_f, x)) \to \cos(\varphi_{\infty}(p_f)) - \sin(\varphi_{\infty}(p_f)) (\varphi(x, p_f) - \varphi_{\infty}(p_f)) \), which leads to

\[ \varphi_{\infty}(p_f) = \varphi(p_f, 0) + \frac{\Delta_{\infty}(p_f)}{\Delta_{\text{max}}} \cos(\varphi_{\infty}(p_f)) A(p_f, \varphi_{\infty}(p_f)), \] (18)

where

\[ A(p_f, \varphi_{\infty}(p_f)) = \frac{2 \Delta_{\text{max}}}{v_{f,x}} \int_0^\infty \exp \left( -\frac{2}{v_{f,x}} \sin(\varphi_{\infty}(p_f)) \int_0^x \Delta(p_f, \tilde{x}) d\tilde{x} \right) \left( 1 - \frac{\Delta(p_f, x)}{\Delta_{\infty}(p_f)} \right) dx. \] (19)

Here, we introduced the quantity \( \Delta_{\text{max}} = \max\{|\Delta_{\infty}(p_f)|\} \).

The condition of weak deviations of the phase from its value on the surface is transformed with the help of Eqs. (14), (15) into the form

\[ \frac{|\Delta_{\infty}(p_f)|}{\Delta_{\text{max}}} |\cos(\varphi_{\infty}(p_f))| |A(p_f, \varphi_{\infty}(p_f))| \ll 1. \] (20)

Thus, the approximation can be justified, for example, for momentum directions for which the order parameter is only slightly suppressed at the surface (where \(|A(p_f, \varphi_{\infty}(p_f))| \) is small), or in the vicinity of nodes of the order parameter (when \(|\Delta_{\infty}(p_f)|/\Delta_{\text{max}} \) is small), or for a small enough \( |\cos(\varphi_{\infty}(p_f))| \).

If condition (21) is valid both for incoming and for outgoing momenta, we get from Eqs. (14), (15), (18) the following equation for the bound state energy,

\[ \frac{\varepsilon_B^2(p_f)}{\Delta_{\infty}(p_f)\Delta_{\text{max}}(p_f)} \text{sgn}(\Delta_{\infty}(p_f)\Delta_{\text{max}}(p_f)) \left( 1 - \frac{\varepsilon_B^2(p_f)}{\Delta_{\infty}^2(p_f)} \right)^{1/2} \left( 1 - \frac{\varepsilon_B^2(p_f)}{\Delta_{\text{max}}^2(p_f)} \right)^{1/2} = \]

\[ = \cos \left( \frac{\varepsilon_B(p_f)}{\Delta_{\text{max}}} \left[ A(p_f, \varphi_{\infty}(p_f)) - A(p_f, \varphi_{\infty}(p_f)) \right] \right). \] (21)

It is easy to see that the condition \( \Delta_{\infty}(p_f)\Delta_{\text{max}}(p_f) < 0 \) implies the existence of a midgap state at \( \varepsilon_B(p_f) = 0 \). We should note that this solution does not depend on the validity of our expansion (18) for the phase \( \varphi_{\infty}(p_f) \). If the order parameter changes sign along a trajectory, then \( \varphi(p_f) = (\pi/2) \text{sgn}(v_{f,x}\Delta_{\text{max}}(p_f)) \) is a solution of Eqs. (13), (14) for \( \varepsilon_B(p_f) = 0 \). The left-hand side of Eq. (21) is equal to zero for this solution. Another consequence of Eq. (21) is the absence of nonzero-energy states near the edge of the continuous spectrum (that is close to the right-hand side of (16)) provided \( \Delta_{\infty}(p_f)\Delta_{\text{max}}(p_f) < 0 \) and \( |A(p_f, \varphi_{\infty}(p_f))\Delta_{\infty}(p_f)|/\Delta_{\text{max}} \ll 1 \). However, bound states may appear near the band edge if the parameter \(|A(p_f, \varphi_{\infty}(p_f))\Delta_{\infty}(p_f)|/\Delta_{\text{max}} \) is not small (see Fig. 4c). In this case, our approximation (18) for the phase \( \varphi_{\infty}(p_f) \) breaks down.

Let us now consider the opposite case, \( \Delta_{\infty}(p_f)\Delta_{\text{max}}(p_f) > 0 \). If the condition \( |\Delta_{\infty}(p_f)A(p_f, \varphi_{\infty}(p_f))|/\Delta_{\text{max}} \ll 1 \) is satisfied for a pair of incoming and outgoing momenta, we see from Eqs. (14) and (21) that bound states occur only for trajectories with \(|\Delta_{\infty}(p_f) - \Delta_{\text{max}}(p_f)| \ll |\Delta_{\infty}(p_f)| \). The energies of these bound states lie close to the continuum. These bound states arise for momentum directions close to the normal or almost parallel to the boundary plane where \( \Delta_{\infty}(p_f) \approx \Delta_{\text{max}}(p_f) \). The latter region of momentum directions, however, is not so interesting because of its comparatively small contribution to the tunneling current. For bound state energies near the edge of the continuum \( \Delta_{\infty}(p_f) \approx \Delta_{\text{max}}(p_f) \) we find from Eq. (15) \( \sin(\varphi_{\infty}(p_f)) \ll 1 \). Therefore, we can approximate Eq. (19) by

\[ A_0(p_f) = A(p_f, 0) = \frac{2 \Delta_{\text{max}}}{v_{f,x}} \int_0^\infty \left( 1 - \frac{\Delta(p_f, x)}{\Delta_{\infty}(p_f)} \right) dx, \] (22)
and obtain the following expression for bound states energies near the band edge:

\[
\frac{\varepsilon_B^2(p_f^f)}{\Delta_{\text{max}}^2} = \frac{\Delta_{\infty}(p_f)\Delta_{\infty}(p_f^f)}{\Delta_{\text{max}}^2} \left( 1 - \frac{\Delta_{\infty}(p_f)\Delta_{\infty}(p_f^f)}{4\Delta_{\text{max}}^2} (A_0(p_f) - A_0(p_f^f))^2 \right) + \\
\left( \frac{\Delta_{\infty}(p_f)}{\Delta_{\text{max}}(p_f)} - \frac{\Delta_{\infty}(p_f^f)}{\Delta_{\text{max}}(p_f^f)} \right) \left( \frac{\Delta_{\infty}(p_f)\Delta_{\infty}(p_f^f)}{4\Delta_{\text{max}}^2} - \frac{1}{(A_0(p_f) - A_0(p_f^f))^2} \right).
\]

(23)

It is of particular interest to consider the momentum direction along the normal to the boundary plane \(p_f^f || \hat{n}\), where the additional relation \(p_f^f = -p_f^f\) holds. Using \(\Delta(p_f) = \Delta(-p_f)\) we get \(\varphi(p_f^f, x) = -\varphi(p_f^f, x)\). Together with the boundary condition \(\varphi=f\) for \(\varphi\) at the wall we find \(\varphi(p_f^f, 0) = 0\). Then one has \(|\varphi_{\infty}(p_f^f) - \varphi(p_f^f, 0)| = |\varphi_{\infty}(p_f^f)| \ll 1\), and obtains from Eqs. \((14)\), \((18)\) the following expression for the bound state energy:

\[
|\varepsilon_B(p_f^f)| = |\Delta_{\infty}(p_f^f)| \cos \left( \frac{\Delta_{\infty}(p_f^f)}{\Delta_{\text{max}}(p_f^f)} A_0(p_f^f) \right) \approx \left( 1 - \frac{\Delta_{\infty}^2(p_f^f)}{2\Delta_{\text{max}}^2} A_0^2(p_f^f) \right) |\Delta_{\infty}(p_f^f)|.
\]

(24)

The asymptotic condition \((14)\) for \(\varphi\) is satisfied for this state for positive values of \(A_0(p_f^f)\), hence

\[
\int_0^\infty \left( 1 - \frac{\Delta(p_f^f, x)}{\Delta_{\infty}(p_f^f)} \right) dx > 0.
\]

(25)

This inequality is fulfilled, in general, for the order parameter with the amplitude near the wall being less than its bulk value. This is true, in particular, for a one-component order parameter. Condition \((25)\) might be violated only if order parameter components with different symmetries appear in the vicinity of the surface due to nonzero coupling constants in subdominant symmetry channels. In the absence of this effect, the function \(\Delta(p_f^f, x)\) is always a monotonously increasing function of the distance from the boundary, which ensures the validity of Eq. \((25)\). Thus, we have shown in Eq. \((24)\) that bound states with nonzero energy do exist for \(p_f^f || \hat{n}\) for any (even tiny) suppression of the order parameter at the surface. If one interprets these states as bound states in the effective potential well formed by the order parameter at the boundary, one can say that for \(p_f^f || \hat{n}\) quasiparticle bound states appear in any shallow potential well.

One can find the dependence of the bound state energy on the momentum direction in the vicinity of perpendicular incidence, i.e., for \(p_f \approx p_f^f\). Assuming that the boundary is a symmetry plane of the Fermi surface of the superconductor, one may write

\[
p_f = (p_f \cdot \hat{n})\hat{n} + \delta p_f = p_f^f + \delta p_f, \quad p_f^f = \delta p_f - p_f^f.
\]

(26)

Furthermore, we expand all the quantities on the right-hand side of Eq. \((23)\) in powers of small deviations \(\delta p_f\). In particular,

\[
\Delta_{\infty}(p_f) = \Delta_{\infty}(p_f^f) + (\delta p_f \cdot \nabla p_f^f) \Delta_{\infty}(p_f^f) + \frac{1}{2} (\delta p_f \cdot \nabla p_f^f)^2 \Delta_{\infty}(p_f^f) + \ldots.
\]

(27)

By keeping only terms up to second order in \(\delta p_f\), expression \((23)\) for the bound state energy can be reduced to

\[
\frac{\varepsilon_B^2(p_f^f)}{\Delta_{\text{max}}^2} = \frac{\Delta_{\infty}^2(p_f^f)\Delta_{\infty}^2(p_f^f)}{\Delta_{\text{max}}^2} \left( 1 - \frac{\Delta_{\infty}^2(p_f^f)\Delta_{\infty}^2(p_f^f)}{4\Delta_{\text{max}}^2} A_0^2(p_f^f) \right) - \\
\frac{(\delta p_f \cdot \nabla p_f^f) \Delta_{\infty}(p_f^f)}{\Delta_{\text{max}}(p_f^f)} \left( \frac{1}{A_0^2(p_f^f)} - \frac{2\Delta_{\infty}^4(p_f^f)\Delta_{\text{max}}^2}{A_0^2(p_f^f)} \right)
\]

\[
+ \frac{\Delta_{\infty}(p_f^f)}{\Delta_{\text{max}}(p_f^f)} \left( \frac{\Delta_{\infty}^2(p_f^f)}{\Delta_{\text{max}}^2} - 2 \frac{\Delta_{\infty}^4(p_f^f)\Delta_{\text{max}}^2}{A_0^2(p_f^f)} \right) + \ldots.
\]

(28)

The linear terms in \(\delta p_f\) cancel each other, and hence the bound state energy has a local extremum for the direction normal to the boundary.
It follows from condition (14), that bound states occur only in a narrow region of the Fermi surface for momentum directions which are close to the normal of the interface. Indeed, expanding Eq. (16) in the vicinity of \( p_f^0 \),

\[
\min \left\{|\Delta_{\infty}^2(p_f)|, |\Delta_{\infty}^2(p_f')|\right\} = \Delta_{\infty}^2(p_f^0) - 2 |\Delta_{\infty}(p_f')| \left(\delta p_f \cdot \nabla p_f'\right) \Delta_{\infty}(p_f^0) + \ldots ,
\]

and keeping only terms up to second order in \( \delta p_f \), we get from (16), (28), (29) the following range for the occurrence of bound states:

\[
\left|\frac{\left(\delta p_f \cdot \nabla p_f^0\right) \Delta_{\infty}(p_f^0)}{\Delta_{\infty}(p_f^0)}\right| \leq \frac{5}{8} \frac{\Delta_{\infty}^2(p_f^0)}{\Delta_{\max}^2} A_0^2(p_f^0) .
\]

One can see from (21) and condition \( |\varphi_{\infty}(p_f^0)| \ll 1 \), that the right-hand side of Eq. (31) is much smaller than 1.

B. Results for d-Wave Superconductors

Now, we consider a tetragonal \( d_{x^2-y^2} \) superconductor with a cylindrical Fermi surface whose \( z_0 \)-axis is parallel to the boundary plane. The order parameter is supposed to have the form

\[
\Delta(p_f, x) = \Delta(x) \cos(2\phi - 2\alpha) ,
\]

where \( \phi \) is the azimuth angle between the Fermi momentum \( p_f \) and the surface normal \( \hat{n} \) (which is taken as the \( x \) direction). The angle \( \alpha \) describes the orientation of the crystalline axis \( \hat{x}_0 \) with respect to the normal of the boundary. For this case, Eq. (28) for the bound state energy takes the form:

\[
\frac{\varepsilon_B^2(\phi)}{\Delta_{\max}^2 \cos^2(2\alpha)} = 1 - A_0^2 \cos^2(2\alpha) - \phi^2 \left(A_0^2 \cos^2(2\alpha) + 4(1 - 2A_0^2) + 4 \tan^2(2\alpha) \right) .
\]

Consequently, the angular range for which bound states exist is limited by

\[
|\phi| < \frac{5A_0^2 \cos^2(2\alpha)}{16 \tan(2\alpha)} , \quad 0 \leq \alpha \leq \frac{\pi}{4} .
\]

The quantity \( A_0 = A_0(\phi = 0) \) depends on the misorientation angle \( \alpha \) as well as on the temperature \( T \). According to (22), bound states for quasiparticles with momentum directions close to the normal of the boundary always appear, with the exception of two obvious crystalline orientations: a) \( \alpha = 0 \) where the order parameter is not suppressed at the interface (\( A_0 \) vanishes for \( \alpha \to 0 \)), and b) \( \alpha = \pm 45^\circ \) where the order parameter for perpendicular incidence is zero.

According to (12), (31) the characteristic length describing the localization of bound states near the surface is of the order of\( v_f \cos \phi/|\Delta_{\infty}(p_f)\sin(|\varphi_{\infty}(p_f)|)| \sim \xi(T) \cos \phi/\sin(|\varphi_{\infty}(p_f)|) \cos(2\phi - 2\alpha) \). For momentum directions, for which the bound levels lie close to the edge of the continuous spectrum, one gets from (13) \( |\sin(|\varphi_{\infty}(p_f)|)| \ll 1 \). The characteristic length is in this case much greater than the temperature dependent coherence length \( \xi(T) \) (provided \( \cos \phi \) is not very small). The factor \( \cos(2\phi - 2\alpha) \) in the denominator may result in an additional increase of the characteristic length.

The results of numerical calculations for the angular dependence of the bound state energy \( \varepsilon_B(\phi) \) are presented in Fig. 2 for various misorientations angles \( \alpha \). The temperature is \( T = 0.1 T_c \). The spatially varying gap amplitude \( \Delta(x) \) was evaluated self-consistently (see Ref. 5). Bound states with nonzero energy \( \varepsilon_B(\phi) \) occur in a comparatively narrow angular region in the vicinity of the surface normal (Fig. 2a). These bound states are also described analytically above. Bound states which occur for lattice to surface orientations \( \alpha \geq 37^\circ \) (Fig. 2b) (it is sufficient to consider \( 0^\circ \leq \alpha \leq 45^\circ \)) correspond to values of the parameter \( |\Delta_{\infty}(p_f)\cos(|\varphi_{\infty}(p_f)|)A_0(p_f, \varphi_{\infty}(p_f))/\Delta_{\max} \) of the order of unity for which condition (21) is violated. They arise for trajectories for which \( \Delta_{\infty}(p_f)\Delta_{\max}(p_f) < 0 \). In general, there are also bound states for glancing angles, i.e., \( \phi \approx \pm 90^\circ \), but they give only a very small contribution to the tunneling current, and we do not plot them here. The limit for bound states with nonzero quasiparticle energy is determined by momentum directions for which discrete bound state levels merge in the continuum. Note that for misorientation angles \( 37^\circ \leq \alpha < 45^\circ \) bound states appear for \( \varepsilon = 0 \) (midgap states), for \( \varepsilon \approx \Delta_{\infty}(\phi = 0^\circ) = \Delta_{\max} \cos(2\alpha) \).
(perpendicular incidence) and for \( \varepsilon \approx \Delta_\infty(\phi = 45^\circ) = \Delta_{\text{max}} \sin(2\alpha) (\phi = 45^\circ) \). As a result one finds three peaks in the conductance (see inset of Fig. 6a).

In Fig. 3 we display the dependence of the bound state energy for perpendicular incidence (\( \phi = 0 \)) on the misorientation angle \( \alpha \) for \( T = 0 \). We included the function \( \Delta_\infty(\phi = 0)/\Delta_{\text{max}} = \cos(2\alpha) \) to demonstrate that the bound states with nonzero energy lie very close to the band edge.

The angle-resolved density of states \( \nu(\phi, x = 0; \varepsilon) \) at clean surfaces \( (\rho = 0) \) is shown in Fig. 4 for the misorientation angles \( \alpha = 0^\circ, 20^\circ \) and \( 45^\circ \). For a \( (100) \) surface \( (\alpha = 0^\circ) \) (Fig. 4a) the order parameter is homogeneous up to the wall, and the surface density of states coincides with its bulk value. In particular, there are no surface bound states. The divergences presented in Fig. 4a lie at the edges of the continuum \( (\varepsilon = \pm \Delta_\infty(\phi)) \). For a lattice to surface orientation \( \alpha = 20^\circ \) (Fig. 4b) bound states occur near the surface. For perpendicular incidence \( (\phi = 0^\circ) \) there is a bound state with nonzero energy near the band edge, while for \( \phi = 30^\circ \) and \( 45^\circ \) midgap states appear (cf. Refs. [5,7]). In Fig. 4c we display the surface density of states for an ideal \( (110) \) surface \( (\alpha = 45^\circ) \). For a quasiparticle moving along a trajectory with angle \( \phi = 45^\circ \) we find both a midgap state and a bound state near the edge of the continuum. Both arise for an ideal boundary under the condition \( \Delta_\infty(p_f)\Delta_\infty(p_r) < 0 \). For this special surface orientation we have \( \Delta_\infty(p_f) = -\Delta_\infty(p_r) \) for all pairs of incoming and reflected trajectories. From Eqs. (13) and (14) we find \( \varphi(p_f, x) = \pi - \varphi(p_r, x) \), and at the surface \( \varphi(p_f, 0) = \varphi(p_r, 0) = \pi/2 \). On the other hand, we obtain from (13) for bound states near the continuum \( \varphi_\infty(p_f) = \pi - \varphi_\infty(p_r) \approx 0 \) or \( \pi \). Hence, the phase \( \varphi \) has to vary comparatively rapidly with spatial position \( x \). For this reason, our analytical approach, based on the approximation (18)-(20), breaks down for this special case.

The influence of surface roughness is shown in Fig. 5 for a lattice to surface orientation \( \alpha = 20^\circ \). We observe the broadening of the bound states with increasing roughness. The midgap state is smeared out faster than the nonzero-energy bound state (Figs. 5a, b). The point is that interference effects at the surface, which are of importance for the midgap states, are destroyed by diffuse scattering of quasiparticles at the boundary. On the other hand, for the existence of the nonzero-energy bound state only the suppression of the order parameter near the wall (even if it is very small) plays a role. For very rough surfaces (Fig. 5c) the midgap state is completely suppressed whereas the nonzero-energy bound state merges in the continuum. A similar behavior of midgap states at rough surfaces was observed in Ref. [1].

IV. TEMPERATURE DEPENDENCE OF THE PEAKS IN THE DIFFERENTIAL CONDUCTANCE

We consider a tunnel junction with transparency \( D \ll 1 \). First, we focus on specularly reflecting interfaces between a normal metal and a clean singlet anisotropically paired superconductor. Let the normal of the junction barrier plane be directed along the \( x \)-axis (\( \hat{n} \parallel \hat{x} \)). The superconductor occupies the left half-space \( (x < 0, \text{index } l) \) and the normal metal the right one \( (x > 0, \text{index } r) \). Then, the dissipative current in first order in the barrier transparency \( D \) may be represented by

\[
I_e(V) = -eA \int_{\nu_f, x > 0} \frac{d^2S_l}{(2\pi)^3} \frac{\nu_f}{|v_f|} D(p_f) \int_{-\infty}^{\infty} d\varepsilon \left( \tanh \left( \frac{\varepsilon - eV}{2T} \right) - \tanh \left( \frac{\varepsilon}{2T} \right) \right) \nu_S(p_f, 0; \varepsilon). \tag{34}
\]

Here, \( \nu_S(p_f, x = 0; \varepsilon) \) is the angle resolved density of states (4) of the superconductor on the left side of the tunneling barrier. It is calculated for zero transparency \( (D = 0) \). The voltage \( V = \Phi_l - \Phi_r \) is the difference between the electric potentials of the left and right electrodes, and \( A \) is the area of the interface. Properties of the normal metal enter only implicitly via the function \( D(p_f) \), which is the probability of a quasiparticle with momentum \( p_f \) to tunnel across the barrier. Note that the charge \( e \) is negative in our notation.

Most experiments measure directly the differential conductance \( G = dI/dV \). From Eq. (34) we get

\[
G(V, T) = \frac{e^2A}{2T} \int_{\nu_f, x > 0} \frac{d^2S_l}{(2\pi)^3} \frac{\nu_f}{|v_f|} D(p_f) \int_{-\infty}^{\infty} d\varepsilon \frac{\nu_S(p_f, 0; \varepsilon)}{\cosh^2 \left( \frac{\varepsilon - eV}{2T} \right)}, \tag{35}
\]

which reduces at zero temperature to

\[
G(V, T = 0) = 2e^2A \int_{\nu_f, x > 0} \frac{d^2S_l}{(2\pi)^3} \frac{\nu_f}{|v_f|} D(p_f) \nu_S(p_f, 0; eV). \tag{36}
\]
Thus, tunneling experiments at low temperatures measure essentially the surface density of states integrated over the Fermi surface. As we will show below the surface density of states of anisotropic superconductors deviates substantially from its bulk value if the surface is pair breaking. Hence, tunneling experiments are extremely sensitive to special features of the surface (orientation and roughness).

We notice, that in case of a real order parameter the density of states is symmetric with respect to the Fermi energy \( \varepsilon_f \), i.e., \( \nu(p_f, R; \varepsilon) = \nu(p_f, R; -\varepsilon) \). Consequently, the conductance in Eq. (33) is symmetric: \( G(V) = G(-V) \). Hence, the asymmetry of the conductance observed experimentally in Ref. [33] is beyond the scope of this article.

A. Surfaces without Pair Breaking

Let us first consider surfaces which are not pair breaking. Then, the density of states at the interface coincides with its bulk value,

\[
\nu_{Ss}(p_f, 0; \varepsilon) = \frac{|\varepsilon|}{\sqrt{|\varepsilon^2 - |\Delta(p_f)|^2|}} \Theta(|\varepsilon| - |\Delta(p_f)|) .
\]

At low temperatures \( (T \ll |eV|) \) we get the following expression for the differential conductance \( (\Delta_0(p_f) = \Delta(p_f, T = 0)) \):

\[
G \approx e^2 A \int_{v_{f,s} > 0} \frac{d^2 S^f}{(2\pi)^2} \frac{v_{f,s}^2}{|v_f^0|} D(p_f) \int_{-\infty}^{\infty} \frac{d\tilde{\varepsilon}}{\cosh^2(\tilde{\varepsilon})} \left| eV |\Theta(|eV| - |\Delta_0(p_f)|) + 2T \tilde{\varepsilon} \mathrm{sgn}(eV) \right| \frac{1}{\sqrt{eV T \varepsilon^2 + (|eV|^2 - |\Delta_0(p_f)|^2)^2}} .
\]

In the case of an isotropic \( s \)-wave superconductor we obtain for \( T \ll |eV| - \Delta_0 \) the well-known result for the conductance,

\[
G = \frac{1}{R_N} \frac{|eV|}{|eV|^2 - \Delta_0^2} \Theta(|eV| - \Delta_0) .
\]

At zero temperature the conductance diverges in the limit \( |eV| \to \Delta_0 \), which is directly associated with the singularity in the BCS density of states at \( \varepsilon = \Delta_0 \). It is worth noting that in the opposite limiting case, \( |eV| - \Delta_0 \ll T \ll \Delta_0 \), we obtain instead of (39) the following low-temperature anomaly in the conductance:

\[
G \approx \frac{0.48}{R_N} \sqrt{\frac{\Delta_0}{T}} .
\]

Hence, for the voltage \( |eV| = \Delta_0 \) there is a divergence of the conductance, \( G \propto 1/\sqrt{T} \), in the low-temperature limit, due to the singularity in the BCS density of states.

It has been known for a long time that anisotropy of the superconducting order parameter washes out structures in the integrated density of states, and correspondingly removes (or at least reduces) the singular behavior of the conductance (see Eq. (30)). This statement is valid, in general, in the absence of pair breaking at the surface. At the same time, in the presence of nodes of the order parameter on the Fermi surface, a nonzero subgap conductance appears. In particular, specific gapless and, in general, non-Ohmic behavior takes place in the limit of small voltages and low temperatures. For three-dimensional \( d \)-wave superconductor the singular behavior of the conductance vanishes in the absence of surface pair breaking. For the low voltage behavior one has, depending on the crystal orientation of such a superconductor relative to the barrier plane, \( G \propto |eV|/(R_N \Delta_0) \) or \( G \propto (|eV|/R_N \Delta_0) \ln(|\Delta_0/|eV|)| \) under the condition \( T \ll |eV| \ll \Delta_0 \), and \( G \propto (T/R_N \Delta_0) \) or \( G \propto (T/R_N \Delta_0) \ln(|\Delta_0/T|) \) if \( |eV| \ll T \ll \Delta_0 \).

Now, we consider a quasi two-dimensional Fermi surface, e.g., a Fermi cylinder with its principal axis parallel to the barrier plane. Let \( s = (s_\parallel, s_\perp) \) be a two-dimensional parameter set which describes the Fermi surface, i.e., \( p_f = p_f(s) \). As all quantities depend only on \( s_\parallel \) the order parameter can be approximated in the vicinity of a local maximum by \( |\Delta(p_f)| = \Delta_{\text{max}}(1 - b s_\parallel^2) \). Substituting this expansion into (33) we find the following singular contribution to the conductance (coming from the region \( b s_\parallel^2 \ll 1 \)):

\[
G_s \approx -e^2 A \sqrt{\frac{2}{b}} \int \frac{ds_{\perp}}{(2\pi)^3} \frac{d^2 p_{f,\perp}}{ds_{\parallel}} \left| \frac{\partial p_{f,\perp}}{\partial s_{\parallel}} \right| \left| \frac{\partial p_{f,\parallel}}{\partial s_{\parallel}} \right| v_{f,\perp} v_{f,\parallel} D(p_f) \left\{ \ln \left| \frac{|eV|}{\Delta_0} - 1 \right|, \ T \ll |eV| - \Delta_0|, \ \Delta_0, \right. \\
\left. \frac{1}{2} \ln \left( \frac{T}{\Delta_0} \right), \ |eV| - \Delta_0| \ll T \ll \Delta_0, \right\}
\]
where $\Delta_0 = \Delta_{\text{max}}(T = 0)$. For the low voltage behavior one finds in this case in the presence of nodes of the order parameter $G \propto |eV|/R_N\Delta_0$ for $T \ll |eV| \ll \Delta_0$ and $G \propto T/(R_N\Delta_0)$ for $|eV| \ll T \ll \Delta_0$.

So, in case of a $d$-wave superconductor with a cylindrical Fermi surface the low-temperature anomaly in the conductance as well as the singular dependence on the voltage turns out to reduce to a logarithmic singularity, $G \propto \ln(T), \ln(|eV| - \Delta_0|)$, which is much weaker compared to the $s$-wave case where we found $G \propto T^{-1/2}, ((eV)^2 - \Delta_0^2)^{-1/2}$.

**B. Surfaces with Pair Breaking**

For ideally smooth surfaces with pair breaking the singular behavior of the conductance of an NIS junction with a $d$-wave superconductor may become comparable or even stronger than for junctions with isotropic $s$-wave superconductors. The main reason for this are contributions from quasiparticle states bound to the barrier plane.

If in the vicinity of a given voltage the dominating contribution to the conductance comes from bound states, one may consider only a singular part (a pole-like term) of the retarded Green function $g_R^B$ at the interface:

$$g_R^B(p_f, x = 0; \varepsilon) = \frac{Q_g(p_f)}{\varepsilon - \varepsilon_B(p_f) + i\eta}, \quad \eta \rightarrow +0.$$  \hfill (42)

This yields a $\delta$-peak in the angle resolved density of states $\nu$. \hfill (43)

Hence, the function $\varepsilon_B(p_f)$ describes the energy dispersion of the quasiparticles bound to the barrier. Note that $\varepsilon_B(p_f)$ always has an extremum for the momentum direction along the normal of the boundary plane $(p_f||\hat{n})$, provided the bound state occurs for this direction (see [38], Fig. 2 and Ref. [10]). Substituting (43) into (45) we obtain the following anomalous contribution to the conductance:

$$G_s(V, T) = \frac{e^2A}{2T} \int_{\nu_{l,z}>0} d^2S_T \frac{v_{l,z}^f}{(2\pi)^3} |v_f^l| D(p_f^l) \frac{Q_g(p_f^l)}{\cosh^2 \left( \frac{\varepsilon_B(p_f) - eV}{2T} \right)}.$$  \hfill (44)

Consequently, the conductance rapidly increases with decreasing temperature, if the voltage is equal to the extremum of $\varepsilon_B(p_f)$. In case of a real order parameter bound states always appear in pairs with energies $\pm \varepsilon_B(p_f)$ (see Eqs. (44), (45)). Thus, we get from Eq. (44) the relation $G_s(V) = G_s(-V)$.

Let us again consider a two-dimensional system. We assume that the dispersion of the bound states can be approximated around its maximum by $\varepsilon_B(s) = \varepsilon_B^{\text{max}} - bs_{\|}^2$ ($b > 0$). Then for $|\varepsilon_B^{\text{max}} - |eV|| \ll T$ we obtain from (44) the following low-temperature anomaly in the conductance:

$$G_s = \frac{\sqrt{2} - 1}{2\sqrt{\pi bT}} e^2A \int_{\nu_{l,z}>0} dS_T \frac{\partial p_{f\|}^l}{\partial s_\|} \left| \frac{\partial p_{f\perp}^l}{\partial s_\perp} \right| \left| v_{l,z}^f \right| D(p_f^l) Q_g(p_f^l).$$  \hfill (45)

It is essential for the derivation of this result, that under the condition $|\varepsilon_B^{\text{max}} - |eV|| \ll T$ only a region $bs_{\|,\text{max}}^2 \ll T$ contributes to the integral over $s_{\parallel}$ (due to the exponential decrease of the $\cosh^{-2}$-function outside), and the condition $T \ll bs_{\|,\text{max}}^2$ permits to carry out the integration to infinity. Thus, making use of only the first two terms in the expansion of $\varepsilon_B(p_f)$ near its maximum may be justified at sufficiently low temperatures. It is assumed for simplicity, that for all values $bs_{\|}^2 \ll T$ the bound state still exists. All other quantities are supposed to change only slightly within the region $bs_{\|}^2 \ll T$.

Provided $T \ll |\varepsilon_B^{\text{max}} - |eV||, bs_{\|,\text{max}}^2$ we obtain instead of (45) the following dependence of the conductance on the voltage near the low-temperature peak:

$$G_s = \frac{2e^2A \Theta(\varepsilon_B^{\text{max}} - |eV|)}{\sqrt{b}} \int_{\varepsilon_B^{\text{max}} - |eV|} dS_T \frac{\partial p_{f\|}^l}{\partial s_\|} \left| \frac{\partial p_{f\perp}^l}{\partial s_\perp} \right| \left| v_{l,z}^f \right| D(p_f^l) Q_g(p_f^l).$$  \hfill (46)

In the case of a three-dimensional Fermi surface we expect the function $\varepsilon_B(p_f)$ to vary around its maximum as $\varepsilon_B(p_f) = \varepsilon_B^{\text{max}} - b_1s_{\|}^2 - b_2s_{\perp}^2$ ($b_1, b_2 > 0$). In contrast to the two-dimensional case $\varepsilon_B(p_f)$ now has an extremal point
instead of an extremal line. Then Eq. (33) is valid only under the condition $b_2 s_{2, \text{max}}^2 \ll b_1 s_{1, \text{max}}^2$ (e.g., for a strongly elongated ellipsoidal Fermi surface) for temperatures $|\varepsilon_B^{\text{max}} - |eV||$, $b_2 s_{2, \text{max}}^2 \ll T \ll b_1 s_{1, \text{max}}^2$. For lower temperatures $T \lesssim b_2 s_{2, \text{max}}^2$ there are no temperature anomalies in the conductance.

Due to the dispersionless character of midgap states ($\varepsilon_B(p_i) = 0$) their influence on the differential conductance differs from the influence of nonzero-energy states. We find from (44)

$$G_s = \frac{e^2 A}{2T} \int_{v_{f,i} > 0} \frac{d^2 S_{\gamma}^i}{(2\pi)^3} \left| v_{f,x}^i \right| D(p_i) Q_g(p_f) , \quad |eV| \ll T ,$$

which is independent on the exact form and the dimensionality of the Fermi surface. The general analytical expression for the function $Q_g(p_f)$ for midgap states via the spatially dependent order parameter as well as the explicit form of this function for a particular surface configuration are given in Ref. 10. In realistic systems the width of this zero-bias anomaly of the conductance is governed, apart from temperature, by the width of the broadened midgap delta-peak in the density of states.

C. Numerical Results

We have carried out numerical calculations of the conductance under various conditions. The angular dependence of the transparency is taken to be $D(\phi) = D_0 \cos^2(\phi)$ where $D_0$ is the transparency for perpendicular incidence and is related to the normal state resistance via Eq. (7). The conductance $G(V)$ at zero temperature is displayed in Fig. 6 for various misorientation angles $\alpha$. Figure 6a shows the results for a smooth surface ($\rho = 0$), whereas in Figs. 6b, c the roughness parameter $\rho$ is chosen to be 0.02 and 0.10, respectively. For $\alpha = 0$ there is no surface pair breaking and no quasiparticle states bound to the interface. In the case of an ideal boundary (Fig. 6a) the corresponding conductance has a logarithmic divergence (see Eq. (46)) at $|eV| = \Delta_0$ from both sides of this point. In contrast to this peak, one can see asymmetrical peaks for $\alpha \not= 0$. For finite misorientation angles $\alpha$ bound states, localized near the surface, arise. The conductance has a square root divergence at $|eV| = \varepsilon_B^{\text{max}}$ (see Eq. (48)) as well as a divergence at $V = 0$ due to midgap states. Surface roughness (Figs. 6b, c) cuts these divergences and leads to finite peaks which become smaller and wider with increasing roughness. It is evident from these figures that the conductance peak at nonzero voltage does not measure the maximum gap $\Delta_{\text{max}}$ but, to a good approximation, the (bulk) gap for perpendicular incidence $\Delta_{\text{bulk}}(p_f)$. We want to stress that the position of the peaks changes only slightly with increasing roughness. Although a direct comparison of our data with the results of Ref. 24 is not possible (they consider the surface density of states and not the conductance) the influence of roughness is similar in both models.

The low-temperature behavior of the conductance peaks is presented in Figs. 7a, b for smooth interfaces ($\rho = 0$) with misorientation angles $\alpha = 20^\circ$ and $30^\circ$. The temperature dependence of the zero-bias anomaly $G(0)$ is described in Fig. 7a, while in Fig. 7b the values of the peak at nonzero voltage $G(V_{\text{max}})$ are shown. We see, for example, that for a lattice to surface orientation $\alpha = 20^\circ$ the zero-bias conductance $G(0)$ is proportional with a good accuracy to $1/T$ up to $T = 0.2T_c$, whereas the temperature dependence of the quantity $G(V_{\text{max}})$ is described by the $(1/\sqrt{T})$–term only for a very small temperature range ($T \lesssim 0.01T_c$).

The influence of finite temperatures on the conductance is plotted in Fig. 8 (Fig. 9) for a lattice to surface orientation $\alpha = 20^\circ$ ($\alpha = 45^\circ$). We present results for different degrees of interface roughness: (a) smooth interface ($\rho = 0$), (b) slightly rough interface ($\rho = 0.02$) and (c) higher degree of roughness ($\rho = 0.10$). The peaks are well pronounced only for $T \lesssim 0.2T_c$ (this corresponds to the temperature of liquid Helium if $T_c = 93$ K is assumed) the reduction of the height of the conductance peaks is evident. At least at low temperatures, the effect of thermal smearing is more pronounced for the nonzero-bias peaks (Fig. 9a). Thus, we would like to encourage experimentalists to do tunneling measurements even below 4.2 K.

Figure 10 compares the results for the conductance at $T = 0$ using a constant order parameter (cf. Ref. 34) with calculations including a self-consistent order parameter. In both cases ($\alpha = 20^\circ$ and $\alpha = 45^\circ$) we find dramatic differences at finite voltages because of the appearance of nonzero-energy bound states due to the depletion of the order parameter near the interface. The presence of the zero-bias conductance peak is unaffected by the self-consistency of the order parameter, although disregarding surface pair-breaking results in overestimating of the weight of the peak up to 50% depending on the crystal orientation.
In summary, we have studied in detail the appearance of surface bound states and their relevance for the tunneling spectrum of NIS junctions. We developed, for the first time, an analytical approach to the surface problem which allows an understanding of the presence of zero-energy as well as nonzero-energy bound states. Numerical calculations have been done for $d$-wave superconductors assuming a cylindrical Fermi surface.

It is well known that zero-energy bound states are a robust phenomenon and will always occur whenever the real order parameter changes sign along a quasiparticle trajectory. So far, it was not clear under which condition nonzero-energy bound states arise. They were only observed numerically. The result of our analytical consideration is that at least some of the nonzero-energy bound states are also of quite general (although not topological) origin and appear, for any (even tiny) suppression of the order parameter, within a narrow region around the surface normal (see Fig. 2a). The reason is that the order parameter amplitudes for the incoming and the outgoing trajectories far away from the surface are approximately the same in this region, i.e., $\Delta_\infty(p_f) \approx \Delta_\infty(p'_f)$. As a consequence, nonzero-energy states around the surface normal occur in the case of $d$-wave superconductors for all lattice to surface orientations with the exception of (100) surfaces (no suppression of the order parameter) and of (110) surfaces ($\Delta(p^0_f) = 0$). In addition, we found numerically nonzero-energy bound states for misorientation angles between $37^\circ$ and $45^\circ$ as shown in Fig. 2b. These states are, however, beyond the validity of our analytical approach.

Furthermore, we have studied the influence of bound states on the tunneling conductance, in particular at low temperatures (Figs. 6a). While zero-energy bound states always result in a $1/T$ divergence of the conductance for $T \to 0$, the influence of nonzero-energy bound states depend on the geometry of the Fermi surface. For quasi two-dimensional Fermi surfaces the conductance diverges as $1/\sqrt{T}$ at voltages determined by the extrema of the bound state energies. Within a few percent, these peaks coincide for $\alpha \leq 37^\circ$ with the bulk order parameter for perpendicular incidence, i.e., $|eV_{\text{max}}| \approx |\Delta_\infty(p_f)|$. Only for higher misorientation angles ($\alpha \gtrsim 37^\circ$) the conductance peaks correspond approximately to the bulk gap $\Delta_{\text{max}} = \max_{p_f} |\Delta_\infty(p_f)|$. By contrast, low-temperature peaks in the conductance at nonzero-bias voltage are absent for three-dimensional systems. Our finite temperature calculations (Figs. 8a, 9a) demonstrate that the peaks can only be observed for temperatures below $0.2T_c$. Finally, we have investigated the influence of surface roughness on the conductance (Figs. 6b, c, 8b, c, 9b, c). The peaks are broadened, but their positions remain essentially untouched. The broadening of the peaks with increasing surface roughness is more crucial for the zero-bias peaks.

We conclude that a systematic experimental study of low-temperature peaks in the conductance of NIS junctions for a series of lattice to surface orientations would give valuable information on the anisotropy of the superconducting order parameter. We stress once more that nonzero-bias peaks give information on the gap amplitude in the bulk, even though the order parameter is suppressed at the surface.

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FIG. 1. Schematic geometry of our interface model: a smooth interface covered by a dirty layer on each side. Also shown are the four Fermi momenta which are involved in the scattering process at the smooth interface ($x = 0$).

FIG. 2. Angular dependence of the bound state energies $\varepsilon_B(\phi)$ near $\phi = 0^\circ$ (a) and near $\phi = 45^\circ$ (b) for various misorientation angles $\alpha$.

FIG. 3. Bound state energy for perpendicular incidence $\varepsilon_B(\phi = 0)$ as a function of the misorientation angle $\alpha$. For comparison, we included the position of the band edge, $\Delta_\infty(\phi = 0)/\Delta_{\text{max}} = \cos(2\alpha)$.

FIG. 4. Angle-resolved density of states at a smooth surface ($\rho = 0$) for various trajectory angles $\phi$. The lattice to surface orientation is taken to be $\alpha = 0^\circ$ (a), $20^\circ$ (b) and $45^\circ$ (c).

FIG. 5. Angle-resolved density of states at rough surfaces ($\alpha = 20^\circ$) for the same trajectory angles $\phi$ as in Fig. 4b. The roughness parameter $\rho$ is 0.02 (a), 0.10 (b) and 0.50 (c).

FIG. 6. Zero-temperature conductance as a function of the bias voltage for various misorientation angles $\alpha$. The surface roughness is $\rho = 0$ (a), 0.02 (b) and 0.10 (c). The inset of (a) demonstrates the presence of three conductance peaks for $\alpha = 40^\circ$.

FIG. 7. Temperature dependence of the zero-bias anomaly $G(V = 0, T)$ (a) and the nonzero-bias anomaly $G(V = V_{\text{max}}, T)$ (b) for two lattice to surface orientation angles $\alpha = 20^\circ$ and $30^\circ$.

FIG. 8. Conductance $G(V)$ for various temperatures $T$. The lattice to surface orientation is taken to be $\alpha = 20^\circ$. The figures display the effect of increasing roughness: $\rho = 0$ (a), 0.02 (b) and 0.10 (c).

FIG. 9. The same as in Fig. 8 but for $\alpha = 45^\circ$.

FIG. 10. Influence of the self-consistency of the order parameter on the zero-temperature conductance of a smooth interface ($\rho = 0$). We show the data for two misorientation angles $\alpha = 20^\circ$ and $45^\circ$. 
\[ \cos(2\alpha) \]

\[ \varepsilon_B(\phi=0)/\Delta_{\text{max}} \]
energy $\epsilon/\Delta_0$

DOS $\nu(\phi, x=0; \epsilon)$

$\phi = 0^\circ$
$\phi = 15^\circ$
$\phi = 30^\circ$
$\phi = 45^\circ$

$\alpha = 0^\circ$

$\alpha = 20^\circ$

$\alpha = 45^\circ$
(a) $\alpha=0$ $\rho=0$ 

(b) $\alpha=20$ $\rho=0.02$ 

(c) $\alpha=35$ $\rho=0.10$
\( G(V_{\max}) R_N (T/T_c)^{1/2} \) vs. \( (T/T_c)^{1/2} \)

- \( \alpha = 20^\circ \)
- \( \alpha = 30^\circ \)
(a) $\rho=0$

(b) $\rho=0.02$

(c) $\rho=0.10$
self-consistent

not self-consistent