Quasiparticle Interface States in Junctions Involving d-Wave Superconductors

Yu. S. Barash

P.N. Lebedev Physical Institute, Leninsky Prospect 53, Moscow 117924, Russia

and

Department of Physics, Åbo Akademi, Porthansgatan 3, FIN-20500 Åbo, Finland

Abstract

Influence of surface pair breaking, barrier transmission and phase difference on quasiparticle bound states in junctions with $d$-wave superconductors is examined. Based on the quasiclassical theory of superconductivity, an approach is developed to handle interface bound states. It is shown in SIS’ junctions that low energy bound states get their energies reduced by surface pair breaking, which can be taken into account by introducing an effective order parameter for each superconductor at the junction barrier. More interestingly, for the interface bound states near the continuous spectrum the effect of surface pair breaking may result in a splitting of the bound states. In the tunneling limit this can lead to a square root dependence of a nonequilibrium Josephson current on the barrier transmission, which means an enhancement as compared to the conventional critical current linear in the transmission. Reduced broadening of bound states in NIS junctions due to surface pair breaking is found.

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I. INTRODUCTION

The important role in the Josephson effect of quasiparticle bound states localized in contacts between isotropic $s$-wave superconductors, is well known from studies of superconductor-normal metal-superconductor (SNS) junctions and quantum point contacts. Even for spatially constant order parameters of equal moduli on the two sides of a junction (no surface pair breaking), Andreev reflection takes place on account of the phase shift between them. Current-carrying interface bound states with phase-dependent energies are formed at the junction\cite{1,2,3,4}. In short symmetric junctions, these bound states are known to carry all the Josephson current, while in asymmetric junctions the contribution from the continuous spectrum is of importance as well.

The situation becomes more complicated in junctions involving $d$-wave superconductors where a quasiparticle, depending on its momentum, can see both substantial modulus distortions or (and) a sign change in the order parameter in a reflection or a transmission process at a junction. Several kinds of bound states occur in this case, each with a different dependence on the quasiparticle momentum according to the incoming and outgoing quasiparticle trajectories as well as the crystalline orientations on the two sides of the junction. In particular, low energy interface bound states are of interest, associated with changes of sign of the order parameter in reflection or transmission events. They become dispersionless zero-energy states both in the limiting case of zero transmission (impenetrable wall) or (and) in the opposite limit of a ballistic junction\cite{5,6,7,8}. In certain conditions, zero-energy (or low-energy) bound states can result in an anomalous low temperature behavior of the Josephson critical current\cite{9,10} and in characteristic peaks and jumps in the I-V curves\cite{11}. In normal metal-insulator-superconductor (NIS) junctions they lead, at sufficiently low temperatures, to a zero-bias conductance peak\cite{5,12,13,14,15}.

As incoming quasiparticles with a momentum along the interface normal see the same $d$-wave order parameter as the outgoing ones, the bound states they occupy are to some extent analogous to those in junctions with isotropic $s$-wave superconductors. These bound
states can dominate the charge transport across a junction for certain orientations of d-wave superconductors if the transmission coefficient is sufficiently selective, limiting the transport of current to quasiparticles with momentum directions close to the interface normal, as is always the case for thick junctions. The difference between s-wave and d-wave cases, in general, is present even for the momentum orientation parallel to the interface normal being associated with surface pair breaking substantially more pronounced in anisotropically paired superconductors. As compared to isotropic s-wave superconductors, boundary conditions for anisotropic order parameters are very different because of surface pair breaking even within the Ginzburg-Landau theory. Depletion of the modulus of the order parameter in the vicinity of a contact modifies the bound state energies seen in non-selfconsistent models with constant absolute values of the order parameters. Besides, additional bound states can appear for quasiparticles in an effective potential well formed by the spatially dependent moduli of order parameters on the two sides of the junction. Since surface pair breaking depends upon crystal-to-interface orientations, it can strongly modify corresponding angular dependences of bound state energies and, in particular, the critical current obtained for a non-selfconsistent spatially constant order parameters.

Assuming order parameters with spatially constant moduli on both sides of a junction, calculations of the energies of current-carrying quasiparticle bound states can be found in the literature admitting the presence of a phase shift and any value of the transmission. The effect of surface pair breaking combined with a phase shift and the influence of a finite transmission on the interface bound states have, however, to the best of my knowledge, not been studied yet. Below, in Section II, I shall develop an analytical approach for studying the combined effects of surface pair breaking, a phase shift and the transmission coefficient on bound states, localized, in particular, at a contact between two d-wave superconductors. The approach is based on the quasiclassical theory of superconductivity focused on the problem of interface bound states. A key point of the consideration is that retarded propagators at the interface take quite large values (pole-like terms) at energies \( \omega \) close to an interface bound state energy \( \varepsilon_B(p_f) \). Expanding propagators in powers of \( (\omega - \varepsilon_B(p_f)) \)
one can introduce, in a first approximation, an ansatz for the bound states, which reduces the Eilenberger equations and the normalization condition to one scalar differential equation for a quasiclassical phase $\eta$ to be completed with asymptotic and boundary conditions for its solutions. This equation was derived earlier in Ref. 15 for the particular case of impenetrable boundary and real order parameter. Actually the equation has a more general character, as it is associated with the approach where the Eilenberger equations transform to a scalar Riccati equation. It has the same form as that obtained on the basis of the Bogoliubov-de Gennes equations within the WKB approximation, being applicable both to discrete and to continuous spectrum. Boundary conditions formulated below for the quasiclassical equation are new. It is remarkable, that the boundary condition for the quasiclassical quantity $\eta$, in accordance as it is with Zaitsev’s boundary conditions, can be formulated separately from all other quantities, just like the one-scalar boundary condition for the equation for $\eta$ mentioned above. It is a great deal simpler as compared to Zaitsev’s original form and admits analytical results. The same boundary condition for $\eta$ can be derived also starting from the boundary conditions for the Andreev equations irrespective of whether a discrete or continuous spectrum is considered.

On this basis I study interface bound states in both SIS’ (see Section III) and NIS (see Section IV) junctions. It is shown for SIS’ junctions that surface pair breaking results in reducing the energies of low energy bound states which can be taken into account by introducing an effective order parameter for each superconductor at the junction barrier. For interface bound states near the edge of the continuous spectrum, the effect of surface pair breaking turns out to be more interesting, resulting in splitting the bound state energies. In the tunneling limit this can lead to a square root dependence of the nonequilibrium Josephson current on the barrier transmission, which means an enhancement as compared to the conventional critical current linear in transmission. For NIS junctions the influence of surface pair breaking on broadening the bound state is considered.
II. QUASICLASSICAL THEORY OF INTERFACE BOUND STATES

A. Ansatz for bound states

Quasiclassical theory of superconductivity is based on Eilenberger’s equations for the quasiclassical matrix propagator. In the case of a clean singlet anisotropically paired superconductor the equations for the retarded propagator $\hat{g}^R$ reduce to the following $2 \times 2$ matrix form:

$$
\left[ \epsilon \tau_3 - \hat{\Delta}(p_f, r), \hat{g}^R(p_f, r; \epsilon) \right] + i v_f \cdot \nabla_r \hat{g}^R(p_f, r; \epsilon) = 0 ,
$$

(1)

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

(2)

Here, $\epsilon$, $p_f$, $v_f$ and $\hat{\Delta}$ are the quasiparticle energy, the momentum at the Fermi surface, the Fermi velocity and the order parameter matrix respectively. A “hat” indicates matrices in Nambu space and $\hat{\tau}_3$ is a Pauli matrix in this space. The propagator $\hat{g}$ and the order parameter matrix $\hat{\Delta}$ have the form

$$
\hat{g} = \begin{pmatrix} g & f \\ f^* & -g \end{pmatrix} \quad \text{and} \quad \hat{\Delta} = \begin{pmatrix} 0 & \Delta \\ -\Delta^* & 0 \end{pmatrix} .
$$

(3)

Henceforth the superscript $R$ is dropped for simplicity. The boundary conditions for the quasiparticle propagators at a smooth interface with transmission $D(p_f) = 1 - R(p_f) \left(R(p_f)\right)$ the reflectivity coefficient of the interface) are given by Zaitsev’s relations (see Refs. 23, 24) which can be written in the following matrix form

$$
\hat{d}_r \hat{s}_l^2 = i\alpha \left[ \hat{s}_l, \hat{s}_r \left( \pi - \frac{i}{2} \hat{d}_l \right) \right] ,
$$

(4)

$$
\hat{d}_l = \hat{d}_r ,
$$

(5)

with $\alpha = (1 - R)/(1 + R)$, $\hat{s}_{l(r)} = \hat{g}_{l(r)}(p_{f,l(r)}) + \hat{g}_{l(r)}(p_{f,l(r)})$, $\hat{d}_l = \hat{g}_l(p_{f,l}) - \hat{g}_l(p_{f,l})$, $\hat{d}_r = -\hat{g}_r(p_{f,l}) + \hat{g}_r(p_{f,l})$, and the propagators are taken on the left or the right side of the interface. Equations (4), (5) connect, at the interface, the propagators of an incoming quasiparticle from the left and the right sides of the interface with momenta $p_{f,l}$, $p_{f,r}$ and the propagators
of the reflected quasiparticles with the momenta $p_{f,l}$, $p_{f,r}$. For specular reflection, the momentum parallel to the interface is conserved, i.e., $p_{f,l}^\parallel = p_{f,r}^\parallel = p_{r,f}^\parallel = p_{f,r}^\parallel$. For a complete determination of the quasiclassical propagator one has to take into account that deep inside the superconductor the propagator approaches its bulk value.

In the presence of a quasiparticle bound state with the energy $\varepsilon_B(p_f)$, manifesting dispersion dependence on the Fermi momentum $p_f$, the quasiclassical propagator $\hat{g}$ has a pole at $\varepsilon = \varepsilon_B(p_f)$. Following Ref. 15, one can introduce the residue of the propagator $\hat{g}$

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

which is finite, satisfies the same transport equation (1) as $\hat{g}$, but completed with the relation

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

rather than the normalization condition (2).

Linear boundary relations (3) being applied to $\hat{d}$, remain unchanged. At the same time nonlinear boundary conditions (4), taken at a bound state energy, simplify in a significant fashion. Terms containing multiplications of three propagators dominate in (4), if each propagator is well described by a large pole-like term. Other terms in Eq.(4), with only two propagators, can be neglected under conditions in question. Then Eq.(4) reduces to

$$\hat{s}_l^2 - \frac{\alpha}{2} \{\hat{s}_l, \hat{s}_r\} = 0 .$$

As the left hand side of matrix equation (8) is proportional to the unit matrix, it leads to one independent scalar equation only.

Eilenberger’s equations for $\hat{g}$ can be solved in terms of the following ansatz:

$$\tilde{f}^+(p_f, x; \varepsilon_B(p_f)) = \hat{g}(p_f, x; \varepsilon_B(p_f)) \exp(-i\eta(p_f, x)) ,$$

$$\tilde{f}(p_f, x; \varepsilon_B(p_f)) = -\hat{g}(p_f, x; \varepsilon_B(p_f)) \exp(i\eta(p_f, x)) .$$

This ansatz was introduced earlier in Ref. 15 for the particular case of a real order parameter and impenetrable wall. In general, the substitution (8), satisfying Eq. (7), allows for the
quantity $\eta$ (as well as $\tilde{g}(\mathbf{p}_f, x; \varepsilon_B(\mathbf{p}_f))$ and $\varepsilon_B(\mathbf{p}_f)$) to take complex values $\eta = \eta' + i\eta''$ ($\varepsilon_B(\mathbf{p}_f) = \varepsilon'_B(\mathbf{p}_f) + i\varepsilon''_B(\mathbf{p}_f)$). Complex values of $\eta$ and $\varepsilon_B(\mathbf{p}_f)$ imply, in particular, broadened quasiparticle bound states (due to finite quasiparticle lifetime) discussed in the last section of the present article for NIS-junctions on account of finite transmission.

Introducing the phase of the complex order parameter $\Delta(\mathbf{p}_f, x) = |\Delta(\mathbf{p}_f, x)|e^{i\phi(\mathbf{p}_f, x)}$, one obtains from (1), (7) with substitution (9):

$$
\tilde{g}(\mathbf{p}_f, x; \varepsilon_B(\mathbf{p}_f)) = \tilde{g}_0(\mathbf{p}_f, \varepsilon_B(\mathbf{p}_f)) \exp \left( -\frac{2}{v_{f,x}} \int_0^x \left| \Delta(\mathbf{p}_f, \bar{x}) \right| \sin (\eta(\mathbf{p}_f, \bar{x}) - \phi(\mathbf{p}_f, \bar{x})) d\bar{x} \right),
$$

(10)

together with the following equation for $\eta$:

$$
-\frac{v_{f,x}}{2} \partial_x \eta(\mathbf{p}_f, x) + \varepsilon_B(\mathbf{p}_f) - |\Delta(\mathbf{p}_f, x)| \cos (\eta(\mathbf{p}_f, x) - \phi(\mathbf{p}_f, x)) = 0.
$$

(11)

According to Eq.(10), under some conditions the residue $\tilde{g}$ vanishes exponentially in the bulk of the superconductor. Then, the quantity $\tilde{g}$ describes a quasiparticle state bound to the interface. Furthermore, equation (11) coincides with one obtained many years ago on the basis of WKB approximation for Bogoliubov-de Gennes equations\textsuperscript{22,3}, being applicable both to discrete and to continuous spectrum. For continuous spectrum $\eta(\mathbf{p}_f, \bar{x}) - \phi(\mathbf{p}_f, \bar{x})$ should be a purely imaginary quantity in accordance with Eq.(10). The same equation (11) is known to appear as well within the approach transforming the Eilenberger equations to a scalar Riccati equation\textsuperscript{21}.

The asymptotic condition for $\eta$, which guarantees solution (11) to vanish in the bulk, takes in the right half space ($x \to +\infty$) the form

$$
v'^{r,x}_f(\mathbf{p}_f,r) \sin \left( \eta'^{r,\infty}_r(\mathbf{p}_f,r) - \phi^{r,\infty}_r(\mathbf{p}_f,r) \right) > 0,
$$

(12)

while in the limit $x \to -\infty$

$$
v'^{l,x}_f(\mathbf{p}_f,l) \sin \left( \eta'^{l,\infty}_l(\mathbf{p}_f,l) - \phi^{l,\infty}_l(\mathbf{p}_f,l) \right) < 0.
$$

(13)
Substitution (9) essentially simplifies relations (5), (8), resulting, in particular, in the following boundary condition for equation (11)

\[ R \sin \left( \frac{\eta_{0,0}(p_{f,l}) - \eta_{0,0}(p_{f,l})}{2} \right) \sin \left( \frac{\eta_{0,0}(p_{f,r}) - \eta_{0,0}(p_{f,r})}{2} \right) = 
\]

\[ D \sin \left( \frac{\eta_{0,0}(p_{f,l}) - \eta_{0,0}(p_{f,r})}{2} \right) \sin \left( \frac{\eta_{0,0}(p_{f,l}) - \eta_{0,0}(p_{f,r})}{2} \right). \]

(14)

This boundary condition holds for any value of the transmission coefficient. In the tunneling limit, \( D \ll 1 \), it is convenient to transform Eq. (14) to the following equivalent relation

\[ D \sin \left( \frac{\eta_{0,0}(p_{f,l}) - \eta_{0,0}(p_{f,r})}{2} \right) \sin \left( \frac{\eta_{0,0}(p_{f,l}) - \eta_{0,0}(p_{f,r})}{2} \right) = 
\]

\[ \sin \left( \frac{\eta_{0,0}(p_{f,l}) - \eta_{0,0}(p_{f,l})}{2} \right) \sin \left( \frac{\eta_{0,0}(p_{f,l}) - \eta_{0,0}(p_{f,r})}{2} \right). \]

(15)

It is remarkable that the boundary condition for the quantity \( \eta \) can be formulated separately from other quantities, simply as a boundary condition for equation (11). Other boundary relations for quantities entering ansatz (9) are given in Appendix.

Relation (14) can also be derived within a more general framework independent of whether a discrete or continuous spectrum is considered. For this purpose one can represent the Andreev amplitudes in the form

\[
\left( \begin{array}{c}
  u(p_{f}, x) \\
  v(p_{f}, x)
\end{array} \right) = \left( \begin{array}{c}
  e^{i\eta(p_{f}, x)/2} \\
  e^{-i\eta(p_{f}, x)/2}
\end{array} \right) e^{i\xi(p_{f}, x)},
\]

(16)

where \( \eta(p_{f}, x) \) and \( \xi(p_{f}, x) \) are, in general, complex. Substituting (16) into the boundary conditions for Andreev amplitudes, one obtains Eq. (14) as a separate boundary condition for \( \eta(p_{f}, x) \). In the particular case of discrete spectrum \( \eta(p_{f}, x) \) is a real quantity, while \( \xi(p_{f}, x) \) is purely imaginary leading to exponentially decaying asymptotic behavior of the Andreev amplitudes. Furthermore, functions entering the expression for the quasiclassical
matrix Green function and satisfying the Riccati equation can, in general, be represented as \( u(p_f, x)/v(p_f, x) = e^{i\eta(p_f, x)} \). Boundary conditions for these functions are evidently directly related with Eq. (14). It is worth noting, in addition, that Eq. (11) transforms to the Riccati form by introducing the new function \( \beta = \tan(\eta/2) \).

If \( \eta(p_f, x) \) is a solution of Eqs. (11), (15) with the energy \( \varepsilon(p_f) \), then \( \pi - \eta(p_f, x) \) is a solution of the same equations with \( -\varepsilon(p_f) \) for the system with a given \( p_f \) and complex conjugated order parameter. So, for a given \( p_f \) quasiparticle discrete spectrum of a system can be, generally speaking, asymmetric with respect to the Fermi surface under the condition \( \phi \neq 0 \).

**B. Positions of poles and residue values**

As it is shown in this section, energies of bound states, entering denominators of pole-like terms in the expressions for the propagators, on the one hand, and residues of those pole-like terms, on the other hand, can be expressed via \( \eta(p_f, x) \) for a given \( \Delta(p_f, x) \).

Since \( \partial_x \eta(p_f, x) \) vanishes in the bulk \( (x \to \pm \infty) \), one immediately gets from Eqs. (11) the relation between the bound state energy \( \varepsilon_B(p_f) \) and the quantities \( \eta_{\infty}(p_f), \Delta_{\infty}(p_f) \) in the bulk of the superconductor:

\[
\varepsilon_B(p_f, r) = |\Delta^r_{\infty}(p_f, r)| \cos (\eta_{r, \infty}(p_f, r) - \phi_{r, \infty}(p_f, r)) = |\Delta^r_{\infty}(p_f, l)| \cos \left( \eta_{r, \infty}(p_f, l) - \phi_{r, \infty}(p_f, l) \right) \\
= |\Delta^l_{\infty}(p_f, l)| \cos (\eta_{l, \infty}(p_f, l) - \phi_{l, \infty}(p_f, l)) = |\Delta^l_{\infty}(p_f, r)| \cos \left( \eta_{l, \infty}(p_f, r) - \phi_{l, \infty}(p_f, r) \right) .
\]

(17)

As a consequence, bound states might exist for a given momentum direction only below the band edges for the momenta \( p_{f,l(r)} \) and \( p_{f,l(r)} \), i.e., for

\[
|\varepsilon_B(p_f)| \leq \min \left\{ |\Delta^l_{\infty}(p_f, l)|, |\Delta^r_{\infty}(p_f, r)|, |\Delta^l_{\infty}(p_f, r)|, |\Delta^r_{\infty}(p_f, r)| \right\} .
\]

(18)

Furthermore, for a frequency near the bound state energy \( \varepsilon_B(p_f) \), the quasiclassical Green’s functions can be expanded in powers of \( (\omega - \varepsilon_B(p_f)) \). Taking into account ansatz (14), one has
\[ g(p_f, x; \omega) = \frac{\tilde{g}(p_f, x; \varepsilon_B(p_f))}{(\omega - \varepsilon_B(p_f) + i\delta)} + \sum_{n=0}^{\infty} g^{(n)}(p_f, x; \varepsilon_B(p_f))(\omega - \varepsilon_B(p_f))^n, \]  

(19)

\[ f(p_f, x; \omega) = -\frac{\tilde{g}(p_f, x; \varepsilon_B(p_f))}{(\omega - \varepsilon_B(p_f) + i\delta)} e^{\nu(p_f, x)} + \sum_{n=0}^{\infty} f^{(n)}(p_f, x; \varepsilon_B(p_f))(\omega - \varepsilon_B(p_f))^n, \]  

(20)

\[ f^+(p_f, x; \omega) = \frac{\tilde{g}(p_f, x; \varepsilon_B(p_f))}{(\omega - \varepsilon_B(p_f) + i\delta)} e^{-\nu(p_f, x)} + \sum_{n=0}^{\infty} f^{+(n)}(p_f, x; \varepsilon_B(p_f))(\omega - \varepsilon_B(p_f))^n. \]  

(21)

Further I introduce the quantities

\[ f_\pm(p_f, x; \omega) = \frac{1}{2} \left( f^+(p_f, x; \omega)e^{\nu(p_f, x)} \pm f(p_f, x; \omega)e^{-\nu(p_f, x)} \right). \]  

(22)

According to (19)-(21), \( f_+(p_f, x; \omega) \) has no singular part (no pole-like term), while the singular part of \( f_-(p_f, x; \omega) \) coincides with the one for \( g(p_f, x; \omega) \), that is

\[ \tilde{f}_-(p_f, x; \varepsilon_B(p_f)) = \tilde{g}(p_f, x; \varepsilon_B(p_f)), \quad \tilde{f}_+(p_f, x; \varepsilon_B(p_f)) = 0. \]  

(23)

In addition, substituting expansions (19)-(21) into the normalization condition (2) and equating terms inversely proportional to \( (\omega - \varepsilon_B(p_f)) \), one finds

\[ f^{(0)}_-(p_f, x; \varepsilon_B(p_f)) = g^{(0)}(p_f, x; \varepsilon_B(p_f)). \]  

(24)

Taking into account (22)-(24) one derives at the following relationship (for \( x > 0 \)) from the Eilenberger equations

\[ f^{(0)}_+(p_f, x; \varepsilon_B(p_f)) = \frac{2i}{v_x} \int_x^\infty dx \tilde{g}(p_f, x; \varepsilon_B(p_f)) + f^{(0)}_+(p_f, \varepsilon_B(p_f)) \]  

(25)

The bulk value of function \( f^{(0)}_+(p_f, x; \varepsilon_B(p_f)) \) can be easily found:

\[ f^{(0)}_+(p_f; \varepsilon_B(p_f)) = -\frac{i\pi|\Delta_\infty(p_f)|}{\sqrt{|\Delta_\infty(p_f)|^2 - \varepsilon_B^2(p_f)}} \sin (\eta_\infty(p_f) - \phi_\infty(p_f)). \]  

(26)

Substituting Eqs. (10), (26) into (25) I get

\[ f^{(0)}_+(p_f, x = 0; \varepsilon_B(p_f)) = i \text{ sgn}(v_x) |\Delta^{-1}(p_f, 0)| \tilde{g}_0(p_f, \varepsilon_B(p_f)) - \frac{i\pi|\Delta_\infty(p_f)|}{\sqrt{|\Delta_\infty(p_f)|^2 - \varepsilon_B^2(p_f)}} \sin (\eta_\infty(p_f) - \phi_\infty(p_f)) \]  

(27)
where
\[
\frac{1}{|\Delta(p_f, 0)|} = \frac{2}{|v_{f,x}(p_f)|} \int_0^\infty \exp \left( - \frac{2}{v_{f,x}(p_f)} \int_0^{x_1} |\Delta(p_f, x_2)| \sin(\eta(p_f, x_2) - \phi(p_f, x_2)) \, dx_2 \right) \, dx_1.
\] (28)

In terms of Eq. (27), (28), one can easily obtain expression for the residue of the propagator taken at the impenetrable wall. According to the boundary conditions for an impenetrable wall, quantities \( f_+(0; \varepsilon_B(p_f)) \) and \( \tilde{g}_0(p_f, \varepsilon_B(p_f)) \equiv \tilde{g}_0(p_f, 0; \varepsilon_B(p_f)) \), taken for incoming momenta are equal to the same quantities of the outgoing ones. Then one obtains from (27), (17) and (12) the following expression for the residue \( \tilde{g}_0(p_f, \varepsilon_B(p_f)) \) of the propagator \( g(p_f, x > 0; \omega) \) taken at the wall (x=0) and at the bound state energy:
\[
\tilde{g}_0(p_f, \varepsilon_B(p_f)) = 2\pi |\Delta(p_f, 0)| |\Delta(p_f, 0)| / |\Delta(p_f, 0)| + |\Delta(p_f, 0)|.
\] (29)

The positive sign of the residue stipulates a positive contribution from each bound state to the angle resolved local density of states at the wall. In accordance with Eqs. (29), (28), the residue is fully determined by the quantities \( \Delta(p_f, x) \), \( \eta(p_f, x) \). The quantity \( \eta(p_f, x) \) obeys differential equation (11), while the position dependent order parameter \( \Delta(p_f, x) \) needs to be determined self-consistently after specifying a particular form of the pairing potential. The problem of self-consistent spatial dependence of d-wave order parameter near the interface was explicitly studied numerically, for example, in Refs. \textsuperscript{13,28,29}. The self-consistent space dependent order parameter \( \Delta(p_f, x) \) is considered to be given throughout this article.

For the particular case of midgap states and real order parameter one has \( \varepsilon_B(p_f) = 0 \), \( \text{sgn}[\Delta_\infty(p_f)] = -\text{sgn}[\Delta_\infty(p_f)] \), \( \eta(p_f, x) = \eta_\infty(p_f) = \frac{\pi}{2} \text{sgn}[v_{f,x}(p_f)] + \phi_\infty(p_f), \phi(p_f, x) = \phi_\infty(p_f) = \frac{\pi}{2} (1 - \text{sgn}[\Delta_\infty(p_f)]) \). Expressions (28), (29) then reduce to those obtained earlier in Ref. \textsuperscript{11}. 

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III. BOUND STATES IN SIS' JUNCTIONS

In order to calculate a bound state energy within the framework of the approach developed in the preceding section, one should first find solutions to equation (11), which satisfy both asymptotic relations (12), (13) and the boundary condition (15). The bound state energy $\varepsilon_B(p_f)$ is directly associated with the asymptotic value $\eta_\infty(p_f)$ according to Eq. (17).

Explicit analytical expressions for the bound state energies $\varepsilon_B(p_f)$ will be found below under certain conditions in terms of spatially dependent order parameters on both sides of the interface. As was demonstrated in Ref. 13 for the particular case of a massive superconductor confined by impenetrable wall, effects of surface pair breaking for various (although not for all) quasiparticle trajectories result only in weak deviations of the space dependent quantity $\eta(p_f, x)$ from its asymptotic value $\eta_\infty(p_f)$: $|\delta \eta(p_f, x)| = |\eta(p_f, x) - \eta_\infty(p_f)| \ll 1$. In the case of finite transparency of a junction of two halfspaces one can assume this condition as well, linearize equation (11) with respect to $\delta \eta(p_f, x)$ and find the solutions of Eq. (11) on account of asymptotic conditions (12), (13) and Eq. (17):

\[
\eta(p_f, x) = \phi_l(p_f, x) - \text{sgn}(v_{f,x}(p_f, x)) \arccos \left( \frac{\varepsilon_B(p_f, x)}{\Delta^l_b(p_f)} \right) + \frac{2\varepsilon_B(p_f, x)}{v_{f,x}(p_f, x)} \int_{-\infty}^x dx_1 \times \left( 1 - \frac{\Delta^l_b(p_f, x_1)}{\Delta^l_b(p_f, x)} \right) \left( 1 - \frac{2}{|v_{f,x}(p_f, x)|} \int_{x_1}^x \frac{dx}{\Delta^l_b(p_f, x)} \right)
\]

\[
\eta_r(p_f, x) = \phi_r(p_f, x) + \text{sgn}(v_{f,x}(p_f, x)) \arccos \left( \frac{\varepsilon_B(p_f, x)}{\Delta^r_b(p_f)} \right) - \frac{2\varepsilon_B(p_f, x)}{v_{f,x}(p_f, x)} \int_{x}^{+\infty} dx_1 \times \left( 1 - \frac{\Delta^r_b(p_f, x_1)}{\Delta^r_b(p_f, x)} \right) \left( 1 - \frac{2}{|v_{f,x}(p_f, x)|} \int_x^{x_1} \frac{dx}{\Delta^r_b(p_f, x)} \right).
\]

Effects of supercurrent flowing across the junction (along the $x$ axis) can be taken into account by adding the spatially depending term $2mv_y x$ into the phases $\phi_l(r)(p_{f,l}(r))$ in (11). Then the corresponding solutions are obtained from (30), (31) after the substitution $\varepsilon_B(p_f, x) \rightarrow \varepsilon_B(p_f, x) - v_{f,l}(p_{f,l}(r))mv_y, \phi_l(r)(p_{f,l}(r)) \rightarrow \phi_l(r)(p_{f,l}(r)) + 2mv_y x$. 

12
Bound state energies can be found now combining solutions (30), (31) and the boundary condition (15). The equation obtained within the approach should be linearized with respect to the effects of surface pair breaking (described by spatial integrals in (30), (31)) both in the right and the left superconductors.

A. Low energy bound states

Let us consider bound states with low energies

\[ \varepsilon_B(p_{f,l}) \ll \min \left\{ |\Delta^{l}_\infty(p_{f,l})|, |\Delta^{l}_\infty(p_{f,l})|, |\Delta^{r}_\infty(p_{f,r})|, |\Delta^{r}_\infty(p_{f,r})| \right\} . \]

Linearizing Eqs. (30), (31) with respect to the small parameters \( \varepsilon_B(p_{f,l})/|\Delta^{l}_{\infty}(p_{f,l})| \) and taking into account the presence of a supercurrent, one gets after simple transformations:

\[ \eta_{l}(p_{f,l}, x) = \phi_l(p_{f,l}) - \frac{\pi}{2} \text{sgn}(v_{l,x}(p_{f,l})) + \left( \frac{\varepsilon_B(p_{f,l}) - v_{l}(p_{f,l})mv_x}{|\Delta^{l}(p_{f,l}, x)|} \right) sgn(v_{l,x}(p_{f,l})) \]

\[ \eta_{r}(p_{f,r}, x) = \phi_r(p_{f,r}) + \frac{\pi}{2} \text{sgn}(v_{r,x}(p_{f,r})) - \left( \frac{\varepsilon_B(p_{f,l}) - v_{r}(p_{f,r})mv_x}{|\Delta^{r}(p_{f,r}, x)|} \right) sgn(v_{r,x}(p_{f,r})) \]

where the following quantities are introduced

\[ \frac{1}{|\Delta^{l}(p_{f}, x)|} = \frac{2}{|v_{l,x}(p_{f})|} \int_{-\infty}^{x} \exp \left( - \frac{2}{|v_{l,x}(p_{f})|} \int_{x_1}^{x} |\Delta^{l}(p_{f}, x_2)| dx_2 \right) dx_1 , \]

\[ \frac{1}{|\Delta^{r}(p_{f}, x)|} = \frac{2}{|v_{r,x}(p_{f})|} \int_{x}^{\infty} \exp \left( - \frac{2}{|v_{r,x}(p_{f})|} \int_{x}^{x_1} |\Delta^{r}(p_{f}, x_2)| dx_2 \right) dx_1 . \]

I first assume that in the limit \( D \to 0 \) midgap states arise on both sides of the barrier plane for given crystal to surface orientations and quasiparticle trajectories considered. For simplicity, let the phases of the order parameters \( \phi_l(p_{f,l}) \), \( \phi_r(p_{f,r}) \) in both superconductors be spatially constant in the absence of a supercurrent.

Then, allowing for the difference \( \delta \) between the phases of right and left complex order parameters, these phases may be written under the conditions considered as follows

\[ \phi_l(p_{f,l}) = \phi_l + 2mv_x, \quad \phi_r(p_{f,r}) = \phi_r + \pi \delta_{i1} + 2mv_x \]

\[ \phi_l(p_{f,l}) = \phi_l + \pi + 2mv_x, \quad \phi_r(p_{f,r}) = \phi_r - \pi \delta_{i2} + 2mv_x \]
where two different cases \( i = 1, 2 \) are taken into account. The superfluid velocity \( v_s \) is assumed to be positive (negative) for the supercurrent flowing along (opposite to) the \( x \)-axis.

Expanding boundary condition \( \text{(15)} \) with the substitution \( \text{(32), (33)} \) with respect to \( (\varepsilon_B(p_{f,t}) - mv_s v_{f,t}^p) \), results in a simple quadratic equation for the bound state energies:

\[
\begin{align*}
\left[ \varepsilon_B(p_{f,r}) \frac{\tilde{\Delta}^l(p_{f,t}, 0) + |\Delta^l(p_{f,t}, 0)|}{|\Delta^l(p_{f,t}, 0)||\Delta^l(p_{f,t}, 0)|} \operatorname{sgn}(v_{f,x}(p_{f,t})) - mv_s \left( \frac{|v_{f,x}(p_{f,t})|}{|\Delta^l(p_{f,t}, 0)|} - \frac{|v_{f,x}(p_{f,t})|}{|\Delta^l(p_{f,t}, 0)|} \right) \right] \times \\
\left[ \varepsilon_B(p_{f,r}) \frac{\tilde{\Delta}^r(p_{f,r}, 0) + |\Delta^r(p_{f,r}, 0)|}{|\Delta^r(p_{f,r}, 0)||\Delta^r(p_{f,r}, 0)|} \operatorname{sgn}(v_{f,x}(p_{f,r})) + mv_s \left( \frac{|v_{f,x}(p_{f,r})|}{|\Delta^r(p_{f,r}, 0)|} - \frac{|v_{f,x}(p_{f,r})|}{|\Delta^r(p_{f,r}, 0)|} \right) \right] \\
= 4D \sin \left( \frac{\phi}{2} + \frac{\pi}{2} \delta_{i1} \right) \cos \left( \frac{\phi}{2} - \frac{\pi}{2} \delta_{i2} \right) . \quad \text{(37)}
\end{align*}
\]

For the sake of simplicity let \( D \ll 1 \) in Eq.\( \text{(37)} \).

Two particular solutions of Eq.\( \text{(37)} \) are of special interest. For a “symmetric” tunnel junction (STJ) identical superconductors with the same orientations are situated on its left and right sides. Subscript \( i = 1 \) in Eqs.\( \text{(38), (37)} \) corresponds to this case. Absolute values of order parameter on both sides of the STJ taken at the same distance from the interface, are equal to each other, even in the presence of a phase difference and supercurrent: \( |\Delta^l(p_{f,t}, -x)| = |\Delta^r(p_{f,r}, x)| \), \( |\Delta^l(p_{f,t}, -x)| = |\Delta^r(p_{f,r}, x)| \). Then analogous equalities follow from Eqs.\( \text{(34), (33)} \) for effective order parameters: \( |\tilde{\Delta}^l(p_{f,t}, -x)| = |\tilde{\Delta}^r(p_{f,r}, x)| \), \( |\tilde{\Delta}^l(p_{f,t}, -x)| = |\tilde{\Delta}^r(p_{f,r}, x)| \). Under these conditions one gets

\[
\varepsilon_{STJ}^B(p_{f,r}) = \pm \frac{2|\tilde{\Delta}^r(p_{f,r}, 0)||\Delta^r(p_{f,r}, 0)|}{|\Delta^r(p_{f,r}, 0)| + |\Delta^r(p_{f,r}, 0)|} \sqrt{D} \left| \cos \frac{\phi}{2} \right| + \\
\frac{v_{f,x}(p_{f,r})|\tilde{\Delta}^r(p_{f,r}, 0)| + v_{f,x}(p_{f,r})|\Delta^r(p_{f,r}, 0)|}{|\Delta^r(p_{f,r}, 0)| + |\Delta^r(p_{f,r}, 0)|} mv_s . \quad \text{(38)}
\]

For a “mirror” tunnel junction (MTJ) \( i = 2 \) orientations of identical superconductors can be obtained from each other, by definition, by a reflection with respect to the junction
barrier plane. Then $|\Delta_l(p_{f,l}, -x)| = |\Delta_r(p_{f,r}, x)|$, $|\Delta_l(p_{f,l}, -x)| = |\Delta_r(p_{f,r}, x)|$ and one obtains the corresponding values of bound state energy from Eqs. (34), (35), (37):

$$
\varepsilon_{MTJ}^B(p_{f,r}) = \pm \frac{|\tilde{\Delta}^r(p_{f,r}, 0)|}{|\Delta^r(p_{f,r}, 0)| + |\tilde{\Delta}^r(p_{f,r}, 0)|} \sqrt{4D \sin^2 \left( \frac{\phi}{2} \right)} + \left( \frac{|v_{f,x}(p_{f,r})|}{|\tilde{\Delta}^r(p_{f,r}, 0)|} - \frac{|v_{f,x}(p_{f,r})|}{|\Delta^r(p_{f,r}, 0)|} \right)^2 (mv_s)^2.
$$

(39)

As $v_s$ can depend upon $\varepsilon_B$, relations (38), (39) still represent, generally speaking, implicit equations for $\varepsilon_B$. However, factors in front of $mv_s$ in Eqs. (38), (39) can be extremely small or even vanish (as in the case $|\tilde{\Delta}^r(p_{f,r}, 0)| = |\Delta^r(p_{f,r}, 0)|$, $v_{f,x}(p_{f,r}) = -v_{f,x}(p_{f,r})$). Then one can disregard the influence of the superflow on the bound state energy, and get fairly simple results from Eqs. (38) and (39)

$$
\varepsilon_B(p_{f,r}) = \pm \frac{2|\tilde{\Delta}^r(p_{f,r}, 0)|}{|\Delta^r(p_{f,r}, 0)| + |\tilde{\Delta}^r(p_{f,r}, 0)|} \sqrt{D} \begin{cases} 
\cos \left( \frac{\phi}{2} \right) & \text{for STJ}, \\
\sin \left( \frac{\phi}{2} \right) & \text{for MTJ}.
\end{cases}
$$

(40)

One should note the relation $\varepsilon_B \propto \sqrt{D}$ and the essentially different dependences of the bound state energies upon the phase difference $\phi$ for STJ and MTJ. According to (38)-(40), zero energy bound states at an impenetrable wall ($D \to 0$) in the absence of supercurrent, split into two low energy levels on account of the effects of nonzero (low) transmission and phase difference. For STJ the bound state energy has its maximum for $\phi = 0$ and the principal reason for the bound state energy shifting away from the midgap position is the finite transmission. For MTJ the bound state energy differs from zero for nonzero $\phi$ taking its maximum value at $\phi = \pi$. This difference is evidently related to the additional phase shift $\pi$ acquired by paired quasiparticles crossing the junction and seeing different signs of the gap functions for the given momentum direction in two superconductors in MTJ. Let now midgap states take place in the limit $D \to 0$ only on one side of the barrier plane, for instance, in the right superconductor for quasiparticle trajectories considered. Then
expressions for the phases of complex order parameters differ from Eq.(36) and have the following form

$$\phi_l(p_{f,l}) = \phi_l + 2mv_s x , \phi_r(p_{f,r}) = \phi_r + \pi\delta_{i1} + 2mv_s x ,$$  \hspace{1cm} (41)

$$\phi_l(p_{f,l}) = \phi_l + 2mv_s x , \phi_r(p_{f,r}) = \phi_r - \pi\delta_{i2} + 2mv_s x .$$

In the case of an impenetrable wall there is no solution to equation (11) in the left half space $x < 0$ for sufficiently small energy. Such a solution arises, however, at finite transmission, being induced by the proximity effect on account of the corresponding solution for the right half space. These solutions have the same form (30), (31) with new relations (41).

Boundary condition (13) then reduces to

$$\left[ \eta_{r,0}(p_{f,r}) - \phi_{r}(p_{f,r}) - \frac{\pi}{2} \text{sgn}(v_{r,x}(p_{f,r})) \right] - \left[ \eta_{r,0}(p_{f,r}) - \phi_{r}(p_{f,r}) - \frac{\pi}{2} \text{sgn}(v_{r,x}(p_{f,r})) \right] = (-1)^{\delta_{i1}} D \sin \phi . \hspace{1cm} (42)$$

In terms of Eqs.(42), (53)-(58), one can justify that, indeed, $\tilde{g}_{l,0} \propto D \tilde{g}_{r,0}$ both for the incoming and outgoing momentum directions.

Substituting $\eta_{r,0}(p_{f,r})$, $\eta_{r,0}(p_{f,r})$ from Eq.(53) into Eq.(12), one gets the following expression for the bound state energy

$$\varepsilon_B(p_{f,r}) = \frac{|\tilde{\Delta}^r(p_{f,r},0)||\tilde{\Delta}^r(p_{f,r},0)|\text{sgn}(v_{r,x}(p_{f,r}))}{|\tilde{\Delta}^r(p_{f,r},0)| + |\tilde{\Delta}^r(p_{f,r},0)|} \left[ (-1)^{\delta_{i1}} D \sin \phi - mv_s \left( \frac{|v_{r,x}(p_{f,r})|}{|\Delta^r(p_{f,r},0)|} - \frac{|v_{r,x}(p_{f,r})|}{|\Delta^r(p_{f,r},0)|} \right) \right] . \hspace{1cm} (43)$$

Results obtained in this section show that the effect of surface pair breaking on the low-energy bound states, can be taken into account by introducing the effective surface values of order parameters defined in Eq.(34), (35). If one disregards for the time being the surface pair breaking at all, considering moduli of the order parameters being independent of spatial coordinates near interfaces, then it follows from Eqs.(34), (35) $|\tilde{\Delta}(p_{f},x)| = |\Delta_\infty(p_{f})| = const(x)$. For crystalline orientations, when $|\Delta_\infty(p_{f,r})| = |\Delta_\infty(p_{f,l})|$, one gets
from Eq.\( (40) \) in this particular case, 

\[ \varepsilon^\text{STJ}_B(p_{f,r}) = \pm |\Delta_\infty(p_{f,r})| \sqrt{D} \left| \cos \frac{\phi}{2} \right|, \quad \varepsilon^\text{MTJ}_B(p_{f,r}) = \pm |\Delta_\infty(p_{f,r})| \sqrt{D} \left| \sin \frac{\phi}{2} \right|. \]

According to \( (34), (35) \), the relation 

\[ |\tilde{\Delta}(p_f, x)| \leq |\Delta_\infty(p_f)| \]

holds as a consequence of surface pair breaking. Disregarding this effect leads to an overestimation of the shift of the zero energy bound states brought about by the finite transmission of the junction barrier. Such an overestimation can be quite noticeable. Moreover, for smooth surfaces the suppression of the order parameters depends on crystal to surface orientation. The effective surface quantities \( (34), (35) \) can manifest qualitatively different dependences upon crystal to interface orientation as compared to the dependences of the order parameters in the bulk.

**B. Splitting from surface pair breaking of the bound states near the edge of the continuous spectrum**

In junctions of isotropic s-wave superconductors, the order parameters with incoming and reflected quasiparticle momenta are identical. In the s-wave case one can usually disregard surface pair breaking and consider the order parameter as spatially constant up to the interface. Then the energies of the interface bound states in symmetric junctions, as it is well known, are as follows:

\[ \varepsilon_B(\theta) = \pm |\Delta| \sqrt{1 - D(\theta) \sin^2(\phi/2)} . \] (44)

It is explicitly indicated here that transmission depends upon the angle \( \theta \) between momentum direction and the interface normal. For tunnel junctions \( (D \ll 1) \) energy \( (44) \) lies close to the edge of continuous spectrum.

In preceding section the presence of quasiparticle trajectories was assumed, where incoming and outgoing quasiparticles see the order parameter values of opposite signs. The corresponding states have quite low energies in the tunneling limit. Interface bound states in the vicinity of continuous spectrum, however, always arise in tunnel junctions between d-wave superconductors as well. This is the case for quasiparticle trajectories with momentum
directions along the interface normal, where incoming and reflected quasiparticles always see the same order parameter of an anisotropic singlet superconductor. Interface bound states in \( d \)-wave superconductors for trajectories in close vicinity of the interface normal are to some extent analogous to the ones in isotropic \( s \)-wave case. For special crystalline orientations such as \( 45^\circ \) in \( d_{x^2-y^2} \) superconductors all those trajectories reduce to the only one along the interface normal.

If one considers a contribution of bound states to the current across the junction, then the particular dependence of a transmission upon \( \theta \) turns out to be especially important. For the transmission gradually diminishing with increasing \( \theta \), like in case of sufficiently thin barriers, trajectories in a wide range of \( \theta \) can substantially contribute to the current. By contrast, if the transmission noticeably differs from zero only for small \( \theta \) (this is the case for thick barriers), the contribution from trajectories with sufficiently small \( \theta \) entirely governs the current. Below bound states in junctions between \( d \)-wave superconductors are considered just for the trajectory along the interface normal.

Bound states (44) are formed due to Andreev reflection processes resulting from a phase difference in the order parameters of a symmetric junction. According to (44), the bound states merge into the continuum in the limit \( D \to 0 \). However, this is not actually the case as a result of a suppression of the moduli of the order parameters in the vicinity of the barrier plane. For a smooth impenetrable wall, the bound states still exist on account of surface pair breaking for momentum direction along (or sufficiently close to) the surface normal for almost all crystal to surface orientations of a \( d \)-wave superconductor. Bound states of this kind arise even for a weak suppression of the order parameter. Then, however, there must be a tiny distance from the energy of a bound state to the continuum. For isotropic \( s \)-wave superconductors this applies to any quasiparticle trajectory.

Inhomogeneous modulus of the order parameter as such near an impenetrable wall can be considered an effective potential well for quasiparticles. Finite transmission across the interface of a junction, as opposed to the impenetrable wall, results in a double well structure and allows for the interplay of the phase difference and the inhomogeneous moduli of the
order parameters in forming interface bound states. It is shown below, that splitting of bound state levels takes place in the double well structure for the quasiparticle trajectory along the surface normal, at least in the tunneling limit.

One can easily see from (17) for positive bound state energies near the continuum, that in “symmetric” or “mirror” tunnel junctions all asymptotic values ($\eta_{\infty}(p_f) - \phi_{\infty}(p_f)$) are small. Assuming in addition $|\eta(p_f, x) - \eta_{\infty}(p_f)| \ll 1$, one can get from Eq.(11) in the first approximation the following expressions for the corresponding interface values $\eta(\eta_{\infty}(p_f))$:

\[
\eta_{l,0}(p_{f,l}) = -\text{sgn}(v_{f,x}(p_{f,l})) \sqrt{1 - \frac{\varepsilon_B^2(p_{f,l})}{|\Delta_{\infty}(p_{f,l})|^2}} + \frac{2\varepsilon_B(p_{f,l})}{v_{f,x}(p_{f,l})} \int_{-\infty}^{0} \left( 1 - \frac{|\Delta^l(p_{f,l}, x)|}{|\Delta_{\infty}(p_{f,l})|} \right) dx ,
\]

\[
(45)
\]

\[
\eta_{r,0}(p_{f,l}) = \phi + \text{sgn}(v_{f,x}(p_{f,l})) \sqrt{1 - \frac{\varepsilon_B^2(p_{f,l})}{|\Delta_{\infty}(p_{f,r})|^2}} - \frac{2\varepsilon_B(p_{f,l})}{v_{f,x}(p_{f,r})} \int_{0}^{\infty} \left( 1 - \frac{|\Delta^r(p_{f,r}, x)|}{|\Delta_{\infty}(p_{f,r})|} \right) dx .
\]

\[
(46)
\]

Substituting these expressions into the boundary condition (15) and linearizing in $\left(\eta_{\infty}(p_f) - \eta_{0}(p_f)\right)$, one obtains for STJ and MTJ the following bound state energies:

\[
\frac{\varepsilon_B^2(p_{f,r})}{|\Delta_{\infty}(p_{f,r})|^2} = 1 - \left[ \frac{2|\Delta_{\infty}(p_{f,r})|}{|v_{f,x}(p_{f,r})|} \int_{0}^{\infty} \left( 1 - \frac{|\Delta^r(p_{f,r}, x)|}{|\Delta_{\infty}(p_{f,r})|} \right) dx \pm \sqrt{D} \sin \left( \frac{\phi}{2} \right) \right]^2 .
\]

\[
(47)
\]

The minus sign in front of the $\sqrt{D}$ term in (47) is admissible only when the modulus of this term is less than that of the first term in the square brackets. This implies a relatively large role of interface pair breaking in forming Andreev bound states as opposed to the contribution from the phase difference. As can be seen in Eq.(17), under these circumstances the combined effect of the phase difference and the interface pair breaking results in a splitting of the bound state energy. In the opposite limit of absence of noticeable surface pair breaking, when $|\Delta(p_f, x)| = |\Delta_{\infty}(p_f)|$, the first term within the square brackets in Eq.(17) vanishes. Then Eq.(17) reduces to the conventional result Eq.(14). On the other hand, for an impenetrable barrier Eq.(17) takes the form found in Ref. 15.
parameters have equal moduli and opposite signs on the two sides of the junction, then the bound state energies are described by Eq. (47) after replacing \( \sin \left( \frac{\phi}{2} \right) \) by \( \cos \left( \frac{\phi}{2} \right) \).

The splitting considered above is formally analogous to the splitting discussed in Ref. 30 for long SIS junctions and specially constructed SNS junctions with double-well or double-barrier structures. However, the physical reasons for the splitting and the conditions for its observations considered in this section, drastically differ from what was studied earlier, where the effect of interface pair breaking was always neglected. The double well structure discussed in this section is inherent in junctions with noticeable interface pair breaking. One should note that the first term in square brackets in Eq. (47) is considerably less than unity both for \( s \)-wave superconductors as well as for \( d \)-wave superconductors. In the former case this is entirely due to a small suppression of the order parameter at the interface. The \( d \)-wave order parameter taken for a momentum along the surface normal, is small in itself for those crystal to interface orientations, which entail substantial surface pair breaking. However, at least for the \( d \)-wave case the first term in square brackets in Eq. (47) can exceed the second one, allowing an observable splitting (the estimations follow from Fig. 3 in 15).

The supercurrent flowing via individual bound state (47) can be written as

\[
I_{\pm} \propto e|\Delta_\infty(p_{fr})|\sqrt{D} \cos \left( \frac{\phi}{2} \right) \left[ \sqrt{D} \sin \left( \frac{\phi}{2} \right) \pm \frac{2|\Delta_\infty(p_{fr})|}{|\nabla_{fr}(p_{fr})|} \int_0^\infty \left( 1 - \frac{|\Delta_r(p_{fr}, x)}{|\Delta_\infty(p_{fr})|} \right) dx \right].
\]

(48)

For sufficiently small transmission the second term in the square brackets dominates, resulting in a supercurrent proportional to \( \sqrt{D} \). As it is known for resonance Josephson coupling in double well structures, in equilibrium such anomalous terms coming collectively from all bound and extended states cancel in the expression for the total current. For nonequilibrium quasiparticle occupation of bound and (or) extended states, however, one can expect observable manifestations of the anomaly discussed above. As compared to the conventional behavior linear in the transmission coefficient, a \( \sqrt{D} \)-term results in an enhancement of nonequilibrium Josephson current from surface pair breaking in the tunneling limit. For \( d \)-wave superconductors, the broadening of bound states on interface roughness
and impurities is of importance, since can smearing out the splitting.

It is not entirely clear whether the $\sqrt{D}$-behavior of the critical current vanishes in equilibrium within more general assumptions than made above. Such a study is in progress now.

IV. BROADEN BOUND STATES IN NIS JUNCTIONS

Andreev bound states, localized near an impenetrable wall in a d-wave superconductor, become slightly broadened in the case of small but finite barrier transmission of an NIS tunnel junction. In this case, the retarded propagators have no singularities at any real value of the energy, since positions of poles move from the real axis in the complex energy plane. This shift is linear in the barrier transmission coefficient, which is assumed to be sufficiently small. A relatively small imaginary part of a pole position is associated with finite quasiparticle lifetime for the quasistationary bound state.

The other important feature of NIS (normal metal - insulator - superconductor) junctions is that the solution for the normal metal halfspace cannot be described by ansatz (32, 33). At the same time the dominating terms in propagators still satisfy Eq. (1) in the superconducting half space in the case of sufficiently small transparency of the barrier.

As it follows from Eilenberger’s equations, the diagonal component of the quasiclassical Green’s function is constant throughout the normal metal up to the interface ($g = -i\pi$). At the same time superconducting correlations are present there due to the proximity effect and known to decrease exponentially toward the bulk normal metal ($x < 0$). Since imaginary part of a pole position should be negative for the retarded propagator, one can write for the anomalous Green’s functions for $x < 0$:

\[
\begin{align*}
    \left\{ \begin{array}{l}
    f_N(p_f,l, x, \varepsilon_B(p_{f,l})) = f_{N0}(p_f,l, \varepsilon_B(p_{f,l})) \exp \left( \frac{2\varepsilon_B(p_{f,l})x}{v_{f,x}(p_{f,l})} \right), \\
    f_N^+(p_f,l, x, \varepsilon_B(p_{f,l})) = f_{N0}^+(p_f,l, \varepsilon_B(p_{f,l})) \exp \left( -i\frac{2\varepsilon_B(p_{f,l})x}{v_{f,x}(p_{f,l})} \right), 
    \end{array} \right.
\end{align*}
\]

while $f_N(p_f,l, x, \varepsilon_B(p_{f,l})) = 0$, $f_N^+(p_f,l, x, \varepsilon_B(p_{f,l})) = 0$. Here and below normal to the
interface velocity component $v_{f,x}^l(p_{f,l}) \ (v_{f,x}^l(p_{f,l}^-))$ is chosen to be positive (negative) for an incoming (outgoing) quasiparticle in the left halfspace.

Evidently, propagators (49) in the left halfspace do not satisfy relation (9). There is, however, another important relation, which strictly holds in the normal metal halfspace and substantially simplifies Zaitsev’s boundary conditions at the NIS interface: diagonal components of matrix $\hat{d}_l$ are equal to zero in the case considered. According to (5), diagonal components of $\hat{d}_r$ vanish in this case as well. Thus, applying ansatz (9) to the right halfspace and taking into account (5), (49), one gets

$$f_{N0}^p(p_{f,l}, \varepsilon_{B}(p_{f,l})) = g_{r,0}(p_{f,r}, \varepsilon_{B}(p_{f,l})) \left[ e^{i\eta_{r,0}(p_{f,r})} - e^{-i\eta_{r,0}(p_{f,r})} \right],$$

$$f_{N0}^+(p_{f,l}, \varepsilon_{B}(p_{f,l})) = g_{r,0}(p_{f,r}, \varepsilon_{B}(p_{f,l})) \left[ e^{-i\eta_{r,0}(p_{f,r})} - e^{i\eta_{r,0}(p_{f,r})} \right].$$

(50)

With relations just mentioned above the matrix boundary condition (4) reduces only to a single scalar equation. In the particular case of this section one should not forget either that equations (9), (51) are valid only for sufficiently small $\alpha$. For these small values of $\alpha$ the estimation $|\eta_{r,0}(p_{f,r}) - \eta_{r,0}(p_{f,r})| \propto \alpha$ holds and the quantity $\alpha g_{r,0}(p_{f,r}, \varepsilon_{B}(p_{f,l}))$ is sufficiently small and vanishes in the limit $\alpha \to 0$. This can be seen, in particular, from (51), since in the limit of impenetrable boundary amplitudes $f_{N0}(p_{f,l}, \varepsilon_{B}(p_{f,l}))$, $f_{N0}^+(p_{f,l}, \varepsilon_{B}(p_{f,l}))$ should vanish. For sufficiently small transmission coefficient and therefore small $[\eta_{r,0}(p_{f,r}) - \eta_{r,0}(p_{f,r})]$ a remarkably simple boundary condition follows from (4)

$$\eta_{r,0}(p_{f,r}) - \eta_{r,0}(p_{f,r}) = -2i\alpha \approx -iD(p_f).$$

(51)

The complex pole $\varepsilon_{B}(p_{f,l})$ can be found now on the basis of equations (11), (12), (51). For broadened zero energy bound states, one should assume $\phi_{r}(p_{f,r}) = 0$, $\phi_{r}(p_{f,r}) = \pi$ ensuring the existence of that state in the limit $D \to 0$ for the trajectory. Then the solution of Eq.(11) for the superconductor coincides with (33) in the absence of a supercurrent across the junction: $\delta \eta_{r}(p_{f,r}, x) = -\varepsilon_{B}(p_{f,r}) \text{sgn} \left( v_{f,x}^r(p_{f,r}) \right) / |\Delta(p_{f,r}, x)|$. The definition
of $|\tilde{\Delta}(p_{f,r}, x)| = |\tilde{\Delta}^r(p_{f,r}, x)|$ is given in (35). Substituting this solution into boundary condition (51) one gets a purely imaginary value $\varepsilon_B(p_{f,r}) = -i\Gamma(p_{f,r})$ for the pole:

$$\Gamma(p_{f,r}) = D(p_f) \frac{|\tilde{\Delta}(p_{f,r}, 0)||\tilde{\Delta}(p_{f,r}, 0)|}{|\Delta(p_{f,r}, 0)| + |\Delta(p_{f,r}, 0)|}. \quad (52)$$

According to (52), the effects of surface pair breaking on the broadening of the zero energy bound state is taken into account by introducing effective order parameter values (35) taken at the interface. This effective order parameter reduces into order parameter of the superconductor when neglecting surface pair breaking. This is entirely analogous to what was obtained in Sec. III.A for the effects of surface pair breaking on the energies of low energy bound states. In the particular case of no surface pair breaking Eq.(52) coincides with the result obtained in Ref. 34 for crystal orientations when $|\Delta(p_{f,r})| = |\Delta(p_{f,r})|$.

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Ansatz (9) works well inside a normal metal layer if Andreev bound states arise there. For instance, in a clean SNS system with fully transparent interfaces one can easily get conventional Andreev discrete quasiparticle subgap levels basing on the equation (11) and asymptotic conditions (12), (13).

In the normal metal halfspace one of two Andreev amplitudes $u(p_f, x)$, $v(p_f, x)$ with a given $p_f$ vanishes. The other one is finite on account of the proximity effect and decreases exponentially toward the bulk normal metal. In this special case Eq. (16) is not suitable.
for describing the Andreev amplitudes.

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APPENDIX

One can derive from the boundary conditions (5), (8) with the substitution (9), the following relations among interface values of the propagator $\tilde{g}$ taken both for incident and (or) for outgoing momenta:

\[
\begin{align*}
\tilde{g}_{l,0}(p_{f,l}) \sin \left( \frac{\eta_{l,0}(p_{f,l}) - \eta_{r,0}(p_{f,r})}{2} \right) \sin \left( \frac{\eta_{l,0}(p_{f,l}) - \eta_{r,0}(p_{f,r})}{2} \right) = \\
\tilde{g}_{l,0}(p_{f,l}) \sin \left( \frac{\eta_{l,0}(p_{f,l}) - \eta_{r,0}(p_{f,r})}{2} \right) \sin \left( \frac{\eta_{l,0}(p_{f,l}) - \eta_{r,0}(p_{f,r})}{2} \right),
\end{align*}
\]

(53)

\[
\begin{align*}
\tilde{g}_{r,0}(p_{f,r}) \sin \left( \frac{\eta_{r,0}(p_{f,r}) - \eta_{l,0}(p_{f,l})}{2} \right) \sin \left( \frac{\eta_{r,0}(p_{f,r}) - \eta_{l,0}(p_{f,l})}{2} \right) = \\
\tilde{g}_{r,0}(p_{f,r}) \sin \left( \frac{\eta_{r,0}(p_{f,r}) - \eta_{l,0}(p_{f,l})}{2} \right) \sin \left( \frac{\eta_{r,0}(p_{f,r}) - \eta_{l,0}(p_{f,l})}{2} \right),
\end{align*}
\]

(54)

\[
\begin{align*}
\tilde{g}_{l,0}(p_{f,l}) \sin \left( \frac{\eta_{l,0}(p_{f,l}) - \eta_{r,0}(p_{f,r})}{2} \right) \sin \left( \frac{\eta_{l,0}(p_{f,l}) - \eta_{r,0}(p_{f,r})}{2} \right) = \\
\tilde{g}_{r,0}(p_{f,r}) \sin \left( \frac{\eta_{r,0}(p_{f,r}) - \eta_{l,0}(p_{f,l})}{2} \right) \sin \left( \frac{\eta_{r,0}(p_{f,r}) - \eta_{l,0}(p_{f,l})}{2} \right),
\end{align*}
\]

(55)
\[ \tilde{g}_{l,0}(p_{f,l}) \sin \left( \frac{\eta_{l,0}(p_{f,l}) - \eta_{r,0}(p_{f,r})}{2} \right) \sin \left( \frac{\eta_{l,0}(p_{f,l}) - \eta_{r,0}(p_{f,l})}{2} \right), \]

(56)

\[ \tilde{g}_{l,0}(p_{f,l}) \sin \left( \frac{\eta_{l,0}(p_{f,l}) - \eta_{r,0}(p_{f,r})}{2} \right) \sin \left( \frac{\eta_{l,0}(p_{f,l}) - \eta_{r,0}(p_{f,l})}{2} \right) = -\tilde{g}_{r,0}(p_{f,r}) \sin \left( \frac{\eta_{r,0}(p_{f,r}) - \eta_{l,0}(p_{f,r})}{2} \right) \sin \left( \frac{\eta_{r,0}(p_{f,r}) - \eta_{r,0}(p_{f,r})}{2} \right), \]

(57)

\[ \tilde{g}_{l,0}(p_{f,l}) \sin \left( \frac{\eta_{l,0}(p_{f,l}) - \eta_{r,0}(p_{f,r})}{2} \right) \sin \left( \frac{\eta_{l,0}(p_{f,l}) - \eta_{r,0}(p_{f,l})}{2} \right) = -\tilde{g}_{r,0}(p_{f,r}) \sin \left( \frac{\eta_{r,0}(p_{f,r}) - \eta_{l,0}(p_{f,r})}{2} \right) \sin \left( \frac{\eta_{r,0}(p_{f,r}) - \eta_{r,0}(p_{f,r})}{2} \right). \]

(58)