Scattering theory of superconductive tunneling in quantum junctions.

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Abstract

We present a consistent theory of superconductive tunneling in single-mode junctions within a scattering formulation of Bogoliubov-de Gennes quantum mechanics. Both dc Josephson effect and dc quasiparticle transport in voltage biased junctions are considered. Elastic quasiparticle scattering by the junction determines equilibrium Josephson current. We discuss the origin of Andreev bound states in tunnel junctions and their role in equilibrium Josephson transport. In contrast, quasiparticle tunneling in voltage biased junctions is determined by inelastic scattering. We derive a general expression for inelastic scattering amplitudes and calculate the quasiparticle current at all voltages with emphasis on a discussion of the properties of subgap tunnel current and the nature of subharmonic gap structure.

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I. INTRODUCTION.

The tunnel Hamiltonian model has for many years been a main theoretical tool for investigation of tunneling phenomena in superconductors. However, interpretation of recent experiments on transmissive tunnel junctions and complex superconductor-semiconductor structures require more detailed knowledge of the mechanisms of the superconductive tunneling than the tunnel model is able to provide. Particularly informative are experiments on superconducting quantum point contacts with controlled number of transport modes and transparency, such as controllable superconducting break junctions and gate controlled superconductor-semiconductor devices. Since only a few transport modes with controlled transparency are involved in the tunnel transport, the experiments provide precise and detailed information which can be directly compared with theory.

The first attempts to develop a theory of superconductive tunneling beyond the tunnel Hamiltonian model were made in generalization of methods applied to SNS junctions and superconducting constrictions based on Green’s function techniques. In these theories, the junction Green’s functions are directly found from Green’s function equations supplemented by special boundary conditions representing the tunnel barrier, or by matching the superconductor and insulator Green’s functions at the superconductor-insulator boundaries.

In the first works on the Josephson effect in SNS junctions, another way of calculation has been used, based on expansion over eigenstates of the Bogoliubov-de Gennes (BdG) equation. A similar method has been also applied to SIS tunnel junctions and superconductor-semiconductor junctions. In the absence of inelastic scattering the method of using the BdG equation gives the same results as the Green’s function technique. One might then expect that the Josephson effects in superconducting junctions can be explained on a rather simple quantum mechanical level. Following this idea, the quantum mechanical approach has been successfully applied to calculation of the dc Josephson current in different kinds of mesoscopic weak links and tunnel junctions. The first
application of the method to voltage biased junctions was done by Blonder, Tinkham, and Klapwijk who considered quasiparticle tunneling in SIN junctions as a scattering problem in BdG quantum mechanics [23]. Later on, the quantum mechanical approach has been found to be helpful in investigations of more complex phenomena of quasiparticle transport and ac Josephson effect in voltage biased SNS junctions [32], mesoscopic SIS tunnel junctions [33] and mesoscopic constrictions [34].

The quantum mechanical approach based on the BdG equation is adequate for describing the physical situation in mesoscopic junctions, where inelastic scattering effects are weak and coherent electron dynamics is of main importance. Moreover, due to the effect of quantization of transverse electron modes in mesoscopic junctions [24,35], 1D models for the current transport through the junction may be appropriate.

In this paper we present a consistent quantum mechanical theory of superconductive tunneling in a one-mode quantum constriction, Fig.1. We consider the dc Josephson effect and also dc quasiparticle tunneling in voltage biased junctions. In the latter case we focus attention on a detailed calculation of the subharmonic gap structure (SGS) of the tunnel current [33].

Following the Landauer approach [36], we consider superconducting electrodes as equilibrium reservoirs which emit quasiparticles into the constriction. Scattering by the junction goes into two channels: (i) the normal channel with outgoing quasiparticles remaining in the same branch of the quasiparticle spectrum, and (ii) the Andreev channel where the quasiparticles change branch due to electron-hole conversions. The current in such a picture results from the imbalance of currents carried by scattering states originating from the left and the right reservoirs, the magnitude of the current being proportional to the transmission coefficient $D$ of the tunnel barrier.

The imbalance of currents in superconducting junctions can be created in two ways: by establishing a difference of the phases of the order parameters in the left and right electrodes, or by applying a voltage bias. The basic fact concerning the flow of equilibrium current in the presence of a phase difference, established by Furusaki and Tsukada [29], is that a bulk
supercurrent, when approaching the tunnel interface, is transformed into current flowing through superconducting bound states which appear at the tunnel interface in the presence of this phase difference [37] and which provide transmission of the Cooper pairs through the tunnel barrier. The balance among currents of different scattering states is not violated, although the scattering amplitudes depend strongly on the phase difference.

Application of a voltage bias gives rise to more far reaching consequences than just imbalance of the elastic scattering modes: the scattering states themselves are modified in a non-trivial way. This follows from the fact that the scattering amplitudes, being phase-dependent in equilibrium, become time-dependent in accordance with the Josephson relation [38], \( \frac{d\phi}{dt} = 2eV \), when voltage is applied. Thus, in the presence of a dc voltage the superconducting junction behaves as an effective nonstationary scatterer whose transmissivity oscillates. This property of superconducting junctions gives rise to ac Josephson effect; however, it is also significant for dc quasiparticle transport because the quasiparticle transmission through such a scatterer is \textit{inelastic}.

The physical mechanism of inelastic quasiparticle transmission through voltage biased superconducting junctions has been first considered in SNS junctions [32] where it has been explained in terms of multiple Andreev reflections (MAR): the normal quasiparticles confined between superconducting walls are permanently accelerated by the static electric field due to sequential electron-hole conversions at the NS interfaces, similarly to acceleration of the electrons in an ordinary potential well by a time dependent electric field. Similar arguments can be extended to the tunnel junctions [39]; however, in tunnel junctions the scattering theory approach is more appropriate because of the quantum nature of quasiparticle transmission through the atomic-size tunnel barrier. This introduces a side-band spectrum of scattered waves where side-band energies are shifted with respect to the energy of the incident wave by integer number of quanta of the scatterer frequency [33]. Such an approach is familiar in the theory of quantum scattering by oscillating potential barriers in normal tunnel junctions (see e.g., Refs. [40,41] and references therein).

The tunneling through all the inelastic channels (normal and Andreev) constitutes a
complete picture of superconductive tunneling in biased Josephson junctions - the incoherent part of side band currents corresponding to the dc quasiparticle current and the side band interference currents corresponding to the ac Josephson current. An important aspect of this picture is that the Andreev bound states are involved in the current transport together with the extended side band states, giving a multiparticle character to the superconductive tunneling in the subgap voltage region. This multiparticle origin of the subgap tunnel current was first pointed out by Schrieffer and Wilkins [42].

The structure of the paper is the following. After formulation of the problem and discussion of the quasiclassical approximation in Sec. II, we consider the problem of elastic scattering in Sec. III as a starting point for construction of inelastic scattering states in biased junctions. The solution of the elastic scattering problem allows us to calculate dc Josephson current, which is done for completeness in Sec. IV. In Sec. V we construct inelastic scattering states and derive a continued-fraction representation for the scattering amplitudes. Sec. VI is devoted to derivation of the nonequilibrium current. In Sec. VII we discuss the origin of the excess tunnel current in the large bias limit. In Sec. VIII we present a general analysis of the subgap tunnel current. Finally, the SGS is analyzed in Sec. IX.

II. FORMULATION OF MODEL.

We consider a superconducting quantum constriction with adiabatic geometry [13]: the cross section varies smoothly with the coordinate \( x \) on the scale of the Fermi electron wave length, \( 1/p_F \), and the size of cross section is comparable with the Fermi electron wave length, Fig. 1. The length \( L \) of the constriction is assumed to be smaller than the superconducting coherence length \( \xi_0 \),

\[ 1/p_F \ll L \ll \xi_0. \]

(2.1)

The Hamiltonian of the constriction is assumed to have the form:
\[ \hat{H} = \left[ \frac{(\hat{p} - \sigma_z e\vec{A}(\vec{r}, t))^2}{2m} + U(\vec{r}) - \mu \right] \sigma_z + [V(x) + e\varphi(\vec{r}, t)] \sigma_z + \hat{\Delta}(\vec{r}, t), \]  

(2.2)

where \(U(\vec{r})\) is the potential confining electrons within the constriction, \(V(x)\) is the potential of the tunnel barrier, \(\vec{A}(\vec{r}, t)\) and \(\varphi(\vec{r}, t)\) are electromagnetic potentials, and \(\hat{\Delta}(\vec{r}, t)\) is the off-diagonal superconducting order parameter given by the matrix:

\[ \hat{\Delta} = \begin{pmatrix} 0 & \Delta e^{i\chi/2} \\ \Delta e^{-i\chi/2} & 0 \end{pmatrix}. \]  

(2.3)

We assume the junction to be symmetric. The choice of the units corresponds to \(c = \hbar = 1\).

It is convenient to eliminate the phase of the superconducting order parameter \(\chi(\vec{r}, t)\) in Eq. (2.3) by means of a gauge transformation:

\[ e^{i\sigma_z \chi/2} \hat{H} e^{-i\sigma_z \chi/2} \rightarrow \hat{H}, \]  

(2.4)

which allows us to introduce a gauge invariant superfluid momentum, \(\vec{p}_s = \nabla \chi/2 - e\vec{A}\) and an electric potential \(\Phi = \dot{\chi}/2 + e\varphi\).

There are different scales of change of potentials in Eq. (2.2): one is an atomic scale over which the confining potential \(U(r_{\perp})\) and the potential of the tunnel barrier \(V(x)\) change. Other scales are related to change of superconducting order parameter, electromagnetic field penetration lengths and length of the contact: all these lengths are large in comparison with the atomic length. It is convenient to separate these two scales, introducing quasiclassical wave functions \([14]\) which vary slowly on an atomic scale, and including rapidly varying potentials in a boundary condition for quasiclassical wave functions. To this end we assume the solution \(\Psi(\vec{r}, t)\) of the Bogoliubov-de Gennes equation \([20]\)

\[ i\dot{\Psi}(t) = \hat{H}\Psi(t), \]  

(2.5)

with the Hamiltonian of Eq. (2.2), to have the quasiclassical form

\[ \Psi(\vec{r}, t) = \sum_{\beta} \psi_{\perp}(\vec{r}_{\perp}, x) \frac{1}{\sqrt{v}} e^{i\beta \int p dx} \psi_{\beta}(x, t), \]  

(2.6)
where $\psi_{\perp}$ is the normalized wave function of the quantized transverse electron motion with the energy $E_{\perp}$,

$$
\left(\frac{\hat{p}_{\perp}}{2m} + V(\vec{r}_{\perp}, x)\right)\psi_{\perp} = E_{\perp}(x)\psi_{\perp}, \quad \psi_{\perp}(r_{\perp} = \infty, x) = 0,
$$

and $p$ is the longitudinal momentum of the quasiclassical electron, $p(x) = \sqrt{2m(\mu - E_{\perp}(x))}$; $\beta = \pm$ indicates the direction of the electron motion. We assume here that the constriction has only one transport mode; an extension to the case of several unmixed modes consists of additional summation over all transport modes in the equation for the current. The coefficients $\psi_{\beta}$ in Eq. (2.6) describe the wave functions slowly varying in the $x$ direction and satisfy the reduced BdG equation

$$
i\dot{\psi}_{L,R}^\beta = (\beta v\hat{p}\sigma_z + \Phi_{L,R}\sigma_z + v\vec{p}_sL,R + \Delta\sigma_x)\psi_{L,R}^\beta \tag{2.7}
$$

in the the left (L) and the right (R) electrodes; $v = p/m$. The potentials $\vec{p}_s$ and $\Phi$ describe the distributions of electromagnetic field and supercurrent in the electrodes. In the point contact geometry these quantities are small due to the effect of spreading out of current [16,45], and we will omit them, $\vec{p}_s = \Phi = 0$. For the same reason, deviation of spatial distribution of the module of the order parameter $\Delta$ from constant magnitude is small in the point contacts, and we will neglect it, $\Delta = const$.

The functions $\psi_{L,R}^\beta$ are matched at the constriction by the boundary condition [31] (see also Appendix A):

$$
\begin{pmatrix}
\psi_{L}^- \\
\psi_{R}^+
\end{pmatrix} = \hat{V}_x
\begin{pmatrix}
\psi_{L}^+ \\
\psi_{R}^-
\end{pmatrix} \quad \text{at} \quad x = 0 , \tag{2.8}
$$

with a matching matrix $\hat{V}_x$

$$
\hat{V}_x = \begin{pmatrix}
\begin{pmatrix}
r \\
d e^{i\sigma_z\phi/2}
\end{pmatrix} & \begin{pmatrix}
d e^{-i\sigma_z\phi/2} \\
r
\end{pmatrix}
\end{pmatrix} . \tag{2.9}
$$

d and $r$ are the normal electron transmission and reflection amplitudes due to the barrier, and $\phi$ is a gauge invariant difference of the superconducting phases of right and left electrodes: $\phi = \chi_R(0) - \chi_L(0)$. The matching matrix in Eq. (2.9) satisfies the unitarity condition
\[ \hat{V} \hat{V}^\dagger = 1. \]  

(2.10)

The boundary condition in Eqs. (2.8), (2.9) is analogous to the boundary condition used in the quasiclassical Green’s functions techniques (see e.g., [11,46]). This is the simplest equation for coupling of superconducting electrodes, while retaining the main features of the Josephson effect, except for effects of the resonant tunneling [30,47,48].

III. ELASTIC SCATTERING

In the absence of time dependence in the phase difference at the junction, \( \dot{\phi} = 0 \), Eqs. (2.7) and (2.8) describe elastic scattering of quasiparticles. The scattering states are to be constructed using stationary solutions of Eq. (2.7) which correspond to elementary propagating waves with energy \( |E| > \Delta \):

\[ \psi^{\beta \alpha}_E = e^{-iEt + i\alpha(\xi/v)x} u^\delta_E, \]  

(3.1a)

\[ u^\delta_E = \frac{1}{\sqrt{2 \cosh \gamma}} \begin{pmatrix} e^{\delta \gamma/2} \\ \sigma e^{-\delta \gamma/2} \end{pmatrix}, \]  

(3.1b)

where

\[ \xi = \sqrt{E^2 - \Delta^2}; \quad e^{\gamma} = \frac{|E| + \xi}{\Delta}; \quad \sigma = \text{sign}E, \quad \alpha = \pm, \quad \delta = \alpha \sigma. \]  

(3.2)

The vector function \( u_E \) is normalized, \( (u, u) = 1 \), the brackets meaning scalar product in electron-hole space. In Eq. (3.1) there are four elementary waves which correspond to the same energy, as illustrated in Fig. 2, which are labeled by quantum numbers \( \beta \) (direction of the Fermi electron momentum) and \( \alpha = \text{sign}(|p| - p_F) \) (electron or hole-like branch of the quasiparticle spectrum). The direction of propagation of each elementary wave is determined by the sign of the probability current. The probability current density \( j_p \), defined by the conservation law (continuity equation) \( \partial |\psi|^2 / \partial t + \partial j_p / \partial x = 0 \) for the BdG equation Eq. (2.7), has the form \( j_p = (\psi, \sigma_z \psi) \). For the elementary waves in Eq. (3.1) one obtains the
explicit result $j_p = \beta \delta \tanh \gamma$. According to this formula, the relation \( \delta = \beta \) is met for for the waves propagating from left to right, \( \delta = -\beta \) for the waves propagating from right to left. Therefore the incoming waves from the left (L) and right (R) have the form

\[
L: \ e^{i\sigma(\xi/v)x}u_E^\beta, \quad R: \ e^{-i\sigma(\xi/v)x}u_E^{-\beta},
\]

while the outgoing waves have the form

\[
L: \ e^{-i\sigma(\xi/v)x}u_E^{-\beta}, \quad R: \ e^{i\sigma(\xi/v)x}u_E^\beta.
\]

Correspondingly, the incoming quasiparticle can be scattered into four outgoing states: two forward scattering states and two back scattering states. One of the reflected waves belongs to the same (electron- or hole-like) branch of the quasiparticle spectrum as the incoming wave and constitutes the normal scattering channel, while the other reflected wave changes spectrum branch and constitutes the Andreev channel. In a similar way transmitted waves constitute normal and Andreev channels. The structure of the scattering states then becomes

\[
\begin{pmatrix}
\psi_L^- \\
\psi_R^+
\end{pmatrix} = \begin{pmatrix}
\delta_{j,1} \\
\delta_{j,2}
\end{pmatrix} e^{i\sigma(\xi/v)x}u_E^\beta + \begin{pmatrix}
a \\
b
\end{pmatrix}_j e^{-i\sigma(\xi/v)x}u_E^{-\beta},
\]

\[
\begin{pmatrix}
\psi_L^+ \\
\psi_R^-
\end{pmatrix} = \begin{pmatrix}
\delta_{j,3} \\
\delta_{j,4}
\end{pmatrix} e^{i\sigma(\xi/v)x}u_E^- + \begin{pmatrix}
c \\
f
\end{pmatrix}_j e^{-i\sigma(\xi/v)x}u_E^\beta.
\]

(for brevity we have omitted the time dependent factors \( e^{-iEt} \)). In Eqs. (3.3) the index \( j = 1(2) \) corresponds to a hole-like quasiparticle coming from the left (right), while index \( j = 3(4) \) corresponds to an electron-like quasiparticle coming from the left (right). According to the structure of the matching matrix Eq. (2.9), there is the following symmetry between the scattering states \( j = 1 \) and \( j = 2 \):

\[
\begin{pmatrix}
a \\
b
\end{pmatrix}_2 (\phi) = \begin{pmatrix}
b \\
a
\end{pmatrix}_1 (-\phi), \quad \begin{pmatrix}
c \\
f
\end{pmatrix}_2 (\phi) = \begin{pmatrix}
f \\
c
\end{pmatrix}_1 (-\phi).
\]

(3.6)
The analogous symmetry exists also for the scattering states $j = 3, 4$. Using the unitarity of the matching matrix Eq. (2.9) one can find the following relation between scattering states $j = 3$ and $j = 1$:

$$
\begin{pmatrix}
a \\
b
\end{pmatrix}_3 \begin{pmatrix}
\gamma, r, d
\end{pmatrix} = \begin{pmatrix}
c \\
f
\end{pmatrix}_1 \begin{pmatrix}
-\gamma, r^*, d^*
\end{pmatrix},
$$

$$
\begin{pmatrix}
c \\
f
\end{pmatrix}_3 \begin{pmatrix}
\gamma, r, d
\end{pmatrix} = \begin{pmatrix}
a \\
b
\end{pmatrix}_1 \begin{pmatrix}
-\gamma, r^*, d^*
\end{pmatrix}.
$$

(3.7)

These symmetry relations allow us to find all the scattering amplitudes if one of the scattering states is known.

Let us find the explicit scattering amplitudes for the scattering state $j = 1$. After substituting Eqs. (3.5) into Eq. (2.8) it is convenient to split the resulting equation, using the orthogonality condition, $(u^+, \sigma_z u^-) = 0$, into two independent equations for the normal scattering amplitudes $c, f$ and for the Andreev scattering amplitudes $a, b$,

$$
(u^-, \sigma_z u^-) \begin{pmatrix}
1 \\
0
\end{pmatrix} = (u^-, \sigma_z \tilde{V} u^-) \begin{pmatrix}
c \\
f
\end{pmatrix}_1,
$$

(3.8a)

$$
(u^+, \sigma_z u^+) \begin{pmatrix}
a \\
b
\end{pmatrix}_1 = (u^+, \sigma_z \tilde{V} u^+) \begin{pmatrix}
c \\
f
\end{pmatrix}_1.
$$

(3.8b)

Calculating the scalar products in Eqs. (3.8) we find explicit expression for the Andreev amplitudes in terms of the normal ones,

$$
\begin{pmatrix}
a \\
b
\end{pmatrix}_1 = \frac{id \sin(\phi/2)}{\sinh \gamma} \begin{pmatrix}
f \\
-c
\end{pmatrix}_1.
$$

(3.9)

The solution of the first equation in Eq. (3.8) is given by

$$
c_1 = \frac{r \sinh^2 \gamma}{Z}, \quad f_1 = -\frac{d \sinh \gamma \sinh(\gamma + i\phi/2)}{Z},
$$

(3.10)

where

$$
Z = -\frac{d}{d^*} \left( R \sinh^2 \gamma + D \sinh(\gamma + i\phi/2) \sinh(\gamma - i\phi/2) \right),
$$

(3.11)
\( D = |d|^2 \) is the normal electron transmission coefficient of the tunnel junction, and \( R = |r|^2 = 1 - D \) is the normal electron reflection coefficient. It follows from Eqs. (3.9), (3.10) that if there is no phase difference across the junction, \( \phi = 0 \), the Andreev scattering channel is closed: \( a = b = 0 \). It is worth mentioning that the Andreev reflection is also absent if the normal transparency of the junction is equal to zero, \( D = 0 \). If, on the other hand, the junction is completely transparent for normal electrons, \( D = 1 \), there is no Andreev forward scattering, \( b = c = 0 \).

In the presence of a phase difference at the junction the quasiparticle scattering is accompanied by the appearance of superconducting bound states [37]. One can establish the existence of bound states by investigating the poles of the scattering amplitudes, Eq. (3.10), at imaginary \( \gamma \) corresponding to energies lying inside the gap \( |E| < \Delta \). Assuming \( \gamma \to i\gamma \) in Eq. (3.11), we have the dispersion equation \( Z(i\gamma) = 0 \), or

\[
\sin^2 \gamma = D \sin^2 \phi / 2. \tag{3.12}
\]

The bound states correspond to a positive magnitude of \( \sin \gamma \): \( \Delta \sin \gamma = \text{Im} \xi > 0 \). This condition selects two roots:

\[
\gamma = \gamma_0 = \arccos(\sqrt{D} \sin \phi / 2), \quad \gamma = \pi - \gamma_0, \tag{3.13}
\]

or

\[
E(\phi) = \pm \Delta \sqrt{1 - D \sin^2 \phi / 2}. \tag{3.14}
\]

The wave functions of the bound states are to be constructed from elementary solutions of Eq. (2.7) with \( |E| < \Delta \) which decay at \( x = \pm \infty \),

\[
\varphi_{E,R}^\beta = e^{-iEt - \zeta x / v} u_E^\nu, \tag{3.15a}
\]

\[
\varphi_{E,L}^\beta = e^{-iEt + \zeta x / v} u_E^{-\nu}, \tag{3.15b}
\]

where
\[ u'_{E} = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{i\nu\gamma/2} \\ \sigma e^{-i\nu\gamma/2} \end{pmatrix}, \quad e^{i\gamma} = \frac{|E| + i\zeta}{\Delta}, \quad \zeta = \sqrt{\Delta^2 - E^2}, \quad \nu = \beta\sigma. \quad (3.16) \]

The bound state ansatz has a form similar to the outgoing part of the scattering states Eq. (3.5) with the coefficients satisfying the homogeneous equations of Eq. (3.8). These coefficients are:

\[ f = -\frac{d \sin(\gamma + \phi/2)}{r \sin \gamma} c, \quad (3.17a) \]

\[ \begin{pmatrix} a \\ b \end{pmatrix} = \frac{d \sin(\phi/2)}{\sin \gamma} \begin{pmatrix} f \\ -c \end{pmatrix}, \quad (3.17b) \]

with \( \gamma \) given by Eq. (3.12). We note that the bound state spectrum is nondegenerate. The coefficient \( c \) in Eqs. (3.17) is obtained from the normalization condition for the bound state wave function,

\[ \int d^2r_{\perp} \int_{-\infty}^{\infty} dx |\Psi|^2 = \frac{1}{\zeta}(|a|^2 + |b|^2 + |c|^2 + |f|^2) = 1, \]

which yields

\[ |c|^2 = \Delta \sin \gamma \left(1 + \frac{D \sin^2(\gamma + \phi/2)}{R \sin^2 \gamma}\right)^{-1}. \quad (3.18) \]

What is the origin of the bound states in a tunnel junction? According to Eq. (3.8) one can regard these states as resulting from hybridization of the bound states in the short ballistic constriction [24] due to the normal electron reflection by the barrier (cf. effect of impurities in the SNS junction [25,26]). Let us consider a smooth constriction with the length exceeding the coherence length, \( L \gg \xi_0 \). In such a constriction the supercurrent density and the superfluid momentum are related by the local equation, \( J_s(x) = (e/m)N_s p_s(x) \), and they are both enhanced in the neck of the constriction due to current concentration (for simplicity we neglect the effect of suppression of the superfluid electron density \( N_s \) by the supercurrent). The local quasiparticle spectrum in the presence of supercurrent has an additional contribution \( \pm v_F p_s(x) \) [20], which gives rise to a shift of the local energy gap,
Fig. 3. The spatial bending of the gap edges forms the potential wells at $E < 0 (E > 0)$ for quasiparticles with electron velocities directed along (opposite) the current. The bound states in these potential wells are similar to the Andreev bound states in the SNS junctions [49], the difference being that here the bound states are caused by the spatial nonhomogeneity of the phase of the order parameter, while the original Andreev states are caused by the spatial nonhomogeneity of the modulus of the order parameter. With decreasing length of the constriction the number of the bound states in the well decreases. The short Josephson constriction corresponds to an infinitely narrow and deep $\delta$-potential well which contains only one Andreev level [24].

IV. DC JOSEPHSON CURRENT

A convenient expression for the tunnel current results from statistical averaging of the current operator written in the Nambu representation [50]:

$$I(x,t) = \frac{e}{2m} \left\{ (\hat{p} - \hat{p}') \int d^2r_\perp \left[ \delta(\vec{r} - \vec{r}') - Tr \langle \hat{\Psi}(\vec{r},t) \hat{\Psi}^\dagger(\vec{r}',t) \rangle \right] \right\}_{\vec{r} = \vec{r}'} ,$$  \hspace{1cm} (4.1)

where $\hat{\Psi}$ is a two-component field operator:

$$\hat{\Psi}(\vec{r},t) = \begin{pmatrix} \hat{\psi}^\uparrow(\vec{r},t) \\ \hat{\psi}^\downarrow(\vec{r},t) \end{pmatrix},$$  \hspace{1cm} (4.2)

and $Tr$ is a trace in electron-hole space. The angular brackets in Eq. (4.1) denote a thermal average of the one-particle density matrix of the superconductor [51]. In equilibrium this matrix has the form

$$\langle \hat{\Psi}(\vec{r}) \hat{\Psi}^\dagger(\vec{r}') \rangle = \sum_\lambda \Psi_\lambda(\vec{r}) n_F(-E_\lambda) \Psi^\dagger_\lambda(\vec{r}'),$$  \hspace{1cm} (4.3)

where $\Psi_\lambda(\vec{r})$ are the eigenstates of the stationary BdG equation Eq. (2.5) with the quantum numbers $\lambda$. We note that the definition of Fermi distribution function $n_F$ here corresponds to the distribution of holes in the normal metal: in the ground state all energy levels above the Fermi level ($E > 0$) are occupied, while energy levels below the Fermi level ($E < 0$) are
empty (see also the discussion in the next section). In the quasiclassical approximation, Eq. (2.6), the average tunnel current calculated at the middle of the junction has the form

$$I = -e \sum \lambda n_F(-E_\lambda) \sum \beta |\psi_\lambda^\beta(0)|^2.$$  

(4.4)

The current in Eq. (4.4) can be calculated either at the left or the right side of the junction because, due to the unitarity of the matching matrix $\hat{V}$ in Eq. (2.10), the equality

$$|\psi^+_L|^2 - |\psi^-_L|^2 = |\psi^+_R|^2 - |\psi^-_R|^2$$  

(4.5)

holds for the each eigenstate. The current in Eq. (4.4) consists of contributions from both the scattering states and the bound states

$$I = -\int |E|>\Delta \frac{dE|E|}{2\pi \xi} n_F(-E) \sum_j I_j(E) - \sum_{|E|<\Delta} n_F(-E)I_{bound}(E),$$  

(4.6)

$$I(E) = e \sum \beta |\psi^\beta(E)|^2.$$  

When calculating the contribution from the scattering states, it is convenient to consider the transmitted current of each scattering mode:

$$I_j(E) = \begin{cases} 
  e(|b_j|^2 - |f_j|^2) & j = 1, 3 \\
  e(|c_j|^2 - |a_j|^2) & j = 2, 4 
\end{cases}.$$  

(4.7)

The symmetry relations Eqs. (3.6), (3.7) yield

$$I_1(E) = I_4(E), \quad I_2(E) = I_3(E), \quad I_2(E) = -I_1(E).$$  

(4.8)

Thus the currents of all the scattering states with a given energy cancel each other in equilibrium [52]. Substitution of equations Eq. (3.17), (3.18) into Eq. (4.6), taken e.g. at the right electrode, yields for the current of the bound state

$$I_{bound}(E) = e(|b|^2 - |f|^2) = -\frac{e\Delta^2}{2E} D \sin \phi.$$  

(4.9)

A useful formula for the current of the single bound state, which allows direct evaluation of the current from the bound state spectrum, is given by equation:
\[ I(E) = 2e \frac{dE(\phi)}{d\phi}, \]  

(4.10)

where \( E(\phi) \) is the bound state energy band, Eq. (3.14). This formula is derived in Appendix B. Taking into account Eqs. (4.9), (4.6), the total current has the form [10–12,53]:

\[ I = e \frac{\Delta D \sin \phi}{2 \sqrt{1 - D \sin^2 \phi/2}} \tanh \frac{\Delta \sqrt{1 - D \sin^2 \phi/2}}{2T}. \]  

(4.11)

Thus, the dc Josephson current in tunnel junctions is carried only by the bound states, which is similar to the situation found in the other kinds of short weak links [30,24–26,28]. It follows from Eqs. (4.6), (4.9) that the nonvanishing total current results from the imbalance of the bound state currents due to a difference in the equilibrium population numbers. Creation of a nonequilibrium population gives rise to a possibility to control the Josephson transport [31,48,28].

V. INELASTIC SCATTERING

Now we proceed to a discussion of inelastic scattering in voltage biased junctions. According to our assumption \( \Phi = 0 \), explained in Sec. II, the applied voltage drop \( V \) is confined to the constriction; we also neglect, in order not to complicate the problem, a small time dependent voltage induced across the junction by the ac Josephson current (self-coupling effect [54]). This implies the following dependence on time of the phase difference:

\[ \phi = \phi_0 + 2eVt. \]  

(5.1)

The appearance of factors with periodic time dependence in the boundary condition, Eqs. (2.8), (2.9), gives rise to a more complex structure of the scattering states than in Eq. (3.5). In order to satisfy the boundary condition, the outgoing part of the scattering states in Eq. (3.5) is to be constructed from the eigenstates of equation Eq. (2.7) with different energies \( E_n = E - neV \) shifted with respect to the energy \( E \) of the incoming wave with an integer \(-\infty < n < \infty\) (sideband structure)
\[
\left(\begin{array}{c}
\psi_L^- \\
\psi_R^+
\end{array}\right)(0) = \left(\begin{array}{c}
\delta_{j,1} \\
\delta_{j,2}
\end{array}\right) u_E e^{-iEt} + \sum_n \left(\begin{array}{c}
a \\
b
\end{array}\right)_{j,n} u_{E_n}^+ e^{-iE_nt},
\]

\hspace{1cm} \text{(5.2a)}

\[
\left(\begin{array}{c}
\psi_L^+ \\
\psi_R^-
\end{array}\right)(0) = \left(\begin{array}{c}
\delta_{j,3} \\
\delta_{j,4}
\end{array}\right) u_E e^{-iEt} + \sum_n \left(\begin{array}{c}
c \\
f
\end{array}\right)_{j,n} u_{E_n}^- e^{-iE_nt}.
\]

\hspace{1cm} \text{(5.2b)}

For brevity we use the notation \( u_n = u_{E_n} \). While the incoming state is itinerant, the outgoing states can be either itinerant [Eq. (5.1) if \( |E_n| > \Delta \)] or bound [Eq. (5.16) if \( |E_n| < \Delta \)]. It is convenient to combine both the equations for the functions \( u_n \) in a single analytical form:

\[
u_n^\pm = \frac{1}{\sqrt{2 \cosh \Gamma_n}} \begin{pmatrix} e^{\pm \gamma_n/2} \\ \sigma_n e^{\mp \gamma_n/2} \end{pmatrix} \]

\hspace{1cm} \text{(5.3)}

\[
e^{\gamma_n} = \frac{|E_n| + \xi_n}{\Delta}, \quad \Gamma_n = \text{Re} \gamma_n, \quad \xi_n = \begin{cases} \sqrt{E_n^2 - \Delta^2}, & |E_n| > \Delta \\ i\sigma_n \sqrt{\Delta^2 - E_n^2}, & |E_n| < \Delta. \end{cases} \]

\hspace{1cm} \text{(5.4)}

To find the scattering amplitudes in Eq. (5.2) we consider the boundary condition Eq. (2.8). It is important to mention, that this boundary condition was derived neglecting the energy dispersion of the normal electron scattering amplitudes \( d \) and \( r \), which means that now this assumption should be valid for the entire interval of relevant energies \( E_n \). Let us first discuss \( j = 1 \) (hole-like quasiparticle coming from the left):

\[
\begin{pmatrix} 1 \\ 0 \end{pmatrix} u_n^- \delta_{n,0} + \begin{pmatrix} a \\ b \end{pmatrix}_{1,n} u_n^+ = r \begin{pmatrix} c \\ f \end{pmatrix}_{1,n} u_n^- + \frac{d}{2} \begin{pmatrix} 1 + \sigma_z & 0 \\ 0 & 1 - \sigma_z \end{pmatrix} \begin{pmatrix} f \\ c \end{pmatrix}_{1,n-1} \]

\hspace{1cm} + \frac{d}{2} \begin{pmatrix} 1 - \sigma_z & 0 \\ 0 & 1 + \sigma_z \end{pmatrix} \begin{pmatrix} f \\ c \end{pmatrix}_{1,n+1} u_n^- + 1, \quad (5.5)

It is convenient to separate the equations for normal and Andreev scattering amplitudes in Eq. (5.5) again using a procedure similar to Eq. (3.8). The equation for the normal scattering amplitudes then becomes

\[
r c_{1,n} + \frac{d}{2} (V_{nm+1}^- f_{1,n+1} + V_{nm-1}^+ f_{1,n-1}) = \delta_{n0} \]

\hspace{1cm} \text{(5.6)}

\[
r f_{1,n} + \frac{d}{2} (V_{nm+1}^+ c_{1,n+1} + V_{nm-1}^- c_{1,n-1}) = 0,
\]

\hspace{1cm} (5.7)
where the coefficients

\[ V_{nm}^\pm = \frac{(u_n^+, \sigma_z \pm 1 u_m^-)}{(u_n^+, \sigma_z u_m^-)} \]  

have the explicit form

\[ V_{nm}^+ = -\frac{e^{-(\gamma_n + \gamma_m)/2}}{\sinh \gamma_n} \sqrt{\frac{\cosh \Gamma_n}{\cosh \Gamma_m}}, \]  

\[ V_{nm}^- = \sigma_n \sigma_m \frac{e^{(\gamma_n + \gamma_m)/2}}{\sinh \gamma_n} \sqrt{\frac{\cosh \Gamma_n}{\cosh \Gamma_m}}. \]  

The equation for the Andreev scattering amplitudes reads

\[ a_{1,n} = (d/2)(U_{nn+1}^+ f_{1,n+1} + U_{nn-1}^- f_{1,n-1}) \]  

\[ b_{1,n} = (d/2)(U_{nn+1}^+ c_{1,n+1} + U_{nn-1}^- c_{1,n-1}) \]  

where the coefficients are defined as

\[ U_{nm}^\pm = \frac{(u_n^{+*}, \sigma_z \pm 1 u_m^-)}{(u_n^{+*}, \sigma_z u_m^-)}, \]  

and have the explicit forms

\[ U_{nm}^+ = \frac{e^{(\gamma_n - \gamma_m)/2}}{\sinh \gamma_n} \sqrt{\frac{\cosh \Gamma_n}{\cosh \Gamma_m}}, \]  

\[ U_{nm}^- = -\sigma_n \sigma_m \frac{e^{-(\gamma_n - \gamma_m)/2}}{\sinh \gamma_n} \sqrt{\frac{\cosh \Gamma_n}{\cosh \Gamma_m}}. \]  

As can be seen from Eqs. (5.6), (5.9), the inelastic scattering possesses a specific asymmetry: the forward scattered waves have odd side band indices and backward scattered waves have even side band indices, as illustrated in Fig. 4. Correspondingly, bound states with odd or even side band indices are induced either in the right or in the left electrode. We note that the scattering to any side band consists of both normal and Andreev components.

It is instructive to compare the superconducting scattering diagram in Fig. 4 with the scattering diagram of normal junctions. In the normal limit \( \Delta = 0 \), all the Andreev
amplitudes in Eq. (5.4) vanish \( U_n^+ = 0 \) in Eq. (5.11) and equations Eq. (5.6) split due to \( V^+ = 0 \) in Eq. (5.8), which yields \( f_n = c_{n-1} = 0 \) for all \( n \neq 1 \). Thus, the side band diagram in Fig. 4 reduces to the elementary fragment shown in Fig. 5a. This fragment corresponds to the scattering of a \textit{true hole}, meaning a particle with spectrum \( E_h = -(p^2/2m - \mu) \) according to the BdG equation Eqs. (2.2), (2.5). In the ground state, \( T = 0 \), these holes fill all positive energy states \( E > 0 \) while the negative energy states are empty. For the electrons, the corresponding diagram is sketched in Fig. 5b. In this diagram the chemical potentials in both electrodes are equal, while the energies of the incident and transmitted states are shifted by \( eV \). This difference from the conventional diagram of normal electron tunneling in Fig. 5c (where the chemical potentials in the electrodes are shifted relative to each other, while the scattering is elastic) appears after separating out the superconducting phase in Eq. (2.4); the conventional picture with shifted chemical potential can be restored by means of the gauge transformation of the normal electron wave function \( \psi \rightarrow \exp(-ieVt)\psi \).

When superconductivity is switched on, \( \Delta \neq 0 \), the incoming quasiparticle consists of both electron and hole components, and therefore the scattering diagram is a combination of the diagrams in Figs. 5a,b. One has also to take into account electron-hole conversions, which lead to the appearance of both electron and hole components in the upper as well as lower transmitted state. Continuation of this process creates the whole superconducting scattering diagram in Fig. 4.

From a mathematical point of view, Eqs. (5.6), (5.9) for the scattering amplitudes are second order difference equations which can not be solved exactly, except in some particular cases, e.g. a fully transparent constriction \( (r = 0) \) where equation Eq. (5.6) reduces to a binary relation [34]. In the general case, it is only possible to find asymptotical solutions using some small parameter. In the present case of a tunnel junction, there is a natural small parameter - the transparency of the tunnel barrier: \( D \ll 1 \). However, a straightforward perturbation expansion with respect to this parameter gives rise to divergences, similar to difficulties of the multiparticle tunneling theory (MPT) [42, 57, 58]. In order to formulate an improved perturbation procedure, it is convenient to rewrite Eqs. (5.6), (5.9) in terms of the
parameter $\lambda = D/4R$, the true small parameter of the theory, as will be seen later. To this end we introduce new scattering amplitudes

$$c_{1,\pm 2k} = \frac{\lambda^k}{r} c_{\pm 2k}, \quad f_{1,\pm (2k+1)} = \frac{\lambda^k d^*}{2R} f_{\pm (2k+1)}, \quad a_{1,\pm 2k} = \lambda^k a_{\pm 2k},$$

$$b_{1,\pm (2k+1)} = \frac{\lambda^k d}{2r} b_{\pm (2k+1)},$$

which satisfy the equations:

$$c_n + \lambda V_{mn+1}^- f_{n+1} + V_{mn-1}^+ f_{n-1} = 0 \quad (5.13a)$$

$$f_n - \lambda V_{mn+1}^+ c_{n+1} - V_{mn-1}^- c_{n-1} = 0,$$

$$a_n = \lambda U_{mn+1}^- f_{n+1} + U_{mn-1}^+ f_{n-1} \quad (5.13b)$$

$$b_n = \lambda U_{mn+1}^+ c_{n+1} + U_{mn-1}^- c_{n-1},$$

for $n > 0$. For $n < 0$ one has to make the change $V_{nm}^\pm \rightarrow V_{n-m}^\mp, U_{nm}^\pm \rightarrow U_{-n-m}^\mp, (n, m > 0)$ in the above equations. The equation for $n = 0$ then reads

$$c_0 + \lambda (V_{01}^- f_1 + V_{0-1}^+ f_{-1}) = 1 \quad (5.13c)$$

Let us now turn to the second scattering case in Eq. (5.2), $j = 2$ (hole-like quasiparticle incoming from the right). According to the symmetry relations of Eq. (3.6) the scattering amplitudes $j = 2$ differ from the scattering amplitudes $j = 1$ by $\phi \rightarrow -\phi$, which in the present time-dependent case means that $n \pm 1 \rightarrow n \mp 1$. Taking into account this symmetry and also the property of scattering amplitudes in Eq. (3.6), we introduce new scattering amplitudes

$$f_{2,\pm 2k} = \frac{\lambda^k}{r} c_{\pm 2k}, \quad c_{2,\pm (2k+1)} = \frac{\lambda^k d^*}{2R} f_{\pm (2k+1)}, \quad b_{2,\pm 2k} = \lambda^k a_{\pm 2k},$$

$$a_{2,\pm (2k+1)} = \frac{\lambda^k d}{2r} b_{\pm (2k+1)},$$

which satisfy the following equations (for $n > 0$):
\[ \tau_n + \lambda V_{nm+1}^+ \bar{f}_{n+1} + V_{nm-1}^- \bar{f}_{n-1} = 0 \quad (5.15a) \]

\[ \bar{f}_n - \lambda V_{nm+1}^- \bar{c}_{n+1} - V_{nm-1}^+ \bar{c}_{n-1} = 0, \]

\[ \pi_n = \lambda U_{nm+1}^+ \bar{f}_{n+1} + U_{nm-1}^- \bar{f}_{n-1} \quad (5.15b) \]

\[ \bar{f}_n = \lambda U_{nm+1}^- \bar{c}_{n+1} + U_{nm-1}^+ \bar{c}_{n-1}, \]

\[ \bar{c}_0 + \lambda (V_{01}^+ \bar{f}_1 + V_{0-1}^- \bar{f}_{-1}) = 1. \quad (5.15c) \]

Equations (5.15) differ from equations Eq. (5.13) by

\[ V^\pm \rightarrow V^\mp, \quad U^\pm \rightarrow U^\mp. \quad (5.16) \]

In the case of electron-like quasiparticles incoming from the left, \( j = 3 \), the symmetry of Eq. (3.7) involves transformation \( \gamma \rightarrow -\gamma \), which means transformation of the coefficients \( V^\pm \rightarrow -\sigma_n \sigma_m V^\mp \), \( U^\pm \rightarrow -\sigma_n \sigma_m U^\mp \) in Eqs. (5.13), (5.15). This allows us to relate the scattering amplitudes of this case to the solutions of Eqs. (5.15):

\[ a_{3, \pm 2k} = \frac{\lambda^k}{r^{*}} \sigma_{\pm 2k} \bar{c}_{\pm 2k}, \quad b_{3, \pm (2k+1)} = -\frac{\lambda^kd^*}{2R} \sigma_{\pm (2k+1)} \bar{f}_{\pm (2k+1)}, \quad c_{3, \pm 2k} = \lambda^k \sigma_{\pm 2k} \bar{\pi}_{\pm 2k}, \quad (5.17) \]

\[ f_{3, \pm (2k+1)} = -\frac{\lambda^kd^*}{2r^{*}} \sigma_{\pm (2k+1)} \bar{b}_{\mp (2k+1)}. \]

In a similar way the scattering amplitudes of electron-like quasiparticles incoming from the right, \( j = 4 \), are related to the solutions of Eqs. (5.13),

\[ b_{4, \pm 2k} = \frac{\lambda^k}{r^{*}} \sigma_{\pm 2k} c_{\pm 2k}, \quad a_{4, \pm (2k+1)} = -\frac{\lambda^kd^*}{2R} \sigma_{\pm (2k+1)} f_{\pm (2k+1)}, \quad f_{4, \pm 2k} = \lambda^k \sigma_{\pm 2k} a_{\pm 2k}, \quad (5.18) \]

\[ c_{4, \pm (2k+1)} = -\frac{\lambda^kd^*}{2r^{*}} \sigma_{\pm (2k+1)} b_{\mp (2k+1)}. \]

According to a symmetry of the coefficients in Eqs. (5.13), (5.15),

\[ V_{nm}^\pm (-E) = V_{n-m}^\mp (E), \quad U_{nm}^\pm (-E) = U_{n-m}^\mp (E), \quad (5.19) \]

all scattering amplitudes with positive and negative incoming energies are related through

\[ a_n(-E) = \bar{\pi}_{-n}^-(E), \quad (5.20) \]
and similarly for the other amplitudes.

Let us now present a formal solution of Eq. (5.13) for \( n > 0 \) on the following form \[55\]:

\[
f_{2k+1} = (-1)^k \prod_{l=0}^{2k+1} S_l c_0, \quad (5.21)
\]

where the quantities \( S_l \) are defined as

\[
S_{2k} = -\frac{c_{2k}}{f_{2k-1}}, \quad S_{2k+1} = \frac{f_{2k+1}}{c_{2k}}, \quad (5.22)
\]

and satisfy the recurrence relations

\[
S_{2k} = \frac{V_{2k-2k-1}}{1 + \lambda V_{2k,2k+1} S_{2k+1}}, \quad S_{2k+1} = \frac{V_{2k+1,2k}}{1 + \lambda V_{2k+1,2k+2} S_{2k+2}}. \quad (5.23)
\]

The quantity \( c_0 \) in Eq. (5.27) is given by

\[
c_0 = \frac{1}{1 + \lambda (V_{01} S_1 + V_{0-1} S_{-1})}. \quad (5.24)
\]

It is convenient to express the functions \( S_n \) in Eq. (5.23) through the relation \( S_n = V_{n,n+1}^\pm /Z_n \), were the denominators \( Z_n \) \((n \neq 0)\) satisfy the recurrence

\[
Z_n = 1 + \lambda a_\pm a_{n+1}^\pm, \quad a_\pm = \frac{e^{\pm \gamma_n}}{\sinh \gamma_n}, \quad (5.25)
\]

\((\pm \) corresponds to even/odd \( n \)), and to define \( Z_0 \) as the denominator of \( c_0 \), Eq. (5.24):

\[
Z_0 = 1 + \lambda a_0^+ a_1^+ + \lambda a_0^- a_{-1}^- /Z_{-1}. \quad (5.26)
\]

Using the above notation, one is able to express the coefficients of the normal forward scattering, \(|f_n|^2\), on the form

\[
|f_n|^2 = e^{\gamma_0} \cosh \gamma_0 |Z_0|^2 e^{\Gamma_n} \cosh \Gamma_n \prod_{l=1}^{n} \frac{1}{|Z_l \sinh \gamma_l|^2}, \quad (5.27)
\]

provided \( a^- \neq 0 \). The equation for the coefficients of the normal backward scattering, \(|c_n|^2\), differs from Eq. (5.27) by \( e^{\Gamma_n} \rightarrow e^{-\Gamma_n} \). The relation between the amplitudes of the Andreev and normal forward scattering in Eq. (5.13), taking into account Eqs. (5.22), (5.23), (5.25), has the form
\[ b_n = -e^{-\gamma_n} \left( 1 - \lambda \frac{2e^{-\gamma_{n+1}}}{\sinh \gamma_{n+1} Z_{n+1}} \right) f_n. \]  

(5.28)

In a similar way, one can express the solution of Eq. (5.15) for \( n > 0 \) on the form

\[ |\tilde{f}_n|^2 = \frac{e^{-\gamma_0}}{\cosh \gamma_0 |Z_0|^2} e^{-\Gamma_n} \cosh \Gamma_n \prod_{l=1}^{n} \left| Z_l \sinh \gamma_l \right|^2; \quad \tilde{b}_n = -e^{\gamma_n} \left( 1 + \lambda \frac{2e^{-\gamma_{n+1}}}{\sinh \gamma_{n+1} Z_{n+1}} \right) \tilde{f}_n, \]  

(5.29)

where

\[ \tilde{Z}_n = 1 + \lambda \frac{a_n^+ a_{n+1}^-}{Z_{n+1}}, \quad \tilde{Z}_0 = 1 + \lambda \frac{a_0^+ a_{-1}^-}{Z_{-1}}. \]  

(5.30)

We note that Eqs. (5.29), (5.30) differ from Eqs. (5.27), (5.28) by \( \gamma_n \to -\gamma_n \) everywhere.

Equations for the scattering amplitudes with negative side band indices, \( n < 0 \), can be derived in a similar way, and the result differs from the above equations for positive side band indices Eqs. (5.25)-(5.30) by the substitution

\[ \gamma_n \to -\gamma_{-|n|}, \quad n \neq 0, \]  

(5.31)

introduced everywhere except in \( Z_0 \) and \( \tilde{Z}_0 \).

VI. QUASIPARTICLE CURRENT

In the nonstationary problem under consideration, the density matrix determining the current Eq. (4.1) is time dependent, and its dynamic evolution can be described by an equation similar to Eq. (4.3),

\[ \langle \hat{\Psi}(\vec{r},t) \hat{\Psi}^\dagger(\vec{r}',t) \rangle = \sum_{\lambda} \Psi_{\lambda}(\vec{r},t) f_{\lambda} \Psi_{\lambda}^\dagger(\vec{r}',t), \]  

(6.1)

\( \Psi_{\lambda} \) are now solutions of the time dependent problem, Eq. (2.7), with initial conditions corresponding to the eigenstates of the initial Hamiltonian with the eigenvalues \( \lambda \), and occupation numbers \( f_{\lambda} \) of these initial states. We consider inelastic scattering states, Eqs. (2.6), (5.2), as the propagators \( \Psi_{\lambda}(t) \) in Eq. (6.1) with \( \lambda \) corresponding to the complete set of the incoming states \( \lambda = (E,j) \); according to the assumption about local equilibrium within
the electrodes, the incoming states possess the Fermi distribution of occupation numbers, 
\( f_{Ej} = n_F(-E) \). Thus the current Eq. (4.4) takes the form:
\[
I(t) = -e \int_{|E| > \Delta} \frac{dE |E|}{2\pi \xi} n_F(-E) \sum_{N=-\infty}^{\infty} e^{iNevt} \sum_{n=-\infty}^{\infty} \sum_{j\beta} \beta(\psi_j^\beta(E, n), \psi_j^\beta(E, N+n)).
\] (6.2)

The current in Eq. (6.2) consists of a time independent part, \( N = 0 \), which is formed by incoherent contributions of all the side bands (the quasiparticle current), and of a time dependent part, \( N \neq 0 \) which results from interference among the different side bands (ac Josephson current). The difference between the side band indices \( N \) is an even number since the side band index is either even or odd depending on the electrode; therefore the time-dependent current oscillates with the Josephson frequency \( \omega = 2eV \).

In this paper we will concentrate on an analysis of the time-independent quasiparticle current. Similarly to Eq. (4.7) we will calculate the current using the transmitted states,
\[
I = \frac{1}{2} e \int_{|E| > \Delta} \frac{dE |E|}{\xi} n_F(-E) \sum_{n=-\infty}^{\infty} \left[ \sum_{j=1,3} (|f_{jn}|^2 - |b_{jn}|^2) + \sum_{j=2,4} (|a_{jn}|^2 - |c_{jn}|^2) \right].
\] (6.3)

Using the scattering amplitudes introduced in the previous section through Eqs. (5.12), (5.14), (5.17) and (5.18) we express the current in Eq. (6.3) in the following form:
\[
I = e \int_{|E| > \Delta} \frac{dE |E|}{\xi} n_F(-E) \sum_{n=0}^{\infty} (K_n - \overline{K}_n),
\] (6.4)

where
\[
K_n = \lambda^{|n|}(R^{-1}|f_n|^2 - |b_n|^2), \quad \overline{K}_n = \lambda^{|n|}(R^{-1}|\overline{f}_n|^2 - |\overline{b}_n|^2) = K_n(-\gamma).
\] (6.5)

The factor of two appears in Eq. (6.4) due to equality of currents \( I_1 \) and \( I_4 \) and of currents \( I_2 \) and \( I_3 \) in Eq. (4.8), equalities which hold also in the nonstationary case. However, there is no balance between currents of these two pairs any more. The symmetry of Eq. (5.20) allows us to reduce the interval of integration in Eq. (6.4) to the semiaxis \( E > 0 \),
\[
I = e \int_{\Delta}^{\infty} \frac{dE E}{\xi} \tanh \frac{E}{2T} \sum_{n=0}^{\infty} (K_n - \overline{K}_n).
\] (6.6)

The side band currents \( K_n \) in Eq. (6.3) are proportional to the powers of the small parameter \( \lambda \), \( K_n \sim \lambda^n \). Therefore Eqs. (5.6), (6.3) present a perturbative expansion of the current,
convenient for analysis in the limit of low barrier transparency. The following sections are devoted to such an analysis of the structure of the current in Eq. (6.6).

**VII. EXCESS CURRENT AT LARGE BIAS**

To make some observations useful for analysis of the subgap current, it is instructive first to discuss the simpler case of large bias $eV \gg \Delta$, which is well studied in literature [17, 11, 23, 12]. Simultaneously we will derive the explicit analytical expression for the current in this limit valid in a whole range of the junction transparency $0 < D < 1$. The asymptotic expansion of the current with respect to the small parameter $\Delta/eV$ has the form [17]:

$$I = e^2 D V \pi + I_{\text{exc}}(D) + O \left( \frac{\Delta}{eV} \right),$$  \hspace{1cm} (7.1)

where the first term is the tunnel current of the normal junction and the second term is a voltage-independent excess current which represents the leading superconducting correction.

A main simplification in this case is that the side band currents $K_n$ and $\overline{K}_n$, $|n| > 1$ diminish when the bias voltage increases. This follows from an estimate of the transmission amplitudes in Eqs. (5.27)-(5.29), which contain products of factors $|\sinh \gamma_k|^{-2}$ which are small at large voltages, $|\sinh \gamma_k|^{-2} \sim (\Delta/eV)^2$, because of the large interval of involved energies, $E \sim eV$. Furthermore, inspection of the amplitudes $f_{-1}$ and $\overline{f}_1$ shows that they are also small due to the factors $e^{-\gamma_0 - \gamma_1}$; therefore the non-vanishing part of the current Eq. (6.6) in the limit $eV \gg \Delta$ becomes

$$I = \frac{e}{\pi} \int_{\Delta}^{\infty} \frac{dE E}{\xi} \tanh \frac{E}{2T} (K_1 - \overline{K}_{-1}).$$  \hspace{1cm} (7.2)

The essential fragments of the scattering diagram in the large bias limit are shown in Fig. 6.

The structure of the current in Eq. (7.2) is essentially determined by the presence of a gap in the spectrum of the side band $n = 1$; this causes different analytical forms of the current $K_1$ in the regions $|E| < \Delta$ and $|E| > \Delta$. We note that the spectrum of the side band
\( n = -1 \) possesses no gap: \( E_{-1} > \Delta \) for \( E > \Delta \). According to this we divide the integral in Eq. (7.2) into three parts:

\[
I = I_\prec + I_\Delta + I_\succ.
\]

The first part corresponds to the current of the states in the side band \( n = 1 \), which lie below the gap, \( E_1 < -\Delta \). The second part corresponds to the current of the states of the same side band lying within the gap, \( -\Delta < E_1 < \Delta \). The third part combines contributions from the remaining states of the side band \( n = 1 \), \( \Delta < E_1 \), and from the all states of the side band \( n = -1 \). Making use of the approximations

\[
|Z_0|^2 = |Z_0|^2 \approx 1, \quad |Z_{-1}|^2 = |Z_1|^2 = |Z^2| = |Z_{-2}|^2 \approx 1, \quad (7.3)
\]

\[
|Z_1|^2 = |Z_{-1}|^2 = |Z_{-2}|^2 = |Z_2|^2 \approx 1/R^2,
\]

it is possible to express the integral \( I_\prec \) on the form (we restrict ourselves to the limit \( T = 0 \)):

\[
I_\prec = e^{\pi} \int_{eV}^{eV-\Delta} \frac{dE}{\xi} K_1 = \frac{8e\lambda}{\pi R} \int_{\Delta}^{\infty} dE \frac{E}{\xi Z_0^2} - \frac{2e\lambda}{\pi R} \int_{\Delta}^{\infty} dE \frac{(E - \xi)}{\xi Z_0^2} \left( 1 - 4\lambda R \frac{E}{\xi} \right) \quad (7.4)
\]

where the limit of integration in the last term is extended to infinity since the main contribution to this integral comes from the energies \( E \sim \Delta \ll eV \). Separating out the normal junction current we may express Eq. (7.4) in the following form

\[
I_\prec = \frac{e^2DV}{\pi} - \frac{8e\lambda^2}{\pi} \int_{\Delta}^{\infty} dE \frac{eV}{Z_0^2\xi} \left[ 4\lambda R \frac{E\Delta^2}{\xi^2} + (2R + 1) \frac{E(E - \xi)}{\xi} + \frac{1}{4\lambda R} \frac{E - \xi}{\xi} \right]. \quad (7.5)
\]

We note that this current is always smaller than the normal current. It is convenient to express the integral \( I_\Delta \) as

\[
I_\Delta = e^{\pi} \int_{eV}^{eV+\Delta} \frac{dE}{\xi} K_1 = \frac{16e\lambda^2}{\pi} \int_{\Delta}^{\Delta} dE \frac{\Delta^2}{\xi|Z_0|^2}, \quad (7.6)
\]

obtained by using the relations between the functions \( Z_n \) [which result from their definition in Eq. (5.25)]

\[
Z_n(E + eV) = \overline{Z}_{n-1}(E), \quad Z_0(E + eV)Z_1(E + eV) = \overline{Z}_0(E)\overline{Z}_{-1}(E). \quad (7.7)
\]
Inspection of the equation for $I_>$,

$$I_> = \frac{e}{\pi} \int_{eV+\Delta}^{\infty} dE \frac{E}{\xi} K_1 - \frac{e}{\pi} \int_{\Delta}^{\infty} dE \frac{E}{\xi K_{-1}},$$

(7.8)

shows that both integrals diverge at the upper limit $E = \infty$, which means that the states lying far from the Fermi level formally contribute to the current, while the quasiclassical approximation of Eq. (2.6) assumes, that all relevant states lie close to the Fermi level. To get rid of this formal divergence one commonly shifts by $eV$ the variable in the first integral in Eq. (7.8). Using again the relations (7.7) we may express this integral on the form

$$\frac{4e\lambda}{\pi R} \int_{\Delta}^{\infty} dE \frac{E}{\xi Z_0 Z_{-1}} + \frac{8e^2}{\pi} \int_{\Delta}^{\infty} dE \frac{E(E - \xi)}{\xi^2 Z_0^2},$$

where the first term has the same analytical form but the opposite sign compared to the divergent term in the second integral in Eq. (7.8),

$$-\frac{4e\lambda}{\pi R} \int_{\Delta}^{\infty} dE \frac{E}{\xi Z_0 Z_{-1}} + \frac{2e^2}{\pi R} \int_{\Delta}^{\infty} dE \frac{(E - \xi)}{\xi Z_0^2}.$$

After elimination of the divergent terms, the integral in Eq. (7.8) takes the form

$$I_> = \frac{2e\lambda}{\pi R} \int_{\Delta}^{\infty} dE \frac{(E - \xi)}{\xi Z_0^2} \left( 1 + 4\lambda R \frac{E}{\xi} \right).$$

(7.9)

The currents in Eq. (7.9) and Eq. (7.6) are positive and overcompensate the missing part of the current in Eq. (7.5). Collecting Eqs. (7.5), (7.6) and (7.9) we find after some algebra the following explicit equation for the excess current in Eq. (7.1),

$$I_{exc} = \frac{16e\Delta^2 R}{\pi} \left[ 1 - \frac{D^2}{2(1+R)\sqrt{R}} \ln \frac{1 + \sqrt{R}}{1 - \sqrt{R}} \right],$$

(7.10)

which is valid in the whole interval of junction transparency $0 < D \leq 1$. Asymptotics of this expression coincide with the results presented in literature [11,23] both in the limit of fully transparent ($D = 1$) constrictions, $I_{exc} = 8e\Delta/3\pi$, and in the limit of low-transparency ($D \ll 1$) tunnel junctions, $I_{exc} = e\Delta D^2/\pi$.

The above calculation reveals an important difference between the structure of the current in normal and superconducting junctions. In normal junctions, the current, e.g. in the
right electrode, see Fig. 5c, results from scattering states lying above the local chemical potential, $E > \mu - eV$, while contribution from the energy interval $E < \mu - eV$ is equal to zero due to mutual cancellation of currents of the scattering states incident from the left and from the right (in Fig. 5a the current carrying energy region corresponds to negative energies $E_h < 0$). Thus the total current coincides with the current of real excitations emitted from the contact, which is consistent with the nonequilibrium origin of the current in the voltage biased junctions. In superconducting junctions, only ”across-the-gap” current $I_<$ is clearly related to the real excitations emitted at the right side of the junction where the current is calculated (Fig. 6a) - the dissipative character of the currents $I_\Delta$ and $I_> \Delta$ is not obvious. However, one should take into account the creation of real excitations at the left side of the junction via back scattering into the side band $n = 2$ (Fig. 6b,c). Although the current of this side band exists only at the left side of the scattering diagram it should have an effect at the right side due to continuity of the current at the interface, Eq. (4.5), and therefore it should be distributed among the states of the side band $n = 1$. As our calculations show, this ”kick” current partially flows through the Andreev bound states, involving the current $I_\Delta$, Fig. 6b, which convert this current into a supercurrent outside the junction. It is also partially distributed among the scattering states with positive energies, current $I_> \Delta$, Fig. 6c, in the form of imbalanced ground state currents.

VIII. SUBGAP CURRENT

In this section we turn to a discussion of the tunnel current in the subgap region $eV < 2\Delta$. A basic property of the subgap current is the presence of temperature independent structures on I-V characteristics - the subharmonic gap structure (SGS). SGS in tunnel junctions was discovered in experiments by Taylor and Burstein [56], and the first theoretical explanation was given by Schrieffer and Wilkins [42] in terms of multiparticle tunneling (MPT). Recently SGS has been observed in a number of experiments on transmissive tunnel junctions [3-5]. Although there is a possibility to attribute SGS in planar junctions to normal shorts, the
observation of SGS in superconducting controllable break junctions provided convincing confirmation of the existence of SGS in the true tunnel regime.

The existence of SGS in tunnel current can be established within the MPT theory by means of rather simple perturbative arguments. On the basis of the tunnel Hamiltonian model, assuming a small perturbative coupling between electrodes, one can calculate the probability of tunneling in $n$-th order of perturbation theory. Such a probability is proportional to a product of filling factors of the initial and the final states: $n_F(E)[1 - n_F(E - n eV)]$. At zero temperature this factor is equal to zero outside the interval $\Delta < E < n eV - \Delta$, which selects the quasiparticle transitions across the gap, i.e. the processes of creation of real excitations relevant for the tunnel current. Such a restriction places the threshold of the $n$-th order current at $eV = 2\Delta/n$, and a sequence of current onsets of magnitudes $\sim D^n$ at the voltages $eV = 2\Delta/n$ forms the SGS of the tunnel current.

In our approach, the filling factors of final states do not enter the equation for the current Eq. (6.6), and the existence of SGS is therefore not obvious, although the side band currents Eq. (5.25) successively diminish with increasing side band index. However, attribution of the nonequilibrium tunnel current in biased junctions to the current of real excitations is a general physical argument which should be automatically met in any correct theory. In fact, and this also follows from the discussion of the previous section, the true tunnel current is hidden in Eq. (6.6): it results from partial cancellation of large contributions of different scattering modes. The cancellation is nontrivial because of mixture of currents of different side bands, the odd side bands containing information about the currents of the even side bands and vice versa. This means that a finite perturbation expansion of Eq. (6.6) is not satisfactory and will not adequately correspond to the perturbative structure of the true tunnel current. To reveal such a structure one must rearrange the series in Eq. (6.6).

To this end we consider a general term $K_n, n > 0$ in Eq. (6.4). It follows immediately from the explicit form of the normal and Andreev transmission coefficients, Eqs. (5.27) and (5.28), that the leading term with respect to $\lambda$ in $K_n$ is proportional to a factor $1 - e^{2\Gamma_n}$.
which is equal to zero if $|E_n| < \Delta$. Having made this observation we express the quantity $K_n$ in the following form:

$$K_n = \frac{2}{R} \lambda^n \theta (E_n^2 - \Delta^2) e^{-\gamma_n} \sinh \gamma_n |f_n|^2 + 4 \lambda^{n+1} e^{-2\Gamma_n} \left| \frac{f_n}{Z_{n+1}} \right|^2 F_{n+1},$$  \hspace{1cm} (8.1a)

$$F_{n+1} = |Z_{n+1}|^2 + \text{Re} \left( \frac{e^{-\gamma_{n+1}} Z_{n+1}^*}{\sinh \gamma_{n+1}} \right) - \lambda \left| \frac{e^{-\gamma_{n+1}}}{\sinh \gamma_{n+1}} \right|^2.$$  \hspace{1cm} (8.1b)

In Eq. (8.1a) the first term represents the main contribution of the $n$-th side band to the current: it is proportional to the probability of normal scattering to the $n$-th side band and it does not contain the contribution of the side band states lying inside the gap $|E_n| < \Delta$. Using the recurrence relation (5.25) and remembering that $\lambda = D/4R$, after some algebra the function $F_n$ in Eq. (8.1b) becomes

$$F_n = \frac{1}{R} \theta (E_n^2 - \Delta^2) \frac{1}{\tanh \gamma_n} - \lambda \left| \frac{e^{\gamma_n}}{\sinh \gamma_n Z_{n+1}} \right|^2 G_{n+1},$$  \hspace{1cm} (8.2a)

$$G_{n+1} = |Z_{n+1}|^2 - \text{Re} \left( \frac{e^{\gamma_{n+1}} Z_{n+1}^*}{\sinh \gamma_{n+1}} \right) - \lambda \left| \frac{e^{\gamma_{n+1}}}{\sinh \gamma_{n+1}} \right|^2.$$  \hspace{1cm} (8.2b)

Substituting Eq. (8.2) into Eq. (8.1a), we find that the second term in the equation for $K_n$, proportional to $\lambda^{n+1}$, has analytical structure similar to the first term in the same equation, proportional to $\lambda^n$, namely, it consists of the probability of normal scattering to the $(n+1)$-th side band [cf. Eq. (5.22)] and it does not include the contribution of the side band states lying inside the gap $|E_{n+1}| < \Delta$. This allows us to associate this term with the effective contribution of the nearest even side band.

A similar transformation of the function $G_{n+1}$ in Eq. (8.2) yields the recurrence:

$$G_{n+1} = -\frac{1}{R} \theta (E_{n+1}^2 - \Delta^2) \frac{1}{\tanh \gamma_{n+1}} - \lambda \left| \frac{e^{-\gamma_{n+1}}}{\sinh \gamma_{n+1} Z_{n+2}} \right|^2 F_{n+2}$$  \hspace{1cm} (8.3)

Combination of Eqs. (8.1a)-(8.3) shows that the next term of the current $K_n$, proportional to $\lambda^{n+2}$, has the same analytical structure as the leading term in the current $K_{n+2}$ of the next odd side band, and therefore it can be regarded as a renormalization of that current.
Continuing this procedure by systematic use of the recurrence Eqs. (8.2), (8.3) we obtain the following expansion for the current $K_n$ in Eq. (8.3):

$$K_n = \frac{2\lambda^n}{R} \theta(E_n^2 - \Delta^2)Q_n + \frac{4\lambda^{n+1}}{R} \theta(E_{n+1}^2 - \Delta^2) e^{-\Gamma_n} \cosh \Gamma_n Q_{n+1}$$  \hspace{1cm} (8.4)

$$+ \frac{4\lambda^{n+2}}{R} \theta(E_{n+2}^2 - \Delta^2) e^{-\Gamma_n + 2\Gamma_{n+1}} \cosh \Gamma_n Q_{n+2}$$

$$+ \frac{4\lambda^{n+3}}{R} \theta(E_{n+3}^2 - \Delta^2) e^{-\Gamma_n + 2\Gamma_{n+1} - 2\Gamma_{n+2}} \cosh \Gamma_n Q_{n+3} + \ldots$$

where we have introduced the quantity $Q_n$ defined for all $n$ as

$$Q_n = e^{\gamma_0} \frac{\sinh \gamma_n \cosh \Gamma_n}{\cosh \gamma_0 |Z_0|^2} \prod_{l=1}^{n} \frac{1}{|Z_l \sinh \gamma_l|^2}$$  \hspace{1cm} (8.5)

One can derive similar expansions for the currents $\bar{K}_n$ as well as for the currents of the side bands with negative $n < 0$. Expanding each term of the series in Eq. (8.6) using Eq. (8.4) and collecting terms with the same factor $\lambda^n$, we can finally express the series in the form

$$\sum_{\text{odd}} (K_n - \bar{K}_n) = \sum_{n \neq 0} (\tilde{K}_n - \tilde{\bar{K}}_n).$$  \hspace{1cm} (8.6)

The last summation is done over all odd and even integer $n$, and the renormalized coefficients have the form

$$\tilde{K}_n = \lambda^n \theta(E_n^2 - \Delta^2)(4Q_n/R) \left[ (1/2) + \cosh \Gamma_{n-2} e^{-\Gamma_{n-2} + 2\Gamma_{n-1}} \right]$$  \hspace{1cm} (8.7a)

$$+ \cosh \Gamma_{n-4} e^{-\Gamma_{n-2} + 2\Gamma_{n-2} - 2\Gamma_{n-3} + 2\Gamma_{n-1} + \ldots + \cosh \Gamma_1 e^{-\Gamma_1 + 2\Gamma_2 - 2\Gamma_3 + \ldots + 2\Gamma_{n-1}} \right]$$

for odd $n > 0$, and

$$\tilde{\bar{K}}_n = \lambda^n \theta(E_n^2 - \Delta^2)(4Q_n/R) \left[ \cosh \Gamma_{n-1} e^{-\Gamma_{n-1}} + \cosh \Gamma_{n-3} e^{-\Gamma_{n-3} + 2\Gamma_{n-2} - 2\Gamma_{n-1} + \ldots + \cosh \Gamma_1 e^{-\Gamma_1 + 2\Gamma_2 - 2\Gamma_3 + \ldots - 2\Gamma_{n-1}} \right]$$  \hspace{1cm} (8.7b)

for even $n > 0$.

The representation of Eqs. (8.6), (8.7) is exact. One can regard a general term of the series as an effective renormalized current of the $n$-th side band. In fact, this effective current
consists of the contributions of all side bands with odd indices smaller than \( n \). An important feature of this representation is the presence of the \( \theta \)-function in the general term, which allows us to separate out in Eq. (6.6) the part of the current which is obviously responsible for the SGS,

\[
I_{SGS} = \sum_{n=1}^{\infty} \frac{e}{\pi} \int_{\Delta}^{n e V - \Delta} dE \frac{E}{\xi} \tanh \frac{E}{2T} (\tilde{K}_n - \tilde{K}_n)
\]  

(8.8)

One might expect (cf. Ref. [55]) that Eq. (8.8) represents the subgap tunnel current at zero temperature and that the remaining part of the current of Eq. (6.6),

\[
I_r = I - I_{SGS} = \sum_{n=1}^{\infty} \frac{e}{\pi} \left[ \int_{n e V + \Delta}^{\infty} dE \frac{E}{\xi} \tanh \frac{E}{2T} (\tilde{K}_n - \tilde{K}_n) + \int_{\Delta}^{\infty} dE \frac{E}{\xi} \tanh \frac{E}{2T} (\tilde{K}_n - \tilde{K}_{n-1}) \right]
\]

(8.9)

corresponds to the current of thermal excitations. However, this separation is not exact: an analysis shows that the current in Eq. (8.9) does not vanish completely at \( T = 0 \), but contributes a small residual part. An important property of this residual current is that it does not contain any structureless component but demonstrates behaviour similar to the current \( I_{SGS} \) in Eq. (8.8), thus resulting in a small correction to Eq. (8.8).

IX. SUBHARMONIC GAP STRUCTURE.

The explicit analytical expressions (8.8) and (8.9) provide a basis for numerical calculation of the subgap current for small \( \lambda \) (low transparency) with any desirable accuracy. However, they are also convenient for qualitative discussion of the SGS. In this section we will analyze the SGS at zero temperature on the basis of Eq. (8.8).

The current-voltage characteristic \( I_{SGS}(V) \) in Eq. (8.8) has a complex form consisting of a sum of renormalized side band currents \( I_n(V, \lambda) \):

\[
I_{SGS}(V, \lambda) = \sum_{n=1}^{\infty} I_n(V, \lambda), \quad I_n(V, \lambda) = \frac{e}{\pi} \int_{\Delta}^{n e V - \Delta} dE \frac{E}{\xi} (\tilde{K}_n - \tilde{K}_n).
\]

(9.1)

The partial current-voltage characteristics \( I_n(V, \lambda) \) are similar to each other, and it is convenient to analyze them independently.
According to Eq. (9.1) the partial current $I_n$ starts with an onset at the threshold voltage $V_n = 2\Delta/en$. In the limit $\lambda \to 0$ the onset is infinitely sharp and the magnitude of the onset is

$$I_n(V_n, \lambda \to 0) = e\Delta D^n \frac{2n}{4^{2n-1}} \frac{n^{2n}}{(n!)^2}. \quad (9.2)$$

The jumps of the current at the thresholds result from the singular denominators in Eqs. (5.27), (5.29), related to the singular density of states at the side band energy gap edges, $\sinh \gamma_k = 0$. Accumulation of these singularities in the high order scattering amplitudes yields a tremendous increase of the partial currents well above the corresponding thresholds - this is what causes the failure of multiparticle tunneling theory [57–59]. In our theory, the singularities are regularized by the factors

$$P_n = \prod_{k=0}^{n} |Z_k|^2 \quad (9.3)$$

in the denominators of the scattering amplitudes Eq. (5.27). These factors are expressed through the continued fractions $Z_n$, Eq. (5.25), which therefore should be calculated with sufficient accuracy to preserve the singular parts of $Z_n$ which provide regularization of the integrals.

The first order current $I_1$ in Eq. (9.1) corresponds to direct one particle scattering to the side band $n = 1$, Fig 7a. The explicit form of the current $I_1$ is

$$I_1 = \frac{2e\lambda}{\pi R} \int_{\Delta}^{eV - \Delta} dE \frac{|E_1|}{\xi \xi_1} \left( \frac{E + \xi}{P_1} + \frac{E - \xi}{P_1} \right). \quad (9.4)$$

In the limit $\lambda \to 0$ this current coincides with the quasiparticle current of the tunnel Hamiltonian model [61,54]. At finite $\lambda$ the threshold onset of the current at $V = V_1$ is washed out. To evaluate the width of the onset we truncate the continued fraction in $P_1$ assuming $Z_{-1} = Z_2 = 1$, obtaining

$$P_1 \approx |(1 + \lambda a_0^- a_1^-)(1 + \lambda a_1^- a_2^-) + \lambda a_0^+ a_1^+|^2. \quad (9.5)$$

The function $\bar{P}_1$ has a similar form. The regularization effect of the threshold singularity is provided by the most singular term $\lambda a_0^1 a_1^+$ in Eq. (9.5). Keeping this term we obtain in the vicinity of the threshold, $e(V - V_1) \ll \Delta$, the following result
\[ I_1(V) = \frac{2e\Delta\lambda}{\pi R} f \left( \frac{eV - eV_1}{\Delta\lambda} \right), \quad f(z) = \int_0^\pi d\theta \frac{\sin^2 \theta}{(\sin \theta + 1/z)^2}. \] (9.6)

According to this formula the onset width is \( e(V - V_1) \sim \lambda \Delta. \)

The second order current \( I_2 \) corresponds to the creation of a real excitation during quasiparticle backscattering into the side band \( n = 2 \), Fig. 7b, and appears as the current of transmitted states of the side band \( n = 1 \) (cf. the excess current in Sec. VII). In the vicinity of the threshold, \( V_2 < V < V_1 \), this current exists only in the form of currents through the bound states and therefore it is completely converted into supercurrent far away from the junction. At larger voltages, \( V > V_1 \), the side band \( n = 1 \) extends outside the energy gap (see Fig. 8a), which also makes the current \( I_2 \) partially consist of contributions from extended states. The explicit expression for the second order current is

\[ I_2 = \frac{4e\Delta^3\lambda^2}{\pi R} \int_\Delta^{2eV-\Delta} dE \frac{|E_2|}{\xi_2\xi_1} \cosh \Gamma_1 \left( e^{-\gamma_0+\Gamma_1} P_2 + e^{\gamma_0-\Gamma_1} \frac{P_2}{\bar{P}_2} \right). \] (9.7)

Omitting the \( \lambda \)-dependence of \( P_2 \) in Eq. (9.7), one gets the two-particle tunnel current of Schrieffer and Wilkins [42,57]. To keep the singular terms in \( P_2 \) one has to truncate the continued fractions in Eq. (5.25) assuming \( Z-1 = Z_3 = 1 \), which yields

\[ P_2 \approx |(1 + \lambda a_{-1}^{-1})(1 + \lambda a_1^- a_2^-) + \lambda a_0^+ a_1^+(1 + \lambda a_2^+ a_3^-)|^2. \] (9.8)

The threshold singularity results from the small product \( \xi \xi_2 \) in denominator of Eq. (9.7). However, there are no singular terms in Eq. (9.8) proportional to \( a_0 a_2 \) among the terms linear in \( \lambda \). Such terms are quadratic in \( \lambda \) and they provide, along with the terms \( \lambda a_0 \) and \( \lambda a_2 \), the width of the onset: \( e(V - V_2) \sim \lambda^2 \Delta. \) This onset is sharper than the onset of the current \( I_1. \)

The threshold singularity in the current \( I_2 \) is typical for all higher order currents \( n > 1. \)

The appearance of the first side band outside the energy gap at \( V = V_1 \) is manifested through a spike in the current \( I_2. \) Indeed, if \( V \approx V_1 \), the nodes of \( \xi \) overlap the nodes of \( \xi \) and \( \xi_2 \) at the lower (\( E = \Delta \)) and at the upper (\( E = 3\Delta \)) limits of integration in Eq. (9.7) respectively (see Fig. 8a). This singularity yields an increase of the current \( I_2 \) when the
voltage approaches \( V_1 \),

\[
I_2 \sim e\Delta \lambda^2 \sqrt{\frac{\Delta}{e(V_1 - V)}}.
\]

Regularization of the integral, which is provided by the singular terms \( \lambda a_1 a_0 \) and \( \lambda a_1 a_2 \) in Eq. (9.8) at the lower the and upper integration limits respectively, yields

\[
\frac{I_2(V_1)}{I_2(V_2)} \sim \frac{1}{\sqrt{\lambda}}.
\]

Further analysis shows that maximal magnitude of the current is achieved slightly above \( V = V_1 \), after which the current rapidly decreases (see Fig. 9). At voltages \( V > V_1 \) the singular point \( \xi_1 = 0 \) remains within the integration region, which gives rise to enhancement of the magnitude of the current by a logarithmic factor in comparison with the current magnitude near the threshold \( V_2 \),

\[
I_2(V > V_1) \sim \frac{e\Delta \lambda^2 \ln \lambda}{R}.
\] (9.9)

At large voltage \( V \gg V_1 \) the current \( I_2 \) forms the excess current Eq. (7.10). It is interesting to note, that in this limit the logarithmic factor is compensated for by the current \( I_r \), Eq. (8.9) which yields the \( \lambda^2 \)-dependence of the excess current.

The third order current \( I_3 \) at voltages close to the threshold \( V_3 \) results from the combination of one-particle tunneling into the side band \( n = 3 \) and excitation of the transmitted Andreev bound states of the side band \( n = 1 \), Fig. 7c. The probabilities of these two processes are related as 1:2 at threshold, Eq. (8.7). Successive emergence of the bound states of the side bands \( n = 1 \) and \( n = 2 \) outside the energy gap at \( V = V_2 \) and \( V = V_1 \), Fig. 8b, gives rise to the current peaks. The current \( I_3 \) has the explicit form

\[
I_3 = \frac{2e\Delta^{3}\lambda^3}{\pi R} \int_{\Delta}^{3eV - \Delta} dE \frac{|E_3|}{\xi_3 |\xi_1 \xi_2|^2} \left[ \frac{e^{\gamma_0}(1 + 2 \cosh \Gamma_1 e^{-\Gamma_1 + 2 \Gamma_2})}{P_3} + \frac{e^{-\gamma_0}(1 + 2 \cosh \Gamma_1 e^{\Gamma_1 - 2 \Gamma_2})}{P_3} \right]
\] (9.10)

with the regularization factor

\[
P_3 \approx \left| (1 + \lambda a_{-1} a_0^-)(1 + \lambda a_1^- a_2^-) + \lambda a_0^+ a_1^+(1 + \lambda a_2^+ a_3^+) \right|^2.
\] (9.11)
The current peak at $V = V_2$ results from the overlap of nodes of $\xi$ and $\xi_2$ at $E = \Delta$ and nodes of $\xi_1$ and $\xi_3$ at $E = 2\Delta$, similarly to the peak of the current $I_2$. These singularities yield again an increase of the current inversely proportional to the square root of the departure from the voltage $V_2$: 

$$I_3 \sim e\Delta^{3/2}\lambda^3/\sqrt{e(V_2 - V)}.$$ 

However, since the factor $P_3$, Eq. (9.11), contains neither a term $\lambda a_0 a_2$ nor a term $\lambda a_1 a_3$, regularization of the singularity is provided, e.g. at $E = \Delta$, by the terms $\lambda a_0$ or $\lambda a_2$, which gives rise to a more pronounced peak with magnitude

$$\frac{I_3(V_2)}{I_3(V_3)} \sim \frac{1}{\lambda}.$$ \hspace{1cm} (9.12)

We note, that the magnitude of this peak is comparable with the magnitude of onset of the current $I_2$. The second peak at $V = V_1$ results from the overlap of nodes of $\xi_2$ and $\xi_3$ at $E = 3\Delta$; this gives rise to increase of the current $I_3$ near the voltage $V = V_1$ inversely proportional to the first power of the distance to this voltage: 

$$I_3 \sim \lambda^3\Delta^2/(V_1 - V).$$ 

The divergence is regularized by the term $\lambda a_2 a_3$ in Eq. (9.11) which results in a peak with magnitude

$$\frac{I_3(V_1)}{I_3(V_3)} \sim \frac{1}{\lambda}.$$ \hspace{1cm} (9.13)

Thus the heights of both peaks of the current $I_3$ are of the same order in $\lambda$, although the peak at $V \approx V_1$ is sharper.

In a similar way, all of the high-order currents result, in the vicinity of their thresholds, either from Andreev bound state currents (even $n$) or from a combination of Andreev bound state currents and the current of a single real excitation (odd $n$). The number of excited Andreev states is correspondingly $n/2$ or $(n-1)/2$. Singularities similar to the singularity of the current $I_3$ at the voltage $V \approx V_1$ exist in all high order currents, where they cause even more pronounced current peaks because of the absence of terms $\lambda a_k a_{k+1}$ in the corresponding smearing functions $P_n$. Due to this property, the magnitudes of such peaks exceed the threshold magnitude of the corresponding current by two orders of $\lambda$: $(I_n)_{\text{max}} \sim e\Delta\lambda^{n-2}/R$.

The above discussion reveals the current peaks to be essential features of the SGS of tunnel current in addition to the current onsets, Fig. 9 (these peaks are seen also in the
numerical results of Refs. [34,39]). It allows us to establish a general classification of singularities causing peaks in partial currents $I_n$. They result from the overlap of singularities of the side band density of states. It is easy to see that the singularities of only two side bands can overlap, the condition of the overlap for $m$-th and $k$-th side bands having the form

$$E - keV = \Delta, \quad E - meV = -\Delta.$$  

This condition is met at voltages $eV = 2\Delta/(m - k)$ for all integer $0 \leq k < m \leq n$. The magnitude of the current peaks depends on whether the overlapping side bands are neighbours or not, and whether the side band index is inside or at the edge of the interval $(0, n)$.

I. $m - k = 1, m = n$ or $k = 0$: edge-type singularity, neighbour side bands. This type of singularity forms the peak of the current $I_2$ at the main threshold $V_1$. The magnitude of the current peak is: $(I_2)_{\text{max}} \sim e\Delta\sqrt{\lambda}/R$.

II. $m - k > 1, m = n$ or $k = 0$: edge-type singularity, non-neighbour side bands. This type of singularity forms the first peak of each current $I_n, n > 2$ at voltage $V_{n-1}$. The magnitude of the current peak is: $(I_n)_{\text{max}} \sim e\Delta\lambda^{n-1}/R$.

III. $m - k = 1, m < n, k > 0$: internal singularity, neighbour side bands. This type of singularity forms the last peak of each current $I_n, n > 2$ at voltage $V_1$. The magnitude of the current peak is: $(I_n)_{\text{max}} \sim e\Delta\lambda^{n-1}/R$.

IV. $m - k > 1, m < n, k > 0$: internal singularity, non-neighbour side bands. This type of singularity forms all intermediate peaks of each current $I_n, n > 3$. The magnitude of the current peaks are: $(I_n)_{\text{max}} \sim e\Delta\lambda^{n-2}/R$.

**X. CONCLUSION**

In this paper we have considered superconductive tunneling as a scattering problem within the framework of Bogoliubov-de Gennes (BdG) quantum mechanics. An essential aspect of this problem is that the scatterer consists not only of the potential of the tunnel
barrier but also of the discontinuity of the phase of the order parameter. In equilibrium (zero bias, dc Josephson current) the scattering problem is elastic. The peculiar feature of the elastic scattering problem in short junctions, considered here, is that the balance of currents of the scattering modes is not violated: the supercurrent flows only through the superconducting bound states (for a more general discussion, see [48]). In the presence of voltage bias the scattering is inelastic due to the time dependence of the component of the scatterer related to the superconducting phase difference. Generally, the currents of all inelastic channels constitute together the components of the tunnel current flowing through the biased junction: the quasiparticle current corresponds to the incoherent part of the inelastic side band contributions, and the ac Josephson current corresponds to the interference of the side band contributions.

There are three distinct components of the quasiparticle tunnel current at zero temperature: (i) the current of quasiparticles excited above the ground state, (ii) the current through Andreev bound states converted to supercurrent outside the junction, and (iii) the imbalance current of the ground state modes. At large bias voltage, $eV \gg 2\Delta$, the first component corresponds to the single particle current of the normal junction, while the other components cause excess current. When voltage is decreased, redistribution of current among the components gives rise to subharmonic gap structure (SGS) in the form of current onsets and current peaks. Within the voltage intervals $2\Delta/n < eV < 2\Delta/(n-1)$ with even $n$, the tunnel current entirely consists of currents through the Andreev bound states [component (ii); e.g. Fig. 7b], the states of all side bands with odd indices smaller than $n$ contributing to the current. If $n$ is odd, a real excitation current of the side band $n$ [component (i); e.g. Fig. 7a,c] is also present in the tunnel current. Opening of new channels of tunneling of real excitations gives rise to current structures. Thus, SGS reveals the discrete nature of the side band spectrum. The structure is the more pronounced the smaller is the transparency of the junction.

Since each Andreev state provides transfer of one Cooper pair through the junction for every incident quasiparticle, $n$ particles will tunnel in the interval $2\Delta/n < eV < 2\Delta/(n-1)$. 
One may be surprised by the participation of a large number of bound Andreev states in current transport at low voltages: this appears to contradict the fact that subgap current diminishes at zero bias. After all, the probability of the scattering into side bands does not depend on the bias and is proportional to powers of $D$. The solution to this paradox results from increasing compensation of currents between the normal and Andreev channels in each side band with decreasing voltage, which gives the required voltage dependence of the total current.

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APPENDIX A: BOUNDARY CONDITIONS

The quasiclassical boundary condition in Eqs. (2.8), (2.9) has been derived in Ref. [31] using the method of Ref. [21]. Here we present simple arguments which lead to this boundary condition. We consider the more general case of asymmetric junction, using an asymmetric version of the Hamiltonian of Eq. (2.2) with the same restriction on the length of the non-superconducting region: $L \ll \xi_0$. We include a contact potential difference into the potential $U(x)$ which implies that this potential may have non-vanishing asymptotic values at infinity: $U(-\infty) \neq U(\infty) \neq 0$. If the junction has more than one transverse transport mode we assume that these modes are not mixed.

A one-dimensional quasiclassical wave function of a given transverse channel in the right electrode has the form [Eq. (2.6)],

$$\Psi_R(x, t) = \sum_{\beta} \frac{1}{\sqrt{v_R}} e^{i\beta} \int p_R dx e^{i\sigma x_R/2} \psi_R^\beta(x, t),$$  \hspace{1cm} (A1)
with similar expression for the left electrode. $\psi^β_R$ are slowly varying two-component wave functions on the scale of $1/p_R$, where $p_R(x) = \sqrt{2m_R(\mu - U_R - E_{\perp R}(x))}$. This equation is valid over the distance $x \gg 1/p_R$ from the junction, and in the spatial region $1/p_R \ll x \ll \xi_0$ the functions $\psi^β_R$ are almost constant.

From another point of view, at large distance from the junction, $|x| \gg 1/p_{R,L}$, the function $\Psi$ can be expressed in the form of a linear combination of the scattering states at the Fermi level,

$$\Psi = C_1\chi_1 + C_2\chi_2 \quad \text{(A2)}$$

$$\chi_1 = \begin{cases} 
(1/\sqrt{v_L})[e^{ip_l x} + r e^{-ip_l x}], & x < 0 \\
(1/\sqrt{v_R}) d e^{ip_R x}, & x > 0,
\end{cases} \quad \text{(A3a)}$$

$$\chi_2 = \begin{cases} 
(1/\sqrt{v_R})[e^{-ip_l x} + \tilde{r} e^{ip_R x}], & x > 0 \\
(1/\sqrt{v_L}) \tilde{d} e^{-ip_l x}, & x < 0.
\end{cases} \quad \text{(A3b)}$$

Comparing Eqs. (A2), (A3) with Eq. (A1) in the region $1/p_F \ll |x| \ll \xi_0$ we have

$$C_1 = e^{i\sigma_x \chi L/2}\psi_L^+ \quad \text{and} \quad C_2 = e^{i\sigma_x \chi R/2}\psi_R^-,$$

$$r C_1 + \tilde{d} C_2 = e^{i\sigma_x \chi L/2}\psi_L^-,$$

$$d C_1 + \tilde{r} C_2 = e^{i\sigma_x \chi R/2}\psi_R^+,$$

which yields the boundary condition

$$\begin{pmatrix} \psi^- \\
\psi^+
\end{pmatrix} = \hat{V} \begin{pmatrix} \psi^+ \\
\psi^-
\end{pmatrix}, \quad \text{(A5)}$$

with the matching matrix

$$\hat{V} = \begin{pmatrix} r & \tilde{d} e^{i\sigma_x \phi/2} \\
\tilde{d} e^{-i\sigma_x \phi/2} & \tilde{r}
\end{pmatrix}, \quad \text{(A6)}$$

where $\phi = \chi_R(0) - \chi_L(0)$. The matrix $\hat{V}$ satisfies the unitarity condition $\hat{V}\hat{V}^\dagger = 1$, provided by the relations among the normal electron scattering amplitudes in Eq. (A3):

$$\tilde{r} = -\tilde{d}(r/d)^*, \quad |d|^2 = |\tilde{d}|^2 = D, \quad |r|^2 = |\tilde{r}|^2 = R = 1 - D.$$
Equation (4.10) for the current of a single bound state can be derived directly from the Bogoliubov-de Gennes equation Eq. (2.5), (2.2). The derivation is valid for junctions with an arbitrary non-superconducting region between superconducting electrodes. We assume for simplicity that the phase of the order parameter, Eq. (2.3), in the electrodes is constant and equal to $\pm \phi/2$ in the right and left electrodes respectively. Let $\Psi(\vec{r}, E)$ to be a normalized wave function of the Andreev bound state with energy $E$,

$$\hat{H}\Psi - E\Psi = 0, \quad \Psi(x = \pm \infty) = 0. \quad (B1)$$

The energy and the wave function of the bound state depend on the phase difference $\phi$. Taking the derivative with respect to $\phi$ of Eq. (B1) and considering a scalar product of the resulting equation with the function $\Psi$, we have

$$\int d^3r (\Psi, \frac{d}{d\phi}(\hat{H} - E)\Psi) = 0, \quad (B2)$$

where the brackets denote a scalar product in electron-hole space, similar to Eq. (3.8). In this equation the derivative of the Hamiltonian has the form

$$\frac{d\hat{H}}{d\phi} = \frac{d\hat{\Delta}}{d\phi} = \frac{i\text{sign}x}{2}\sigma_z\hat{\Delta}, \quad (B3)$$

in accordance with Eqs. (2.2), (2.3). Substituting relation (B3) into Eq. (B2) and taking into account that the function $\Psi$ is normalized, we get

$$\frac{dE}{d\phi} = \int d^3r (\Psi, \frac{d\hat{\Delta}}{d\phi}\Psi). \quad (B4)$$

The continuity equation for the charge current,

$$I(x, E) = \frac{e}{2m}(\hat{p}_x - \hat{p}'_x) \int d^2r_\perp (\Psi(x'), \Psi(x))_{x=x'}, \quad (B5)$$

in accordance with Eq. (B1) has the form

$$i\frac{d}{dx}I(x, E) = e \int d^2r_\perp (\Psi(x), [\sigma_z, \hat{\Delta}]\Psi(x)). \quad (B6)$$
Substituting relation (B3) into Eq. (B6) and performing integration of this equation over the whole $x$ axis we get

$$I(0, E) = 2e \int d^3r \langle \Psi, \frac{d\Delta}{d\phi} \Psi \rangle.$$  \hspace{1cm} (B7)

In equation (B7) the current at infinity drops out because of decay of the bound state wave function, $I(\pm \infty) = 0$. The magnitude $I(0)$ is formally taken in the middle of the junction; however, the current has the same magnitude along the whole non-superconducting region according to the conservation equation (B6). Comparison of Eqs. (B4) and (B7) finally yields

$$I(E) = 2e \frac{dE}{d\phi}.$$  \hspace{1cm} (B8)
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FIGURES

FIG. 1. SIS tunnel constriction.

FIG. 2. Quasiparticle spectrum and position of the incoming states: 1(3) - hole (electron)-like quasiparticle incident from left; 2(4) - hole (electron)-like quasiparticle incident from right.

FIG. 3. Spatial configuration of the edges of the superconducting energy bands in a long constriction: \( E_{\text{min}}, E_{\text{max}} = \pm \Delta + p_s(x)v \). A potential well appears in upper (lower) band for electrons moving in a direction opposite to (along) the supercurrent.

FIG. 4. Scattering diagram of voltage biased superconducting tunnel junctions. Solid (dotted) arrows indicate scattering in the normal (Andreev) channel. Filled triangles indicate superconducting bound states. Transmission (reflection) occurs into side bands with odd (even) indices.

FIG. 5. Scattering diagrams of voltage biased normal tunnel junctions. a) scattering of normal holes with spectrum \( E_h = \mu - (p^2/2m) \); represents an elementary fragment of the diagram in Fig. 4 for \( j = 1 \). b) scattering of the normal electrons with spectrum \( E_e = p^2/2m \). c) conventional diagram of elastic electron scattering in biased tunnel junctions; the local chemical potentials in the electrodes are then shifted by \( eV \).

FIG. 6. Three kinds of processes contributing to the tunnel current at large bias \( eV \gg \Delta \): a) creation of a real excitation across the gap by forward scattering; b) excitation of the Andreev bound state due to creation of a real excitation via backward scattering (dashed arrow); c) imbalance of ground state modes due to creation of a real excitation via backward scattering. Excess current is caused by processes b) and c).
FIG. 7. Scattering processes contributing to the subgap current. a) single particle scattering into side band \( n = 1 \) gives the main contribution at \( eV > 2\Delta \). b) excitation of the Andreev bound state \( (n = 1) \) due to backward scattering into side band \( n = 2 \) gives the main contribution at \( eV > \Delta \). c) single particle scattering into side band \( n = 3 \) and simultaneous excitation of the Andreev bound state in side band \( n = 1 \) gives the main contribution at \( eV > 2\Delta/3 \).

FIG. 8. a) Density of states \( \nu(E) = |E_n/\xi_n| \) of the side bands \( E_0, E_1, E_2 \) at applied voltage \( V > V_1 \) (right), position of singularities of side band density of states as function of applied voltage for current \( I_2 \) (left), \( 1^\pm : E_1 = \pm\Delta, 2^- : E_2 = -\Delta \). b) Density of states of the side bands \( E_0, E_1, E_2, E_3 \) at applied voltage \( V_2 < V < V_1 \) (right), position of singularities of side band density of states as function of applied voltage for current \( I_3 \) (left), \( 1^\pm : E_1 = \pm\Delta, 2^\pm : E_2 = \pm\Delta, 3^- : E_3 = -\Delta \).

FIG. 9. Schematic picture of partial \( I_n - V \) characteristics.