Circuit theory of unconventional superconductor junctions

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We extend the circuit theory of superconductivity to cover transport and proximity effect in mesoscopic systems that contain unconventional superconductor junctions. The approach fully accounts for zero-energy Andreev bound states forming at the surface of unconventional superconductors. As a simple application, we investigate the transport properties of a diffusive normal metal in series with a $d$-wave superconductor junction. We reveal the competition between the formation of Andreev bound states and proximity effect, that depends on the crystal orientation of the junction interface.

In the last decade the mesoscopic superconducting systems have been the subject of intensive experimental and theoretical research. The transport in these system is essentially contributed by the so-called Andreev reflection\textsuperscript{[1]}, a unique process specific for normal metal/superconductor interface. Each electron reflected from the interface may transfer a charge 2e to the superconductor\textsuperscript{[2]}\textsuperscript{[3]}\textsuperscript{[4]}. The phase coherence between incoming electrons and Andreev reflected holes persists in the normal metal at mesoscopic length scale. This results in strong interference effects on Andreev reflection rate.\textsuperscript{[1]}

The transport properties of mesoscopic $N/S$ junctions have been theoretically investigated with various approaches, \textit{e.g.}, traditional nonequilibrium superconductivity approach\textsuperscript{[1]}, tunneling Hamiltonian approach\textsuperscript{[1]}, scattering formalism\textsuperscript{[1]} and computer simulation\textsuperscript{[1]}.\textsuperscript{[12]}

One of the authors has proposed a generic circuit theory of non-equilibrium superconductivity which accounts for the effects abovementioned. The mesoscopic system is presented as a network of nodes and connectors. A connector is characterized by a set of transmission coefficients and can present anything from ballistic point contact to tunnel junction. Full isotropization of electrons is assumed in the nodes. This approach considerably simplifies a practical transport calculation, numerical as well as analytical. The circuit theory is based on conservation laws for so-called spectral currents. These additional conservation laws present interference of electrons and holes. The spectral currents through each connector are functions of spectral vectors in the nodes. There is one-to-one correspondence between spectral vectors and and Keldysh Green functions in the underlying microscopic approach.\textsuperscript{[1]} Kirchoff-type equations determine spectral currents and vectors in each node and connector, and, consequently, electric current in the circuit.

Unconventional superconductors bring about very unusual interface physics. The transport through the interface is influenced by formation of Andreev bound states (ABS) at this interface.\textsuperscript{[1]}\textsuperscript{[1]}\textsuperscript{[12]}. Those result from the interference of injected and reflected quasiparticles. The ABS manifest themselves as a zero-bias peak in tunneling conductance (ZBCP)\textsuperscript{[1]}\textsuperscript{[1]}. Indeed, ZBCP has been reported in various superconductors that have anisotropic pairing symmetry.\textsuperscript{[1]} The proper theory of transport in the presence of ABS has been formulated\textsuperscript{[1]}\textsuperscript{[1]} for conditions of ballistic transport only. This theory has to be revisited to account for diffusive transport in the normal metal. The point is that the diffusive transport provides an Andreev reflection mechanism for ZBCP which does not involve any unconventional superconductivity. This mechanism may compete with the formation of ABS. The anomalous size dependence of transport in YBCO junctions reported in recent experiment\textsuperscript{[13]} seems to arise from this competition.

All this has motivated us to extend the circuit theory to the systems containing unconventional superconductor junctions. We stress that this extension is by no means straightforward. The circuit theory can not be directly applied to an unconventional superconductor since it requires the isotropization. The latter is just incompatible with mere existence of unconventional superconductivity. Fortunately, there is a way around. We concentrate on the matrix currents via the unconventional superconductor junction to/from diffusive parts of the system. If one knows the relation between these currents and the spectral vectors (isotropic Green functions) in the diffusive part, one is able to use Kirchoff rules to complete the evaluation of the matrix currents everywhere in the system.

This relation shall be derived from microscopic theory and presents the main result of this work. We stress that applicability of this relation is not restricted to circuit theory. One can regard our result as a boundary condition for the traditional Keldysh-Usadel equations of non-equilibrium superconductivity.\textsuperscript{[1]} As an immediate application, we study a $d$-wave superconductor junction in series with normal metal. The resistance of the system appears to depend strongly on the angle $\alpha$ be-
between the normal to the interface and the rote direction of \(d\)-wave superconductor (misorientation angle). This reveals the competition between the effect of ABS and proximity-induced reflectionless tunneling.

To derive the relation between matrix current and Green functions, we make use of the method proposed in \(\text{[3]}\). The method puts the older ideas \(\text{[3]}\) to the framework of Landauer-Büttiker scattering formalism. One expresses the matrix current in a constrictor in terms of one-dimensional Green functions \(\tilde{G}_{n,n',\sigma;\sigma'}(x,x')\), where \(n,n'\) and \(\sigma,\sigma'\) denote the indices of transport channels and the direction of motion along \(x\) axis, respectively. The "check" represents the Keldysh-Nambu structure. These Green functions are to be expressed in terms of the transfer matrix that incorporates all information about the scattering, and asymptotic Green functions \(\tilde{G}_{1,2}\) presenting boundary conditions deep in each side of the constriction. The isotropization assumption requires that these \(\tilde{G}\) do not depend on channel number. Under this assumption, the current is universal depending on transmission eigenvalues only. Although the isotropization assumption is good for conventional superconductors and normal metals, it fails to grasp the physics of unconventional superconductor where the Green function essentially depends on the direction of motion and thus on channel number. To avoid this difficulty, we restrict the discussion to a conventional model of smooth interface, assuming momentum conservation in the plane of the interface. Within the model, the channel number eventually numbers possible values of this in-plane momentum and the transfer matrix becomes block-diagonal in the channel index. We thus solve Green functions \(\tilde{G}_{n,n',\sigma;\sigma'}(x,x')\) separately for each channel. Asymptotic Green function in the unconventional superconductor does depend on the direction of motion \(\sigma\),

\[
\tilde{G}_2;n,\sigma;n,\sigma = \tilde{G}_{2+}^{(n)} \frac{1 - \sigma}{2} + \tilde{G}_{2-}^{(n)} \frac{1 + \sigma}{2}
\]

reflecting different asymptotic conditions for incoming \((\tilde{G}_{2+}^{(n)})\) and outgoing \((\tilde{G}_{2-}^{(n)})\) wave in each channel. The asymptotic Green function \(\tilde{G}_1\) in normal metal is the same for both waves and all channels (see Fig. 1). All these matrices satisfy unitary relation \((\tilde{G}_{2+}^{(n)})^2 = \tilde{G}_2^2 = 1\).

After some algebra we obtain the matrix current in the following form

\[
\tilde{I} = \frac{4e^2}{h} \sum_m [\tilde{G}_1, \tilde{B}_m],
\]

\[
\tilde{B}_m = \{ -\Xi_m [\tilde{G}_1, \tilde{H}_{-}^{(m)-1}] + \tilde{H}_{-}^{(m)} \tilde{H}_{+}^{(m)} - \Xi_m^2 \tilde{G}_1 \tilde{H}_{-}^{(m)-1} \tilde{H}_{+}^{(m)} \tilde{G}_1 \}^{-1}
\]

\[
\times [\Xi_m (1 - \tilde{H}_{-}^{(m)-1}) + \Xi_m^2 \tilde{G}_1 \tilde{H}_{-}^{(m)-1} \tilde{H}_{+}^{(m)}],
\]

\[
\tilde{H}_{\pm}^{(m)} = (\tilde{G}_{2+}^{(m)} \pm \tilde{G}_{2-}^{(m)}) / 2.
\]

Here \(\Xi_m \equiv T_m/(1 + \sqrt{1 - T_m})\) is related to the transmission coefficient \(T_m\) in a given channel \(m\). The above relation reduces to isotropic result of Ref. \(\text{[3]}\) provided \(\tilde{G}_{2+}^{(n)} = \tilde{G}_{2-}^{(n)} = \tilde{G}_2\). The above \(4 \times 4\) matrix relation is the main result of the present work. It incorporates the most general situation and allows for many applications that involve unconventional superconductors. Below we provide a simple but extensive application example that both illustrates circuit theory method and demonstrates an interesting interplay of ABS and proximity effect.

The circuit is the one given in Fig. 1: diffusive conductor of resistance \(R_D\) in series with unconventional superconductor junction. We disregard decoherence between electrons and holes in the diffusive conductor, ("leakage" current in terms of Ref.\(\text{[3]}\)), this is justified at energies not exceeding Thouless piece of normal metal. We restrict our attention to \(d\)-wave superconductor, being the most practical example of the singlet unconventional superconductor that preserves time reversal symmetry. For simplicity, we have in mind a "two-dimensional" superconductor made from the layers stacked in \(z\)-direction. \(z\)-axis lies in the plane of the interface and is normal to the plane of Fig. 1. The interface normal \((x\)-axis) makes an angle \(\alpha\) with the main crystal axis. The propagation directions of the waves are thus in \(xy\)-plane and are parameterized by the angle \(\theta\) with \(x\)-axis. The angular dependence of the superconducting order parameter is thus given by \(\Delta(\theta) = \Delta_0 \cos(2(\theta - \alpha))\). A scattering channel consists of an incoming wave in direction \(\pi - \theta\) and outgoing wave in the direction \(\theta\). The sums over channels can be reduced to integrals over \(\theta\):

\[
\sum_m \propto \int_{-\pi/2}^{\pi/2} d\theta \cos \theta \quad (3)
\]

The Green functions are fixed in "US" terminal and in "N" terminal, the voltage \(V\) is applied to "N" terminal. The Green function in the node "DN", \(\tilde{G}_1\) is not fixed and shall be determined from the balance of the matrix currents. There is a natural separation of balance equations for \(2 \times 2\) spectral currents that set advanced or retarded part of \(\tilde{G}_1\) and for particle current at a given energy that set the distribution function in the node "DN\).

We address the balance of the spectral currents first. The advanced \(2 \times 2\) Green functions are fixed in "N" and "US" terminals and read \(\tilde{G}_N = \tau_x\), \(\tilde{G}_{2\pm} = (\Delta_\pm \tau_x - i\epsilon \tau_z)/\sqrt{\Delta_\pm^2 - \epsilon^2}\), \(\tau\) being Pauli matrices, \(\Delta_\pm = \Delta_0 \cos(2(\theta \pm \alpha))\) being superconducting order parameters that correspond to direction of incoming(outgoing) wave. This suggests that the corresponding Green function in the "DN" node assumes a form \(\sin \gamma \cdot \tau_x + \cos \gamma \cdot \tau_z\) where \(\gamma\) is yet to be determined. \(\gamma\) is the measure of proximity effect. All spectral currents are proportional to \(\tau_y\). The spectral current \(i_D^{(s)}\) through diffusive conductor is
Here is a compact form. These expressions are essentially different for \( \Delta^+ \) and \( \Delta^- \) concrete expressions for \( 0 \), this manifesting the formation of ABS in the latter case. The full resistance of the diffusive metal and the interface resistance is determined from Eq. 2. This yields

\[
\begin{align*}
\dot{i}_{B}^{(s)} + \dot{i}_{D}^{(s)} &= 0 \tag{4} \\
\dot{i}_{B}^{(p)} + \dot{i}_{D}^{(p)} &= 0 \tag{5}
\end{align*}
\]

Under conditions considered, the transport is determined by energy-symmetric distribution function, that is conventionally called \( f_j \). The balance of particle currents at each energy determines this distribution function in "DN" node. We will assume that the temperature \( 1/\beta \) is much smaller than the typical value of superconducting energy gap, so we can disregard quasiparticle excitations in the superconductor. The particle current through diffusive conductor is given by the drop of the distribution function at its ends, the particle current via the interface is given by the corresponding block of Eq. 2. This yields

\[
\begin{align*}
\dot{i}_{B}^{(p)} &= f_t \frac{2e^2}{h} \sum_m T^* (\gamma, \epsilon, T_m), \quad \dot{i}_{D}^{(p)} = (f_t - f_0)/R_D
\end{align*}
\]

with \( f_0 \) being the symmetrized distribution function in the normal reservoir, \( f_0 = \frac{1}{2} [\tanh(\beta(\epsilon + eV)/2) - \tanh(\beta(\epsilon - eV)/2)] \). The above relation becomes especially transparent if one regards \( T^* \) as effective transmission coefficients in each channel. It just shows that the full (energy-dependent) resistance of the system is the sum of the resistance of diffusive metal and the interface resistance, the latter being influenced by proximity effect.

The degree of proximity effect is determined from Eq. 4. If we define the average over the angle as

\[
\langle A(\theta) \rangle = \frac{1}{\pi} \int_{-\pi/2}^{\pi/2} d\theta \cos \theta A(\theta)/\int_{-\pi/2}^{\pi/2} d\theta T(\theta) \cos \theta
\]

with \( T(\theta) = T_m \), both balance equations can be rewritten in a compact form.

\[
\begin{align*}
R &= R_D + R_B / < T^*(\gamma, \epsilon, T_m) >, \tag{6} \\
\gamma &= < F(\gamma, \epsilon, T_m) > R_D / R_B. \tag{7}
\end{align*}
\]

Here \( R_B \) is the interface resistance in normal state, \( R \) is the full resistance. It may depend on energy, so that the full electric current is given by \( I_{el} = \int d\epsilon f_0(\epsilon)/R \).

To reveal the underlying physics, we present the concrete expressions for \( F = < F(\gamma, \epsilon, T_m) > \) and \( T^* = T^*(\gamma, \epsilon, T_m) \) assuming \( | \epsilon | \ll | \Delta_{\pm} | \). It turns out that these expressions are essentially different for \( \Delta^+ \), \( \Delta^- \) > 0, this manifesting the formation of ABS in the latter case. For \( \Delta^+ \), \( \Delta^- \) < 0 (ABS channels) we have:

\[
\begin{align*}
F &= \frac{-2T_m \sin \gamma}{T_m \cos \gamma - i(2 - T_m)\epsilon/\Delta} = \epsilon \rightarrow 0 \rightarrow -2 \tan \gamma \tag{8} \\
T^* &= \frac{T_m^2 (1 + \cos \gamma)^2 + | \sin \gamma |^2}{T_m^2 \cos^2 \gamma + (2 - T_m)2(\epsilon/\Delta)^2} = \epsilon \rightarrow 0 \rightarrow \frac{2}{\cos^2 \gamma} \tag{9}
\end{align*}
\]

with \( \tilde{\Delta} = (2 | \Delta_+ || \Delta_- |)/(| \Delta_+ | + | \Delta_- |) \). It is somewhat counterintuitively that the zero-energy limit does not depend on the actual transmission, giving finite currents even for insulating interfaces. This is the signature of the resonance forming precisely at zero energy [11].

If the transmission is low, the resonance feature persists in a narrow energy interval \( T_m \Delta_{\pm} \) only. The spectral current \( F \) eventually suppresses the proximity effect. \( F \) is given by the corresponding block of Eq. 2. This yields

\[
\begin{align*}
\dot{i}_{B}^{(p)} &= f_t \frac{2e^2}{h} \sum_m T^* (\gamma, \epsilon, T_m), \quad \dot{i}_{D}^{(p)} = (f_t - f_0)/R_D
\end{align*}
\]

The effective transmission coefficient \( T^* \) at resonance is always bigger than 2, and is enhanced by proximity effect. One can understand this as a multiple Andreev reflection induced by the corresponding ABS.

In the case of \( \Delta^+, \Delta^- > 0 \) ("conventional" channels) the resonance feature is absent and energy dependence can be safely disregarded. The expressions are identical to those of conventional superconductor

\[
\begin{align*}
F &= \frac{2T_m s \cos \gamma}{2 - T_m + T_m \sin \gamma} \tag{10} \\
T^* &= \frac{2T_m [T_m + (2 - T_m) \sin \gamma]}{2 - T_m + T_m \sin \gamma} \tag{11}
\end{align*}
\]

Here \( s \equiv \text{sgn}(\Delta_+) = \text{sgn}(\Delta_-) \). The spectral current \( F \) thus induces proximity effect of the corresponding sign \( s \). The effective transmission \( T^* \) does not exceed 2 (which is the limiting case of ideal Andreev reflection). Being compared with the transmission in the normal state, the effective transmission is suppressed (enhanced) at \( T_m < (>)/3 \). The fully developed proximity effect \( (\gamma = \pi/2) \) restores the normal transmission.

To summarize, the proximity effect originates from the "conventional" channels and is suppressed by ABS channels. While the proximity effect is present, it enhances transmission via ABS channels. It restores the effective transmission of "conventional" channels to that in the normal state. The full resistance of the structure is determined by competition of all these effects. It is essential that one can tune the relative number of "conventional" and ABS channels by changing the misorientation angle \( \alpha \). As one can see from the Fig.1, the ABS channels are there in the angle interval \( \pi/4 - | \alpha | < | \theta | < \pi/4 + | \alpha | \). If \( \alpha = 0 \), there are no such channels. If \( \alpha = \pi/4 \), there are no "conventional" channels. This gives no chance to proximity effect.

To illustrate this further, we calculate with Eqs. (3, 5) the zero-voltage resistance \( (\epsilon \rightarrow 0) \) at different values of \( \alpha \) as a function of \( R_B/R_D \). The angular dependence of the transmission coefficient was assumed to be \( T(\theta) = \cos^2 \theta/(\cos^2 \theta + Z) \) with barrier parameter \( Z \). The results are presented in Figs. 2, 3. At \( R_B = 0 \) there is no proximity effect in "DN" and the resistances are given by the quasi-ballistic formulas of Ref. [11]. The proximity effect may develop with increasing \( R_D \) and decreases the
Although this becomes exact only at the proximity effect very efficiently at transmission in ABS channels. The ABS channels quench low its normal state value. This manifests the enhanced demonstration interface conductance reduced slightly being Ref. [15], we regard the counterintuitive negative sign of (dR/dR_D)_R_D=0 as a signal of importance of the proximity effect [or reflectionless tunneling (RLT)]. We evaluate this sign at different Z and α. (Fig. 3) The sign of dR/dR_D is negative for junctions of low transmissivity in a relatively narrow range of α.

In conclusion, we have extended the circuit theory of superconductivity to include unconventional superconductor junctions. We have derived a general relation for matrix current to/from unconventional superconductor. An elaborated example demonstrates the interplay of ABS and proximity effect in a d-wave junction. The theory presented will facilitate the analysis of more complicated mesoscopic systems that include unconventional superconductors.

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