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Quasiclassical Theory of Spin Imbalance in a Normal Metal-Superconductor Heterostructure with a Spin-Active Interface

O Shevtsov and T Löfwander

Department of Microtechnology and Nanoscience – MC2, Chalmers University of Technology, SE-412 96 Göteborg, Sweden

E-mail: `shevtsov@chalmers.se, tomas.lofwander@chalmers.se`

Abstract. Non-equilibrium phenomena in superconductors have attracted much attention since the first experiments on charge imbalance in the early 1970's. Nowadays a new promising line of research lies at an intersection between superconductivity and spintronics. Here we develop a quasiclassical theory of a single junction between a normal metal and a superconductor with a spin-active interface at finite bias voltages. Due to spin-mixing and spin-filtering effects of the interface a non-equilibrium magnetization (or spin imbalance) is induced at the superconducting side of the junction, which relaxes to zero in the bulk. A peculiar feature of the system is the presence of interface-induced Andreev bound states, which influence the magnitude and the decay length of spin imbalance. Recent experiments on spin and charge density separation in superconducting wires required external magnetic field for observing a spin signal via non-local measurements. Here, we propose an alternative way to observe spin imbalance without applying magnetic field.

1. Introduction

Studying non-equilibrium phenomena in mesoscopic systems is a challenging yet important task as it paves a way towards microscopic understanding of the underlying physical processes. In particular, non-equilibrium effects in superconducting hybrid structures have been an active direction of research since the pioneering experiments on charge imbalance by Clarke et al. [1]. They observed a voltage drop in the superconductor (S) close to the interface with a normal metal (N) subject to finite bias voltage. Theoretical picture proposed to explain this effect [2] was based on imbalance between the number of electron-like and hole-like quasi-particles in the superconductor when the bias was higher than the superconducting gap. This non-equilibrium quasi-particle distribution has to relax as we move towards the bulk of the superconductor, and it was shown [3] that any pair-breaking mechanism can be responsible for this.

An obvious extension of the previous effect is a situation when there is an imbalance between quasi-particles with opposite spin-projections, which can be achieved by using a ferromagnet (F) as an injector, or applying an external magnetic field. It would create an induced magnetization in the superconductor which relaxes away from the interface, or so-called spin imbalance. In recent experiments [4–6] this possibility has been investigated via non-local transport measurements in N-S-F and F-S-F structures. It is important to emphasize that for all the experiments it was necessary to apply an external magnetic field in order to see

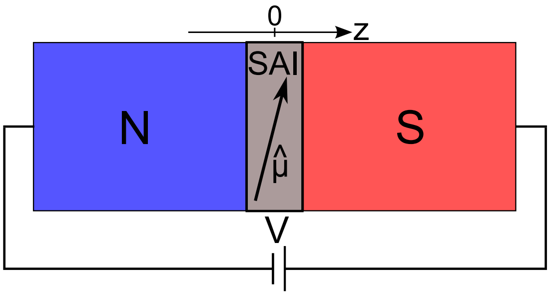

Figure 1. (Color online) Cartoon of the setup: normal metal (N) - superconductor (S) junction with a spin-active interface (SAI) characterized by an intrinsic magnetic moment directed along $\hat{\mu}$. Finite bias V is applied across the junction.

a significant spin imbalance signal. In our work we focus on a system consisting of a normal metal (N) connected to a superconductor (S) via a spin-active interface[1] (SAI) [8, and references therein], see Fig. 1. The system is kept under finite bias voltage V. One can imagine the spin-active interface as a magnetic barrier, which has different transparencies for quasi-particles with opposite spins and is able to rotate the spin of a quasi-particle via Larmor precession around its magnetic moment. Such an interface can host a pair of in-gap spin-polarized Andreev bound states, which has been observed in recent experiments [9]. We use quasiclassical Green's function method [10, 11, and references therein] to calculate the induced magnetization profile in the superconductor. It turns out that it is possible to observe significant spin imbalance signal in this system without applying external magnetic field for voltages below the superconducting gap due to presence of the bound states. Moreover the properties of the observed signal can be tuned by the parameters of the interface. For the reader interested in the physics of the processes responsible for such behavior we refer to Ref. [8]. In this paper we explain some details of calculations left out from Ref. [8]. In Sec. 2, we briefly describe the general theoretical framework we use. In Sec. 3, we describe the theoretical model of our system. In Sec. 4 we demonstrate the self-consistent procedure for calculating bulk superconducting properties in presence of magnetic and scalar impurities. Sec. 5 concludes the paper.

2. Methods

All the relevant information necessary to describe our system is contained in the quasiclassical Green's function $\check{g}(\epsilon, \mathbf{p}_{\mathrm{F}}, \mathbf{r}, t)$. Here ϵ is the quasi-particle energy, $\mathbf{p}_{\mathrm{F}}$ is the quasi-particle momentum on the Fermi surface, $\mathbf{r}$ is the spatial coordinate, and t is the time. This function satisfies the quasiclassical Eilenberger equation,

$$[\epsilon\hat{\tau}_3\check{1} - \check{h}, \check{g}]_{\otimes} + i\hbar\mathbf{v}_{\mathrm{F}} \cdot \boldsymbol{\nabla}\check{g} = \check{0}, \tag{1}$$

accompanied by the normalization condition[2] $\check{g} \otimes \check{g} = -\pi^2\check{1}$. Here and below we will suppress function arguments for brevity. Note that $\check{g}$ and the self-energy $\check{h}$ are matrices in multidimensional space: they have a 2×2 matrix structure in Keldysh space denoted by "check", a 2×2 matrix structure in particle-hole space denoted by "hat", and in general a 2×2 matrix structure in spin space[3],

$$\check{\chi} = \begin{pmatrix} \hat{\chi}^{\mathrm{R}} & \hat{\chi}^{\mathrm{K}} \\ 0 & \hat{\chi}^{\mathrm{A}} \end{pmatrix}, \; \chi = \{g, h\}, \tag{2}$$

$$\hat{h}^{\mathrm{R,A}} = \begin{pmatrix} \Sigma & \Delta \\ \tilde{\Delta} & \tilde{\Sigma} \end{pmatrix}^{\mathrm{R,A}}, \; \hat{h}^{\mathrm{K}} = \begin{pmatrix} \Sigma & \Delta \\ -\tilde{\Delta} & -\tilde{\Sigma} \end{pmatrix}^{\mathrm{K}}. \tag{3}$$

[1] Such interfaces can be engineered with the help of ferromagnetic materials, see Ref. [7].
[2] The $\otimes$ operation is defined by $\check{A} \otimes \check{B}(\epsilon, t) = e^{i\hbar(\partial_\epsilon^A\partial_t^B - \partial_t^A\partial_\epsilon^B)/2}\check{A}(\epsilon, t)\check{B}(\epsilon, t)$.
[3] The "tilde" or particle-hole conjugation operations is defined as $\tilde{Y}(\epsilon, \mathbf{p}_{\mathrm{F}}, \mathbf{r}, t) = Y(-\epsilon, -\mathbf{p}_{\mathrm{F}}, \mathbf{r}, t)^*$.

Finally, $\hat{\tau}_3$ and $\check{1}$ are third Pauli matrix in particle-hole space and unit matrix in Keldysh space, respectively. We will use $\{\sigma_i, i = 1, 2, 3\}$ Pauli matrices for spin. There is a convenient and numerically stable method for solving Eq.(1) by using the so-called Riccati parametrization [11, and references therein] for the elements of the matrix in Eq.(2),

$$\hat{g}^{\mathrm{R,A}} = \mp 2\pi i \begin{pmatrix} \mathcal{G} & \mathcal{F} \\ -\tilde{\mathcal{F}} & -\tilde{\mathcal{G}} \end{pmatrix}^{\mathrm{R,A}} \pm i\pi\hat{\tau}_3, \tag{4}$$

$$\hat{g}^{\mathrm{K}} = -2\pi i \begin{pmatrix} \mathcal{G} & \mathcal{F} \\ -\tilde{\mathcal{F}} & -\tilde{\mathcal{G}} \end{pmatrix}^{\mathrm{R}} \otimes \begin{pmatrix} x & 0 \\ 0 & \tilde{x} \end{pmatrix} \otimes \begin{pmatrix} \mathcal{G} & \mathcal{F} \\ -\tilde{\mathcal{F}} & -\tilde{\mathcal{G}} \end{pmatrix}^{\mathrm{A}}. \tag{5}$$

Here functions $\mathcal{G}$ and $\mathcal{F}$ are in turn parametrized as

$$\mathcal{G} = (1 - \gamma \otimes \tilde{\gamma})^{-1}, \; \mathcal{F} = (1 - \gamma \otimes \tilde{\gamma})^{-1} \otimes \gamma, \tag{6}$$

while their particle-hole conjugated counterparts are obtained by applying the "tilde"-operation. The $\gamma^{\mathrm{R,A}}$ and $\tilde{\gamma}^{\mathrm{R,A}}$ are *coherence functions* describing the electron-hole coherence in the superconducting state, while x and $\tilde{x}$ are *distribution functions*. So, using this parametrization the Eq.(1) simplifies to the following Riccati-type differential equations,

$$(i\hbar\mathbf{v}_{\mathrm{F}} \cdot \boldsymbol{\nabla} + 2\epsilon)\gamma^{\mathrm{R,A}} = \left[\gamma \otimes \tilde{\Delta} \otimes \gamma + \Sigma \otimes \gamma - \gamma \otimes \tilde{\Sigma} - \Delta\right]^{\mathrm{R,A}}, \tag{7}$$

$$\begin{aligned}&(i\hbar\mathbf{v}_{\mathrm{F}} \cdot \boldsymbol{\nabla} + i\hbar\partial_t)x - [\gamma \otimes \tilde{\Delta} + \Sigma]^{\mathrm{R}} \otimes x - x \otimes [\Delta \otimes \tilde{\gamma} - \Sigma]^{\mathrm{A}} \\ &= -\gamma^{\mathrm{R}} \otimes \tilde{\Sigma}^{\mathrm{K}} \otimes \tilde{\gamma}^{\mathrm{A}} + \Delta^{\mathrm{K}} \otimes \tilde{\gamma}^{\mathrm{A}} + \gamma^{\mathrm{R}} \otimes \tilde{\Delta}^{\mathrm{K}} - \Sigma^{\mathrm{K}},\end{aligned} \tag{8}$$

and the corresponding particle-hole conjugated equations obtained applying "tilde"-operation. They have to be supplemented by the corresponding boundary conditions in order to find unique solution. It is important to mention the symmetry relations for coherence and distribution functions,

$$\gamma^{\mathrm{A}} = \left[\tilde{\gamma}^{\mathrm{R}}\right]^{\dagger}, \; x = x^{\dagger}. \tag{9}$$

In equilibrium[4],

$$x^{\mathrm{eq}} = (1 - \gamma^{\mathrm{R}}\tilde{\gamma}^{\mathrm{A}}) \tanh\left(\frac{\epsilon}{2k_B T}\right), \tag{10}$$

and in the non-superconducting (or normal) case $\gamma^{\mathrm{R,A}}$=0. Finally, since the method we use is a mean field theory, equations (7)-(8) have to be in general solved self-consistently together with the corresponding self-consistency equations for self-energies. In particular, the order parameter for a spin-singlet s-wave superconductor $\Delta_0^{\mathrm{R}}(\mathbf{r}) = i\sigma_2\Delta_0(\mathbf{r})$ satisfies,

$$\Delta_0(\mathbf{r}) = -\frac{i\lambda N_{\mathrm{F}}}{8\pi} \int_{-\epsilon_c}^{\epsilon_c} d\epsilon \int \frac{d\Omega_{\mathbf{p}_{\mathrm{F}}}}{4\pi} \operatorname{Tr}\left[i\sigma_2(\hat{\tau}_1 - i\hat{\tau}_2)\hat{g}^{\mathrm{K}}(\epsilon, \mathbf{p}_{\mathrm{F}}, \mathbf{r})\right], \tag{11}$$

where $\lambda < 0$ is the electron-phonon coupling constant and ϵ_c is the high-energy cut-off of the order of the Debye frequency. As soon as the Riccati equations are solved we can find various physical observables as[5],

$$\text{spin imbalance: } \mathbf{M}(\mathbf{r}) = 2\mu_{\mathrm{B}}^2 N_{\mathrm{F}}\mathbf{B}(\mathbf{r}) + \frac{i\mu_{\mathrm{B}}N_{\mathrm{F}}}{8\pi} \int d\epsilon \int \frac{d\Omega_{\mathbf{p}_{\mathrm{F}}}}{4\pi} \operatorname{Tr}\left[\hat{\boldsymbol{\alpha}}\hat{g}^{\mathrm{K}}(\epsilon, \mathbf{p}_{\mathrm{F}}, \mathbf{r})\right], \tag{12}$$

$$\text{local density of states: } \mathrm{N}(\epsilon, \mathbf{r}) = -\frac{N_{\mathrm{F}}}{2\pi}\operatorname{Im}\left\{\int \frac{d\Omega_{\mathbf{p}_{\mathrm{F}}}}{4\pi}\operatorname{Tr}\left[\hat{\tau}_3\hat{g}^{\mathrm{R}}(\epsilon, \mathbf{p}_{\mathrm{F}}, \mathbf{r})\right]\right\}. \tag{13}$$

[4] Here k_B is the Boltzmann constant and T is the temperature.
[5] Here $\hat{\boldsymbol{\alpha}} = \mathrm{diag}(\boldsymbol{\sigma}, \boldsymbol{\sigma}^*)$ is a block-diagonal matrix in Nambu space, $\mathbf{B}(\mathbf{r})$ is the external magnetic field, μ_{B} is the Bohr magneton, $|e|$ is the elementary charge, and N_{F} is the density of states at Fermi level in the normal state.

3. Model for N-SAI-S junction

Let us now specify our theoretical model. We consider a conventional spin-singlet s-wave superconductor S. We assume translational invariance in the plane of the interface so that all physical quantities depend only on one spatial coordinate z. In order to achieve spin relaxation in S we consider a dilute concentration of magnetic spin-flip impurities (SFI) [12], and for completeness we also allow the presence of scalar impurities (SI). Both contributions are described in the Born approximation as

$$\check{h}_{\mathrm{sf}}(\epsilon, z) = \frac{\hbar}{2\pi\tau_{\mathrm{sf}}}\int \frac{d\Omega_{\mathbf{p}_{\mathrm{F}}}}{4\pi}(\hat{\tau}_3\check{1})\check{g}(\epsilon, \mathbf{p}_{\mathrm{F}}, z)(\hat{\tau}_3\check{1}),\;\; \check{h}_{\mathrm{s}} = \frac{\hbar}{2\pi\tau_{\mathrm{s}}}\int \frac{d\Omega_{\mathbf{p}_{\mathrm{F}}}}{4\pi}\check{g}(\epsilon, \mathbf{p}_{\mathrm{F}}, z), \tag{14}$$

where τ_{sf} and τ_{s} are the spin-flip and mean free times, respectively. To simplify the calculation we further assume low transparency of the interface and therefore approximate all self-energies by their *bulk self-consistent values* constant in space. The s-wave order parameter is then defined by a real constant[6]: $\Delta_0^{\mathrm{R}} = i\sigma_2\Delta_0$, $\Delta_0 = \mathrm{const}$. So, with the approximations mentioned above we have to solve Eqs.(7)-(8). Solutions with $\mathbf{p}_{\mathrm{F}}$ pointing towards the interface are called *incoming* and according to our approximation they are given by the bulk self-consistent values $\gamma^{\mathrm{R}}_{\mathrm{S,in}} \equiv \gamma^{\mathrm{R}}_{\mathrm{S,bulk}}$, see Sec.4. The coherence function in N is assumed $\gamma^{\mathrm{R}}_{\mathrm{N}} = 0$, i.e. we neglect the proximity effect. The interface is usually described by a scattering matrix, which defines (via boundary conditions) together with the incoming solution $\gamma^{\mathrm{R}}_{\mathrm{S,in}}$ the corresponding interface value of the *outgoing* solution $\gamma^{\mathrm{R}}_{\mathrm{S,out}}(z = 0)$, i.e. with $\mathbf{p}_{\mathrm{F}}$ pointing away from the interface. This value is then used as the initial condition for Eq.(7) for calculating the spatial dependence of $\gamma^{\mathrm{R}}_{\mathrm{S,out}}(z)$. The same algorithm holds for the distribution function x_{S} with the bulk value given by Eq.(10). We refer the reader to Refs.[8, 11, and references therein] for further details on the description of the interface and the boundary conditions. In the next section we will show how to find the self-consistent bulk value $\gamma^{\mathrm{R}}_{\mathrm{S,bulk}}$ for the coherence function, as this is the main initial ingredient one needs to know, according to our model, in order to find any physical observable.

4. Self-consistent solution in the bulk of superconductor

We now consider the bulk of the superconductor in presence of self-energies Eq.(14) and the order parameter defined in Eq.(11). Since we are looking for the bulk homogeneous solution we can omit the derivative on the left hand side of Eq.(7), which also makes the coherence function isotropic, $\gamma^{\mathrm{R}}_{\mathrm{bulk}} = \gamma^{\mathrm{R}}(\epsilon)$. Taking into account the spin-singlet pairing in the superconductor, both the order parameter and the coherence function have the same spin structure: $\Delta_0^{\mathrm{R}} = i\sigma_2\Delta_0$ and $\gamma^{\mathrm{R}}(\epsilon) = i\sigma_2\gamma(\epsilon)$. Therefore we can easily solve the Riccati equation demanding that $\gamma(\epsilon) \to 0$ if $\Delta_0 \to 0$. So we find,

$$\gamma = -\frac{\Delta}{\Sigma + \sqrt{\Delta^2 - \Sigma^2}},\;\; \tilde{\gamma} = -\gamma \tag{15}$$

$$\Sigma = \epsilon + \left(\frac{\hbar}{\tau_{\mathrm{sf}}} + \frac{\hbar}{\tau_{\mathrm{s}}}\right)\frac{\Sigma}{2\sqrt{\Delta^2 - \Sigma^2}},\;\; \Delta = \Delta_0 - \left(\frac{\hbar}{\tau_{\mathrm{sf}}} - \frac{\hbar}{\tau_{\mathrm{s}}}\right)\frac{\Delta}{2\sqrt{\Delta^2 - \Sigma^2}}. \tag{16}$$

Finally, we have to simplify the self-consistency equation for the order parameter Eq.(11). Using Eq.(5) and Eq.(10) we obtain,

$$\Delta_0 = \frac{|\lambda| N_{\mathrm{F}}}{2}\int_{-\epsilon_c}^{\epsilon_c} d\epsilon\, \mathrm{Im}\left[\frac{\Delta}{\sqrt{\Delta^2 - \Sigma^2}}\right]\tanh\frac{\epsilon}{2k_{\mathrm{B}}T}. \tag{17}$$

Finally we have to eliminate the high-energy cut-off ϵ_c in favor of the experimentally measurable critical temperature [10] by demanding that $\Delta_0 \to 0$ if $T \to T_{\mathrm{C}}$. Introducing the dimensionless quantities Z_1 and Z_2 via $\Sigma = \epsilon Z_1$ and $\Delta = \Delta_0 Z_2$, we obtain

[6] Phase of the order parameter is irrelevant because, for simplicity, we neglect bulk superflow.

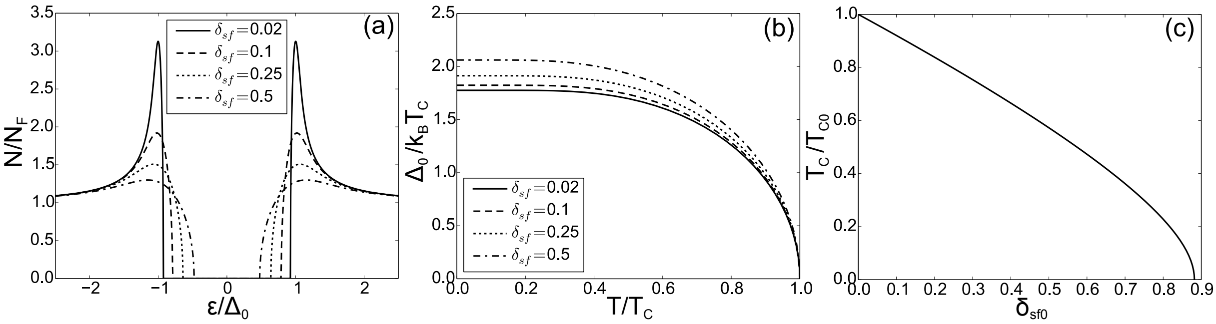

Figure 2. (a),(b),(c) Density of states $N(\epsilon)$, order parameter Δ_0, and critical temperature $T_{\rm C}$ in presence of magnetic impurities calculated self-consistently. Impurity strength is characterized by the dimensionless parameters $\delta_{\rm sf} = \hbar/\tau_{\rm sf} k_{\rm B} T_{\rm C}$ in (a)-(b) and $\delta_{\rm sf0} = \hbar/\tau_{\rm sf} k_{\rm B} T_{\rm C0}$ in (c). $T_{\rm C0}$ is the critical temperature for a clean system.

$$\ln\frac{T}{T_{\rm C}} = \int_0^\infty \frac{d\epsilon}{\epsilon}\left\{ \mathrm{Im}\left[\frac{\epsilon Z_2}{\sqrt{\Delta_0^2 Z_2^2 - \epsilon^2 Z_1^2}}\right] - \frac{1}{1+\frac{\hbar^2}{\tau_{\rm sf}^2\epsilon^2}}\right\}\tanh\frac{\epsilon}{2k_{\rm B}T}$$
$$-\int_0^\infty \frac{d\epsilon}{\epsilon}\left[1 - \frac{1}{1+\frac{\hbar^2}{\tau_{\rm sf}^2\epsilon^2}}\right]\left(\tanh\frac{\epsilon}{2k_{\rm B}T} - \tanh\frac{\epsilon}{2k_{\rm B}T_{\rm C}}\right). \quad (18)$$

By solving together Eq.(16) and Eq.(18) one can obtain the dependence $\Delta_0 = \Delta_0(T, T_{\rm C}, \tau_{\rm sf})$ and calculate, for example, the density of states, see Fig. 2. One can also verify with Eq.(18) that the bulk value Δ_0 is independent of the presence of scalar impurities [13].

5. Conclusions

The algorithm described in this paper has to be considered as a first iteration in a fully self-consistent solution to the problem of N-SAI-S junction. In general, all self-energies are spatially dependent as well as both incoming and outgoing solutions to Riccati equations. However, our simple analysis helps to capture qualitatively the most essential physical features of the model.

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