The influence of the spin-dependent phases of tunneling electrons on the conductance of a point ferromagnet/isolator/d-wave superconductor contact

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Abstract

The influence of the spin-dependent phase shifts (SDPSs) associated with the electronic reflection and transmission amplitudes acquired by electrons upon scattering at the potential barrier on the Andreev reflection probability of electron and hole excitations for a ferromagnet/isolator/d-wave superconductor (FIS) contact and on the charge conductance of the FIS contact is studied. Various superconductor orientations are considered. It has been found that for strong ferromagnets and ultrathin interface potential for the \{110\} oriented d-wave superconductor the presence of the SDPS can lead to the appearance of finite-voltage peaks in the charge conductance of the F/I/d-wave superconductor contact. On the contrary, for the \{100\} orientation of the d-wave superconductor the presence of the SDPS can lead to restoration of the zero-voltage peak and suppression of finite-voltage peaks. The spin-dependent amplitudes of the Andreev reflection probability and energy levels of the spin-dependent Andreev bound states are found.

1. Introduction

The oscillating character of the spatial dependence of the anomalous Green function (GF) in a ferromagnet in various hybrid structures containing a ferromagnet/superconductor with a singlet order parameter (F/S) interface is due to the presence of electron spin subbands with different values of Fermi momenta \( p_\alpha \) in a ferromagnetic metal (F) [1–4] (\( \alpha \) is the spin index, which denotes the projection of the electron spin on the direction of the magnetic moment of a ferromagnet, \( \alpha = \uparrow, \downarrow \)). Such a manifestation of the proximity effect is the basis for the creation of the \( \pi \)-Josephson junction [5], various spin-valve schemes [6–10], being the main elements of promising superconducting electronics [11–13].

The supression of the Andreev reflection [14] in point F/S contacts [15] due to the decrease of the number of conducting channels is another consequence of the presence of spin subbands in a ferromagnetic metal. This fact is used to determine the spin polarization of ferromagnetic materials [16–20], to study the order parameter symmetry of high-temperature superconductors [21–24] and to control the spin-polarized currents [25–27].

Recently attention has been paid to one more property of hybrid F/S structures: the influence of the SDPSs \( \theta^d_\alpha \) and \( \theta^r_\alpha \) associated with the electronic reflection and transmission amplitudes \( r_\alpha \) and \( d_\alpha \) acquired by electrons upon scattering on the potential barrier on thermodynamic [28] and transport [29, 30, 33] characteristics of hybrid structures with a spin-active interface:

\[
d_\alpha = \sqrt{D_\alpha v^F_{\alpha,x}/v^S_{\alpha,x}} \exp(i\theta^d_\alpha); \quad r_\alpha = \sqrt{R_\alpha} \exp(i\theta^r_\alpha).
\]

Here \( d_\alpha \) is the amplitude of transmission from a ferromagnet into a superconductor; \( D_\alpha \) and \( R_\alpha = 1 - D_\alpha \) are transmission and reflection coefficients, respectively; \( v^F_{\alpha,x} \) and \( v^S_{\alpha,x} \) are the Fermi velocity projections on the x-axis, being perpendicular to the plane of the F/I/d contact.

It has been found that the difference of the SDPSs due to the difference of potential barriers for electrons with various
spin projections $\alpha$ results in the appearance of a $\pi$ state in the S/F/I/S junction (FI is a ferromagnetic isolator) without taking into account the proximity effect [29, 30]. Recently [31, 32] as a result of numerical calculations it has been established that in the N/F/I/S structure (N is a normal metal) for any interface spin polarization there is a critical interface resistance, above which the conventional even-frequency proximity component vanishes completely at the chemical potential, while the odd-frequency component remains finite.

The presence of the SDPS also leads to the formation of the spin-dependent Andreev bound states in the superconducting layer of the N/F/s-wave superconductor contact [33]. In the tunneling limit these states appear as resonance peaks in the conductance of the ballistic charge conductance on the applied bias voltage $V$ if $V$ is smaller than a superconducting gap.

The influence of the SDPSs on the charge conductance of a single-channel quantum point contact of an F/s-wave superconductor and on the charge conductance of a multichannel ballistic contact of an F/I/s-wave superconductor (I is an isolator) was studied in [34, 35], respectively. In [34] it has been found that for a weakly transparent contact, the SDPS induces subgap resonances in the charge conductance of the quantum point contact. For high transparencies, these resonances are smoothed, but the shape of the signals remains extremely sensitive to the SDPS. In [35] it has been found that when F is strongly polarized, the peak in the conductance of the F/I/s-wave superconductor contact can be restored at zero voltage.

Such a strong influence of the SDPS on the transport properties of hybrid structures with ferromagnetic elements allows one to suppose that they may be successfully used in experiments on Andreev spectroscopy of ferromagnets, superconductors and in various applications in the field of spintronics.

This paper is devoted to the theoretical study of the SDPS influence on the Andreev reflection and charge conductance of a point F/I/d-wave superconductor contact.

Superconductors with d-wave symmetry (the d$_{x^2-y^2}$ symmetry of the order parameter is considered) have an internal, momentum-dependent phase, which strongly influences the transport properties of contacts between them and other materials. In [36] it was shown that when the angle $\gamma$ between the $a$ axis of a superconducting crystal and the normal to the surface of the high-order interface is $\pi/4$ (the [110] orientation of the d-wave superconductor), then a bound state is formed on the Fermi level near the high-ohm interface. This zero-energy bound state resulting from the repeated Andreev reflections [37, 38] causes a sharp peak at a zero voltage in the dependence of the charge conductance of the N/I/d-wave superconductor on the applied bias voltage [39].

The first theoretical study of spin-polarized tunneling spectroscopy of F/I/d-wave superconductor junctions was performed in [40–42]. It has been found that the subgap charge conductance behavior is qualitatively different from a nonmagnetic case. In particular, it has been found that for the [110] orientation of the d-wave superconductor the zero-voltage peak in the charge conductance is suppressed by the exchange interaction due to the suppression of Andreev reflections and that it splits into two peaks under the influence of the exchange interaction in the insulator.

The influence of the SDPSs $\theta_d^a$ and $\theta_\alpha^a$ on the charge conductance of the F/I/d-wave superconductor contact in [40–42] was not studied.

The main result of this paper is that the presence of the SDPS leads to the lifting of the spin degeneracy of the bound state on the Fermi level for the [110] orientation of the d-wave superconductor and to the formation of spin-dependent Andreev bound states inside the superconductor gap. For strong ferromagnets and ultrathin interface potential, it can lead to additional (by a factor of two or more) suppression of the zero-voltage peak in the dependence of the conductance of the F/I/d-wave superconductor contact on the applied bias voltage and to the appearance of finite-voltage peaks. For the [100] orientation of the d-wave superconductor, spin-dependent Andreev bound states inside the superconductor gap are formed. As a result, the finite-voltage peaks can be suppressed and the zero-voltage peak can be restored. Spin-dependent amplitudes of the Andreev reflection probability and energy levels of the spin-dependent Andreev bound states are found.

This work illustrates that the study of the influence of the SDPS on the charge conductance of the point F/I/d-wave superconductor contact can provide an interesting insight into spin-dependent transport.

A theoretical possibility to study the influence of the SDPSs on the $I$–$V$ characteristics of superconducting weak links with ferromagnetic elements appeared after the boundary conditions (BCs) for the quasiclassical GF were obtained. In [43], BCs for the quasiclassical GF for two metals in contact via a magnetically active interface in terms of an interface scattering matrix were derived. In [29], BCs for the retarded and advanced quasiclassical GFs were obtained in terms of Riccati amplitudes [44, 45]. In [33], BCs in terms of Riccati amplitudes were obtained for the nonequilibrium quasiclassical GF. In [46], quasiclassical equations of superconductivity for metals with a spin-split conduction band were derived and BCs for the temperature quasiclassical GF for the F/S interface were obtained. The model interface was the same as in [43, 47].

In this paper, calculations are carried out using quasiclassical GFs and the relevant BCs obtained in [46].

2. Finding differential conductance of a point FIS contact

2.1. The general expression for differential conductance of a point contact through quasiclassical GF

In hybrid F/S structures the Andreev reflection is modified. The reflected hole has some parameters (for example, the velocity modulus and the phase shift) different from those of the incident electron because it moves in a subband with an opposite spin. Such spin-discriminating processes due to the exchange interaction in a ferromagnet lead to the formation of spin-dependent Andreev bound states inside the gap [30, 29]. As a result, the spectral density of the charge conductance $G_{FIS}$ of the FIS contact at a zero voltage is no longer a symmetrical
function of energy $\varepsilon$. The generalization of the charge conductance expression \[48\] for this case results in the following formula for $G_{\text{FIS}}(V)$ \[35\]:

$$G_{\text{FIS}}(V) = \frac{e^2}{2\pi^2 T} \sum_a \text{Tr} \int \frac{dp_i}{(2\pi)^2} \int_{-\infty}^{\infty} \frac{de}{\coth \left( \frac{e}{2T} \right)} \left[ 1 - \bar{\hat{\rho}}_a \hat{e}_a \hat{e}_a \right] \times \left[ 1 - \bar{\hat{\rho}}_s \hat{e}_s \hat{e}_s \right].$$

(1)

In equation (1), $V$ is the applied bias voltage; $\alpha$ is the contact area; $\varepsilon$ is the electron charge; $T$ is the temperature; $\hat{e}_a$ is the Pauli matrix; $p_i$ is the momentum in the contact plane; $\hat{\rho}_a$, $\hat{\rho}_s$, $\hat{\rho}_g$ are quasiclassical retarded ($R$) and advanced ($A$) GFs symmetric (s) and antisymmetric (a) \[35\] with respect to the projection of the momentum $\vec{p}$ on the Fermi surface on the $x$ axis, being perpendicular to the contact plane, composed according to the rule $T_{\text{sym}}(a) = T_{\text{sym}}(\tau - p_z)$.

Besides the matrix quasiclassical GF $\hat{g}$, the equation for which is analogous to that derived in \[50\], equation (1) includes the matrix GF $\hat{\hat{g}}$, describing the interference of waves incoming to the interface and outgoing from it. The function relation with the matrix one-particle temperature GF and the equations that the function obeys are presented in the appendix. Calculations in equation (1) are to be carried out on the boundary of any contacting metal.

2.2. Finding the quasiclassical GF

Let us assume that the barrier with width $d$ is located in the region $-d/2 < x < d/2$, the superconductor occupies the region $x > d/2$, and the ferromagnet occupies the region $x < -d/2$. To find GFs for each metal, one has to solve quasiclassical equations of superconductivity for metals with a spin-split conductivity band simultaneously with their BCs derived in \[35\]. These quasiclassical equations and the boundary conditions to them are valid only for contacts of ferromagnets with singlet superconductors:

$$\text{sign}(\hat{p}_x) \frac{\partial}{\partial x} \hat{g} + \frac{\partial}{\partial \rho} \left( \hat{\hat{g}}^{-1} \hat{g} + \hat{g} \hat{\hat{g}}^{-1} \right) + [K, \hat{g}]_+ = 0,$$

$$\text{sign}(\hat{p}_x) \frac{\partial}{\partial x} \hat{\hat{g}} + \frac{\partial}{\partial \rho} \left( \hat{\hat{g}}^{-1} \hat{\hat{g}} + \hat{g} \hat{\hat{g}}^{-1} \right) + [K, \hat{\hat{g}}]_+ = 0,$$

$$\hat{K} = -i \hat{v}_z \hat{\hat{g}} \left( \theta \hat{\hat{g}} \right) + \Delta - \hat{\Sigma} \hat{v}_z \hat{\hat{g}} - i(\hat{p}_x - \hat{\hat{p}}_x \hat{\hat{\hat{g}}}_x) / 2;$$

$$\hat{\Delta} = \hat{\Delta}(x, \rho) \times [a, b]_\pm = ab \pm ba.$$ (2)

In this section, $\varepsilon = (2n + 1)\pi T$ is the Matsubara frequency; $\hat{\hat{\hat{g}}}$ and $\hat{\hat{\hat{g}}}$ are the Pauli matrices; $\rho = (x, y)$ are coordinates in the contact plane; $\hat{\Sigma}$ is the self-energy part; $\hat{\Delta}$ is matrix temperature GFs:

$$\hat{g} = \begin{pmatrix} g_{\alpha, \alpha} & f_{\alpha, -\alpha} \\ f_{\alpha, \alpha} & -g_{\alpha, -\alpha} \end{pmatrix}, \quad \hat{\hat{g}} = \begin{pmatrix} \hat{g}_> \quad \hat{g}_< \\ \hat{g}_< \quad \hat{g}_> \end{pmatrix} \quad \text{for} \quad \hat{p}_x > 0,$$

$$\hat{\Delta} = \begin{pmatrix} 0 & \Delta(x, \rho) \\ -\Delta^*(x, \rho) & 0 \end{pmatrix}, \quad \hat{p}_x = \begin{pmatrix} p_{x, a} & 0 \\ 0 & p_{x, -a} \end{pmatrix}.$$

Moreover, $\Delta(x, \rho)$ is the order parameter; $p_{x, a}$ and $p_{x, -a}$ are projections of the momentum on the Fermi surface on the $x$ axis and the contact plane, respectively; $\hat{v}_x = \hat{p}_x / m$ and $\hat{v}_y = p_y / m$.

BCs for a specular reflection of electrons from the boundary $p_x = p_x \sin \theta_x = p_x \sin \theta_x = p_{y, a} \sin \theta_{y, a}$ have the form \[35\]:

$$\hat{\Delta}_S = \begin{pmatrix} \hat{\Delta}_S^+ \quad 0 \\ 0 \quad \hat{\Delta}_S^- \end{pmatrix}, \quad \hat{\Delta}_S^+ = \hat{\Delta}_S^-(\hat{\hat{g}}_S),$$

where $\hat{\Delta}_S^+$ is the order parameter; $p_x, a = p_{x, a} / m$ and $p_y, a = p_{y, a} / m$.

The diagonal parts of matrices $\hat{g}$ are equal to the corresponding matrices $\hat{\hat{g}}$. Coefficients $\alpha$ are:

$$\alpha_1(2) = 1 + \sqrt{R_1 R_2} \pm \sqrt{D_1 D_2},$$

$$\alpha_3(4) = 1 - \sqrt{R_1 R_2} \pm \sqrt{D_1 D_2}.$$
finite in the superconductor. Then for S metal the solution is as follows:

\[
\hat{g}(x, p) = e^{-i\text{sign}(\hat{p}_z)\hat{K}(x - \frac{d}{2})} \hat{C}(p) e^{i\text{sign}(\hat{p}_z)\hat{K}(x - \frac{d}{2})} + \hat{C}_0(p),
\]

\[
\hat{\Gamma}(x, p) = e^{-i\text{sign}(\hat{p}_z)\hat{K}(x - \frac{d}{2})} \hat{\Gamma} e^{-i\text{sign}(\hat{p}_z)\hat{K}(x - \frac{d}{2})};
\]

(5)

\[
\hat{\Gamma} = \hat{\Gamma}(x = 0, p).
\]

Matrices \(\hat{C}_0(p)\) are the values of GFs \(\hat{g}\) far from the F/S boundary:

\[
\hat{C}_0^S(p) = \begin{pmatrix} \hat{g}_s^S & f \hat{g}_s^S + \hat{g}_d^S \end{pmatrix} = \frac{1}{\sqrt{\varepsilon_n + |\Delta(p)|^2}} \begin{pmatrix} \varepsilon_n; & -i\Delta(p) \end{pmatrix},
\]

\[
\Delta(p) = \Delta_d(T) \cos(2\theta_S - 2\gamma).
\]

(6)

In equation (6) \(\Delta_d(T)\) is the maximum value of the order parameter at temperature \(T\); \(\theta_S\) is the angle between the electron momentum in the superconductor and the x axis, being perpendicular to the contact plane, and \(\gamma\) is the angle between the crystal \(a\) axis of the d-wave superconductor and the x axis.

For F metal the solution has the same form as equation (5) except for changing the exponent argument from \((x - d/2)\) to \((x + d/2)\); \(\hat{C}_0^F(p) = \hat{C}_0^S(p)\).

GFs \(\hat{g}_s^S\) in equation (5) have to tend to \(\hat{C}_0^S\) at \(x \to +\infty\) and GFs \(\hat{g}_s^F\) to \(\hat{C}_0^F(p)\) at \(x \to -\infty\). By matrix multiplication in equation (5) and in the corresponding equation for \(\hat{g}_s^F\), we find that for the above to hold it is necessary that at \(x = +d/2\) and at \(-d/2\) the relationships

\[
\hat{C}_0^S(p)\hat{C}_0^S(p) = -\hat{C}_0^S(p)\hat{C}_0^S(p) = \text{sign}(\hat{p}_z)\hat{C}_0^S(p),
\]

\[
\hat{C}_0^F(p)\hat{C}_0^F(p) = -\hat{C}_0^F(p)\hat{C}_0^F(p) = -\text{sign}(\hat{p}_z)\hat{C}_0^F(p)
\]

are fulfilled respectively. It follows from these relationships that

\[
\hat{g}_s^S = \hat{X}\hat{C}_0^S + \hat{X};
\]

\[
\hat{g}_d^S = \hat{C}_0^S + \hat{C}_0^S;
\]

(7)

\[
\hat{g}_s^F = \hat{X}\hat{C}_0^F + \hat{X};
\]

\[
\hat{g}_d^F = \hat{C}_0^F + \hat{C}_0^F
\]

(8)

where

\[
\hat{X} = (1 + \hat{C}_0^S|\hat{C}_0^S|^{-1}, \hat{X} = \hat{C}_0^S|\hat{C}_0^S|^{-1};
\]

\[
\hat{X} = \hat{C}_0^F|\hat{C}_0^F|^{-1}.
\]

In equation (8) \(\hat{C}_0^S|\hat{C}_0^S|^{-1}\) are symmetric and antisymmetric combinations of the matrix \(\hat{C}_0^S(p)\) with respect to the projection of the Fermi momentum on the x axis: \(\hat{C}_0^S(\hat{p}_0) = 1/2[\hat{C}_0^S(p_0) + \hat{C}_0^S(-p_0)], \hat{X} = \hat{I}\). Matrices \(\hat{\Gamma}^S,F\) satisfy the relationships:

\[
\hat{C}_0^F(p)\hat{\Gamma}^F(p) = \hat{\Gamma}^F(p)\hat{C}_0^F(p) = -\text{sign}(\hat{p}_z)(\hat{p}_z)\hat{\Gamma}^F(p),
\]

\[
\hat{C}_0^S(p)\hat{\Gamma}^S(p) = \hat{\Gamma}^S(p)\hat{C}_0^S(p) = \text{sign}(\hat{p}_z)(\hat{p}_z)\hat{\Gamma}^S(p),
\]

(9)

being the condition for the functions \(\hat{\Gamma}^F(x, p)\) and \(\hat{\Gamma}^S(x, p)\) to tend to zero when \(x\) tends to \(-\infty\) and \(+\infty\), respectively.

The \(\hat{g}_s^F\) function appears in the ferromagnet due to the proximity effect. The absence of the \(\hat{g}_s^S\) function in a ferromagnet leads to zero value of the \(\hat{\Gamma}^F\) function.

This result can be obtained if, at first, one finds \(\hat{g}_s^F\) and \(\hat{g}_s^S\) FGs from equation (2) and BCs (3) having excluded the function \(\hat{\Gamma}^F\) from BCs (3).

Then from the BCs (3) and relationships (4) it follows that:

\[
\alpha_3(\hat{g}_s^F) = \alpha_4(\hat{g}_s^S) + \alpha_1(\hat{g}_s^F), \quad \alpha_3(\hat{g}_s^S) = \alpha_2(\hat{g}_s^F).
\]

(10)

From the first equality in equation (10) we find the relation between functions \((\hat{g}_s^F)\) and \((\hat{g}_s^S)\):

\[
(\hat{g}_s^F) = \frac{\sqrt{D_1D_1}}{1 - \sqrt{R_1R_1}}(\hat{g}_s^S).
\]

(11)

By substituting this relation into the second equality in equation (10) and using the relations (4) and (8) we find \((\hat{g}_s^F)\):

\[
\hat{g}_s^F = \hat{g}_s^F e^{-i\hat{g}_s^S \text{sign}(\hat{p}_z)} = \frac{\sqrt{D_1D_1}}{1 - \sqrt{R_1R_1}}(\hat{g}_s^S).
\]

(11)

Kno 2.3. Differential conductance of a point FIS contact

After carrying out the analytical continuation in functions \((\hat{g}_s^F), (\hat{g}_s^S), \hat{\Gamma}^F, \hat{\Gamma}^S\) (substituting \(\varepsilon_n\) for \(\varepsilon \pm \delta\) for retarded and advanced GFs, respectively), we obtain an expression for the charge conductance \(\sigma_{p/S}(V)\). For angles \(\gamma = 0\) and \(\pi/4\)\(\sigma_{p/S}(V)\) is as follows:

\[
\sigma_{p/S}(V) = \frac{e^2A}{(2\pi)^2} \int dp_z \left\{ \right. \right.
\]

\[
\int_{|\Delta(\theta)|} \frac{d\varepsilon}{2\varepsilon} \left[ \frac{1}{\cos^2(\frac{\varepsilon + V}{2\varepsilon})} + \frac{1}{\cos^2(\frac{\varepsilon - V}{2\varepsilon})} \right] \times
\]

\[
\int_{|\Delta(\theta)|} \frac{d\varepsilon}{2\varepsilon} \left[ \frac{D_1 + D_1}{\cos^2(\frac{\varepsilon + V}{2\varepsilon})} + \frac{D_1 + D_1}{\cos^2(\frac{\varepsilon - V}{2\varepsilon})} \right] \left[ |\Delta(\theta)| \right]^2
\]

(12)

For \(\gamma = 0\):

\[
\Delta(\theta) = |\Delta_\alpha| \cos(2\theta_S);
\]

\[
Z_\theta = \left[ |e_1 - W + \xi(1 + W)^2 + 4W|\Delta(\theta)\right] \sin^2(\theta_S);\]

\[
\int_{|\Delta(\theta)|} \frac{d\varepsilon}{2\varepsilon} \left[ \frac{D_1 + D_1}{\cos^2(\frac{\varepsilon + V}{2\varepsilon})} + \frac{D_1 + D_1}{\cos^2(\frac{\varepsilon - V}{2\varepsilon})} \right] \left[ |\Delta(\theta)| \right]^2
\]

(13)
For $\gamma = \pi/4$: 
\[
\Delta(\theta_s) = |\Delta_d| \sin(2\theta_s);
\]
\[
Z_\theta = [\epsilon(1 + W) + \xi(1 - W)]^2 - 4W|\Delta(\theta_s)|^2 \sin^2(\theta_s);
\]
\[
Z_\theta = [1 - 2W \cos(2\theta_d) + W^2]|\Delta(\theta_s)|^2 + 4W^2 \cos(2\theta_d)
\]
\[+ 16W^2(|\Delta(\theta_s)|^2 - \epsilon^2)\sin^2(2\theta_d) - 16W^2(|\Delta(\theta_s)|^2 - \epsilon^2)\sin^2(2\theta_d).
\]

For $\gamma = 0$, when $\theta_s = 0$, the expression for the conductance obtained in [35] follows from equation (12). In the case of a nonmagnetic metal, when $D_1 = D_2$, this expression is the same as that obtained in [47], and for $D = 1/(1 + Z^2)$ this expression is the same as that obtained in [48]. For $\gamma = \pi/4$, when $\theta_s = 0$, the expression for the conductance obtained in [49] follows from equation (12).

### 3. Andreev reflection

The calculation of quasiclassical GFs in the expression for the conductance allows one to conclude that for energies lower than $|\Delta(\theta_s)| (\epsilon^2 < |\Delta|^2)$, the following relation is true:
\[
[1 - \frac{\Delta^R}{\Delta} \tau_{\theta} \frac{R}{g^R} \tau_{\theta} - \frac{\Delta^R}{\Delta} \tau_{\theta} \frac{R}{g^R} \tau_{\theta} + \frac{\Delta^A}{\Delta} \tau_{\theta} \frac{R}{g^A} \tau_{\theta} - \frac{\Delta^A}{\Delta} \tau_{\theta} \frac{R}{g^A} \tau_{\theta}] = 4i \frac{\Delta A}{\Delta \theta} \tau_{\theta} \frac{R}{g^A} \tau_{\theta} \sim 1.
\]

Comparison of the form of under-gap conductances in equation (1) and that of the corresponding equation (25) in [48] shows that the matrix elements of $\frac{g^R}{\Delta}$ and $\frac{A^R}{\Delta}$ are the amplitudes of the Andreev reflection probability $a(\epsilon, \theta_s)$ in FIS contacts. Let us take the matrix elements of $\frac{g^R}{\Delta}$ given by equation (11) as $a(\epsilon, \theta_s)$:
\[
a(\gamma, \epsilon, \theta_s) = \frac{\sqrt{D_1 D_2 |\Delta(\theta_s)|}}{Z(\gamma)},
\]
where
\[
Z(0) = \left(1 - \sqrt{R_1 R_2}\right)[\epsilon \cos(\theta_s) - \sqrt{|\Delta(\theta_s)|^2 - \epsilon^2} \sin(\theta_s)]
\]
\[+ i(1 + \sqrt{R_1 R_2})[\sqrt{|\Delta(\theta_s)|^2 - \epsilon^2} \cos(\theta_s) + \epsilon \sin(\theta_s)].
\]

The presence of the imaginary part in functions $a(\gamma, \epsilon, \theta_s)$ means that Andreev reflection is accompanied by the phase shift. The Andreev reflection probability $A_\alpha(\gamma, \epsilon)$ ($A_\alpha(\gamma, \epsilon) = a(\gamma, \epsilon, \theta_s) a^*(\gamma, \epsilon, \theta_s)$) is:
\[
A_\alpha(\gamma, \epsilon) = \frac{D_1 D_2 |\Delta(\theta_s)|^2}{|Z(\gamma)|^2},
\]
\[
|Z(0)|^2 = \left[1 - \sqrt{R_1 R_2}\right]^2 |\Delta(\theta_s)|^2
\]
\[+ 4\sqrt{R_1 R_2}\left[\sqrt{|\Delta(\theta_s)|^2 - \epsilon^2} \cos(\theta_s) + \epsilon \sin(\theta_s)\right]^2,
\]
\[
|Z(\pi/4)|^2 = \left[1 - \sqrt{R_1 R_2}\right]^2 |\Delta(\theta_s)|^2
\]
\[+ 4\sqrt{R_1 R_2}\left[\sqrt{|\Delta(\theta_s)|^2 - \epsilon^2} \sin(\theta_s) - \epsilon \cos(\theta_s)\right]^2.
\]

From this equation it follows that: (1) the spin-mixing angle $\Theta$ used in [28, 29] corresponds, in our notations, to $\theta_s$ (for S/F/S and N/F/S contacts $\Theta = \theta^e_r - \theta^h_r = \theta^e_r - \theta^h_r$ [30, 29]); (2) for $\gamma = 0$, when $\theta_s < 0$ the Andreev reflection probability of the electron excitation with the spin projection $\alpha$ is larger than that of the hole excitation; when $\theta_s > 0$, the Andreev reflection probability of the hole excitation with the spin projection $\alpha$ is larger than that of the electron excitation; for $\gamma = \pi/4$, the relation is reversed; (3) the Andreev reflection probability has maxima at $\epsilon = \epsilon^b(\gamma)$ (at values of the energy of electron (hole) excitations corresponding to the energy levels of spin-dependent Andreev surface bound states).

The energy of spin-dependent bound states is:
\[
\epsilon^b(\gamma) = \begin{cases} 
-|\Delta(\theta_s)| \cos(\theta_s) & \text{for } (\pi/2) > \theta_s > 0, \\
|\Delta(\theta_s)| \cos(\theta_s) & \text{for } -(\pi/2) \leq \theta_s \leq 0, 
\end{cases}
\]
\[
\epsilon^b\left(\frac{\pi}{4}\right) = \begin{cases} 
-|\Delta(\theta_s)| \sin(\theta_s) & \text{for } (\pi/2) > \theta_s \geq 0, \\
|\Delta(\theta_s)| \sin(\theta_s) & \text{for } -(\pi/2) \leq \theta_s < 0.
\end{cases}
\]

Spin-dependent Andreev surface bound states are formed in a superconductor due to the interference of electron-like and hole-like particles with different SDPSs. One may demonstrate this by using a phenomenological argument in [38]. Let us consider diagrams in figure 1 corresponding to Andreev reflection of an electron with the spin projection $\alpha$ and energy less than $|\Delta|$ transmitted from a ferromagnet into a superconductor. The analysis of these diagrams and their summation makes it possible to obtain the following expression for a phenomenological expression of the amplitudes of the
Andreev reflection probability \( a(\varepsilon, \theta_a) \):

\[
a(\varepsilon, \theta_a) = d_a \tilde{d}_a \rho_{b, a}^{\text{eh}} \left[ 1 + \tilde{r}_a \rho_{b, a} \rho_{a, a}^{\text{eh}} \right] \]

\[
+ \left( \tilde{r}_a \rho_{b, a} \rho_{a, a}^{\text{eh}} \right)^2 + \cdots \right] = \frac{d_a \tilde{d}_a \rho_{b, a}^{\text{eh}}}{1 - \tilde{r}_a \rho_{b, a} \rho_{a, a}^{\text{eh}}}.
\]

The corresponding probability of Andreev reflection is:

\[
A(\varepsilon, \theta_a) = \frac{D_a D_{-a} \rho_{a, a}^{\text{eh}}}{1 + R_{a, a} \rho_{a, a}^{\text{eh}} - \tilde{r}_a \rho_{b, a} \rho_{a, a}^{\text{eh}}}.
\]

By comparing formulae (16), (17), derived using quasiclassical GFs, with formulae (19), (20), obtained using phenomenological arguments, we find the expressions for the vertices \( \rho_{b, a}^{\text{eh}} \) and \( \rho_{b, a}^{\text{be}} \). So for \( \gamma = \pi/4 \):

\[
\rho_{b, a}^{\text{eh}} = \frac{P_{b, a}^{\text{eh}}}{P_{b, a}^{\text{eh}}} \varepsilon - i \frac{\Delta(\varepsilon)}{\Delta(\varepsilon)} \Delta(\varepsilon) \]

\[
\rho_{b, a}^{\text{be}} = \frac{P_{b, a}^{\text{be}}}{P_{b, a}^{\text{be}}} \varepsilon - i \frac{\Delta(\varepsilon)}{\Delta(\varepsilon)} \Delta(\varepsilon) \cos(\theta_a) \sin(\theta_a)
\]

For \( \gamma = 0 \) the expression for the vertex \( \rho_{b, a}^{\text{be}} \) is of an opposite sign. It follows from formulae (20) and (21) that in the absence of the interferential term \( Q \) the probability of Andreev reflection is a constant (independent of the energy \( \varepsilon \) quantity). The interference of electron-like and hole-like particles reflected by the pair potential and the interface results in the formation of spin-dependent Andreev surface bound states. For \( \gamma = 0 \) at \( \theta_a = 0 \) the maximum in the probability of Andreev reflection is at \( \varepsilon = \pm \Delta_{\gamma} \) as in [48]. At \( \theta_a = \pm \pi/2 \) spin-dependent Andreev surface bound states with width \( \Gamma \):

\[
\Gamma = \frac{1 - \frac{1}{\sqrt{R_F R_F}} \Delta(\varepsilon)}{2 \sqrt{R_F R_F}}
\]

are formed at \( \varepsilon = 0 \) on the Fermi level. For \( \gamma = \pi/4 \) the spin degeneracy of the level on the Fermi surface [36] at \( \theta_a \neq 0 \) is removed. Two energy levels symmetric with respect to the Fermi level are formed inside the energy gap.

### 4. Appearance of Andreev bound states in the conductance of the FIS contact

We present below the results of numerical calculations of the charge conductance of the FIS contact taking into account the phase shifts. In the numerical calculations the relation between Fermi momenta of contacting metals was the following: \( p_S = \eta p_t + (1 - \eta) p_i \). Calculations are carried out for a rectangular barrier with a height \( U \) counted from the bottom of the conduction band of a superconductor. The electron wavefunction in the isolator \( \chi(x) \) is as follows:

\[
\chi(x) = C_1 \exp(\mu x) + C_2 \exp(-\mu x),
\]

where \( \mu = \sqrt{k^2 + p_t^2}; k^2 = 2m_S(U - E_F) \); \( E_F \) is the Fermi energy of a superconductor, \( m_0 \) is the mass of an electron in a barrier. In this case the expressions for \( \theta_d^\alpha \) and \( \theta_d^\beta \) have the following form:

\[
\theta_d^\alpha = \theta_a^\alpha - i \frac{1}{2} \left( p_{x, a}^{\text{eh}} + p_{x, a}^{\text{be}} \right) d; \quad \theta_d^\beta = \theta_a^\beta - i \frac{p_{x, a}^{\text{eh}}}{d};
\]

\[
\bar{\theta}_d^\alpha = \arctan \left( \frac{p_{x, a}^{\text{eh}} p_{y, a}^{\text{eh}} - \mu^2}{\mu_x (p_{x, a}^{\text{eh}} + p_{y, a}^{\text{eh}})} \right) \sin(\theta_d^\beta)
\]

\[
\bar{\theta}_d^\beta = \arctan \left( \frac{1 - p_{x, a}^{\text{eh}} p_{y, a}^{\text{eh}}}{\mu_x (p_{x, a}^{\text{eh}} + p_{y, a}^{\text{eh}})} \right) - \frac{\pi}{2}
\]

so that the angle \( \theta_d^\alpha = (\theta_d^\alpha - \theta_a^\alpha)/2 \) is independent of the electron trajectory for strong ferromagnets. With increasing \( \delta = p_i/p_t < 1 \), the values of the \( \theta_d^\alpha \) angle decrease. At \( \mu x d \sim k(p_t d)/p_t > 1 \), the angle \( \theta_a \ll 1 \).

Figure 2 shows dependences of the angle \( \theta_\alpha \) on \( \cos(\theta_\beta) \). All angles are connected by a specular reflection \( p_S = p_t \sin \theta_\beta = p_t \sin \theta_\beta = p_i \sin \theta_S \). Figure 2 shows the angle \( \theta_\alpha \), being a combination of phase shifts \( \theta_d^\alpha \) and \( \theta_d^\beta \), is almost independent of the electron trajectory for strong ferromagnets. With decreasing polarization of a ferromagnet (increasing \( \delta = p_i/p_t < 1 \)), the values of the \( \theta_\alpha \) angle decrease. At \( \mu x d \sim k(p_t d)/p_t > 1 \), the angle \( \theta_a \ll 1 \).

Figure 3 shows the results of numerical calculations of the normalized conductance of the FIS contact \( \sigma_x/(2V) \) at \( \sigma_0 \) for the \{110\} oriented d-wave superconductor \( \gamma = \pi/4 \). As follows from equations (18) and figure 4(a), in the presence of the SDPS only a narrow area of electron trajectories (and not all electron trajectories as in the case of absence of the SDPS), corresponding to \( \sin(2\theta_\beta) \sim 0 \) determines the conductance magnitude at \( V \sim 0 \). The majority of electron trajectories contribute to the conductance magnitude at finite voltage values. This results in splitting of the peak in conductance at zero voltage. With decreasing parameter \( p_t d \) the splitting...
Figure 3. Normalized conductance $\sigma_{FS}(V)/\sigma_0$ derived from equations (12) and (13) as a function of the applied bias voltage $V$ for the $\{110\}$-oriented d-wave superconductor ($\gamma = 0$) for various values of the parameter $p_1d$ not taking into account (dotted lines) and taking into account (solid lines) the phase shifts.

Figure 4. Dependence of the angles $\sin(2\theta_S)$ and $|\cos(2\theta_S)|$ on $\cos(\theta_\perp)$ for various values of the polarization of a ferromagnet $\delta$ ($\delta = p_1/p_1 < 1$) at $\eta = 0.3$.

Figure 5. Normalized conductance $\sigma_{FS}(V)/\sigma_0$ derived from equations (12) and (14) as a function of the applied bias voltage $V$ for the $\{100\}$-oriented d-wave superconductor ($\gamma = \pi/4$) for various values of the parameter $p_1d$ not taking into account (dotted lines) and taking into account (solid lines) the angle $\theta_\perp$. For all curves, $\Delta_d(T)/2T = 20$; $\eta = 0.3$.

The behavior of the finite and zero-voltage peaks in the conductance at other orientations of a superconducting crystal axis is of particular interest at high polarizations of the ferromagnet conduction band. It depends on the parameter $p_1d$. At $p_1d = \pi$, upon variation of the angle $\gamma$ from zero to $\pi/4$, the finite-voltage peaks shown in figure 5 (solid line) will move towards each other, and at $\gamma = \pi/4$ the solid line in
a manifestation of the bound state emerging at two peaks with a small spacing between them. This splitting is due to lifting of the spin degeneracy of the conduction band:  
\[ \delta = \frac{\pi}{2} \]  

Figure 3 will be reproduced. Upon reduction of the parameter \( p_1d \), the finite-voltage peaks at \( \gamma = 0 \) will move towards each other because the energy of bounded states tends to zero. The zero-voltage peak for the \( d \)-wave superconductor due to lifting of the spin degeneracy will move towards each other because the energy of bounded states tends to zero. The zero-voltage peak splits into four, the finite-voltage peaks at \( \gamma = 0 \) will move towards each other because the energy of bounded states tends to zero. The finite-voltage peaks at \( \gamma = \pi/4 \) (see equation (18)).

5. Conclusion

In this paper, the influence of the SDPSs associated with the electronic reflection and transmission amplitudes acquired by electrons upon scattering at the potential barrier on the Andreev reflection probability of electron and hole excitations for a FIS contact and the charge conductance of the FIS contact as a function of the applied bias voltage have been studied. Analytical expressions for spin-dependent Andreev bound states in a superconductor are found. It is found that for strong ferromagnets and ultrathin interface potential with parameter \( \mu, d \), the SDPS has a tremendous effect on the charge conductance of the FIS contact. The zero-voltage peak for the [110] orientation of the \( d \)-wave superconductor due to lifting of the spin degeneracy can be additionally suppressed, by a factor of two or more, and finite-voltage peaks in the charge conductance can appear.

On the contrary, the finite-voltage peaks for the [100] orientation of the \( d \)-wave superconductor can be suppressed and the zero-voltage peak can be restored.

The fitting of equation (12) to the experimental dependence of the charge conductance of the FIS contact on the applied bias voltage makes it possible to determine the polarization of a ferromagnet.

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Appendix A. Determining quasiclastic GFs  \( \hat{g} \) and  \( \hat{\Upsilon} \).

Deriving equation (2)

Let us start with equations for equilibrium thermodynamic GFs  \( \hat{g} \) and  \( \hat{\Upsilon} \).

\[ \hat{G}(\varepsilon_n, \mathbf{r}, \mathbf{r}') = \frac{G_{\alpha\alpha} F_{\alpha-a}^-}{F_{\alpha-a}^+ G_{\alpha-a}^-} ; \quad \hat{\mu} = \frac{1}{2m} \left( \frac{p_\alpha^2}{p_{\alpha-a}^2} \right). \]  

\( \hat{\varepsilon}_n \) is the Pauli matrix;  \( \varepsilon_n = (2n + 1)\pi T \) is the Matsubara frequency,  \( \alpha \) is the spin index;  \( \hat{\Delta}(\mathbf{r}) \) is the order parameter (as defined below equation (2));  \( p_\alpha \) is the Fermi momentum;  \( m \) is the electron mass;  \( \mathbf{r} = (x, \mathbf{R}) \),  \( \mathbf{R} = (y, z) \);  \( x \)-axis is perpendicular to the contact plane.

Passing to coordinates  \( \hat{\rho} \) and  \( \rho(\hat{\rho} = \rho - \hat{\rho}', 2\rho = R + R') \) in equation (A.1) and performing Fourier representation with respect to the  \( \hat{\rho} \) coordinate, the following equation for  \( \hat{G}(x, x') = \hat{G}(x, x', \rho, p_\alpha, \varepsilon_n) \) (\( p_\alpha \) is the momentum in the contact plane) is obtained:

\[ \left( \frac{i}{2m} \frac{\partial^2}{\partial x^2} + i \frac{v_\parallel}{2} \frac{\partial}{\partial \rho} + \hat{\mu}^2 + \hat{\Delta} - \hat{\Sigma} \right) \hat{G}(x, x') = \delta(x - x'). \]  

In equation (A.2):  \( v_\parallel = p_\parallel/m \),  \( \hat{\rho}_x = [p_{\alpha}^2 - p_{\alpha-a}^2]^{1/2} \).

Then the Zaitsev representation generalized for the description of metals with a spin-split conduction band is used for the function  \( \hat{G}(x, x') \):

\[ \hat{G}(x, x') = \sum_{n, m=1}^2 \hat{A}_k(x) \hat{G}_{n,m}(x, x') \hat{A}_k^*(x'), \]  

\[ \hat{A}_k(x) = e^{-i(1)^k \hat{\rho}_x}, \quad \hat{\rho}_x = \left( \begin{array}{c} p_{x,a} \\ p_{x,-a} \end{array} \right); \quad \hat{\rho}_x = m \hat{v}_x. \]  

Representation (A.3) explicitly takes account of oscillating terms present in the function  \( \hat{G}(x, x') \) and waves of the  \( \exp[\pm i (p_{x} x + p_{x} x') \] type, arising from partial reflection of the first electron of the superconducting pair from the interface [51]. Functions  \( \hat{G}_{n,m}(x, x') \) change at distances of...
an order of the mean free path of electrons in a metal. By substituting equation (4.3) into equation (4.2) and neglecting the second x-derivative, we obtain an equation for slow changing functions $\hat{G}_{k_0}(x, x')$:

$$\hat{A}_k(x) \left( i\epsilon_n \tau_c - \left(1 - \frac{1}{2}\right) \hat{v}_x \frac{\partial}{\partial x} + i \frac{\hat{v}_y}{2} \frac{\partial}{\partial \rho} + \Delta(x) - \hat{\Sigma} \right)$$

$$\times \hat{G}_{k_0}(x, x') \hat{A}_k(x') = \delta(x - x').$$

(A.4)

Analogously, an equation conjugate to (A.1) gives:

$$\hat{A}_k(x) \frac{\partial \hat{G}_{k_0}(x, x')}{\partial x} \hat{A}_k(x') \left( i\epsilon_n \tau_c + i \frac{\hat{v}_y}{2} \frac{\partial}{\partial \rho} + \Delta(x') - \hat{\Sigma} \right)$$

$$\times \hat{A}_k(x) \frac{\partial \hat{G}_{k_0}(x, x')}{\partial x'} \hat{A}_k(x') = \delta(x - x').$$

(A.5)

In equations (A.4) and (A.5) let us pass to functions $\hat{g}_0 \equiv \hat{g}_0(x, x') = \hat{g}_0(x, x', \rho, p_\parallel, \epsilon_n)$ and $\hat{\gamma}_0 \equiv \hat{\gamma}_0(x, x') = \hat{\gamma}_0(x, x', \rho, p_\parallel, \epsilon_n)$, being continuous at a point $x = x'$, by using formulae:

$$\hat{\hat{g}}_0 = \begin{cases} \hat{g}_0^+ &= 2i\sqrt{v_x} \hat{G}_{11}(x, x')\sqrt{v_x} - \text{sign}(x - x') & \text{for } \hat{\rho}_x > 0 \\ \hat{g}_0^- &= 2i\sqrt{v_x} \hat{G}_{22}(x, x')\sqrt{v_x} + \text{sign}(x - x') & \text{for } \hat{\rho}_x < 0 \end{cases}$$

$$\hat{\gamma}_0 = \begin{cases} \hat{\gamma}_0^+ &= 2i\sqrt{v_x} \hat{G}_{12}(x, x')\sqrt{v_x} & \text{for } \hat{\rho}_x > 0 \\ \hat{\gamma}_0^- &= 2i\sqrt{v_x} \hat{G}_{21}(x, x')\sqrt{v_x} & \text{for } \hat{\rho}_x < 0 \end{cases}$$

(A.6)

Let us call the obtained equations (A.4') and (A.5'), respectively. By subtracting equation (A.5') from equation (A.4') when $n = k$ and adding equations (A.4') and (A.5') when $n \neq k$, one may get equations for functions $\hat{g}_0(x, x')$ and $\hat{\gamma}_0(x, x')$. In these equations we set $x = x'$. Finally, the following equations are obtained:

$$\text{sign}(\hat{\rho}_x) \hat{B}(x) \frac{\partial \hat{g}_0}{\partial x}(x, x') + \frac{\hat{v}_y}{2} \frac{\partial}{\partial \rho} \hat{B}(x)(\hat{v}_x^{-1}, \hat{g}_0(x)) \hat{B}(x)$$

$$+ [\hat{K}_0, \hat{B}(x) \hat{g}_0 \hat{B}(x)] = 0,$$

$$\text{sign}(\hat{\rho}_x) \hat{B}(x) \frac{\partial \hat{\gamma}_0}{\partial x}(x, x') + \frac{\hat{v}_y}{2} \frac{\partial}{\partial \rho} \hat{B}(x)(\hat{v}_x^{-1}, \hat{\gamma}_0(x)) \hat{B}(x)$$

$$+ [\hat{K}_0, \hat{B}(x) \hat{\gamma}_0 \hat{B}(x)] = 0,$$

$$\hat{B}(x) = e^{-i\hat{g}_0 \hat{\rho}_x} \hat{\rho}_x, \quad \hat{K}_0 = -i\hat{v}_x \tau_z (i\epsilon_n \hat{\tau}_z + \Delta - \hat{\Sigma}) \hat{v}_x^{-1} \hat{g}_0^{-1},$$

$$[a, b]_k = ab \pm ba.$$

(A.7)

Considering that the expression for $\hat{B}(x)$ the matrix $\hat{\rho}_x$ can be written with the help of the Pauli matrix $\hat{\tau}_z$ as a sum of two components proportional to the unit matrix and Pauli matrix $\hat{\tau}_z$:

$$\hat{\rho}_x = (\hat{\rho}_x + \hat{\tau}_z \hat{\rho}_x \hat{\tau}_z)/2 + (\hat{\rho}_x - \hat{\tau}_z \hat{\rho}_x \hat{\tau}_z)/2,$$

(A.8)

and putting in equations (A.7) functions $\hat{g}(\hat{\rho}_0 \equiv \hat{g}(\epsilon_n, p_\parallel, \rho, x)$ and $\hat{\gamma}(\hat{\gamma}_0 \equiv \hat{\gamma}(\epsilon_n, p_\parallel, \rho, x)$, by formulæ:

$$\hat{g} = e^{i \rho \hat{\rho}_0} \hat{\rho}_0^{-1} \hat{g}_0^{-1} e^{-i \rho \hat{\rho}_0 \hat{\hat{g}}_0^{-1}},$$

$$\hat{\gamma} = e^{i \rho \hat{\rho}_0} \hat{\rho}_0^{-1} \hat{\hat{\gamma}}_0^{-1} e^{-i \rho \hat{\rho}_0 \hat{\hat{\gamma}}_0^{-1}},$$

(A.9)

one obtains equations (2). If quasiclassic GFs $\hat{g}$ and $\hat{\gamma}$ are independent of the coordinate, the condition $\hat{g}^2 = 1$ is met.
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