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Andreev spectrum and supercurrent in a multilayer ferromagnetic clean Josephson junction

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Abstract

In this work we consider a ballistic superconductor/multilayer–ferromagnet/superconductor junction, with interface scattering potential, which can be different in strength. We develop, for an arbitrary number of layers, compact analytic formulae for the Andreev bound state spectrum and the supercurrent. The phase dependence of the supercurrent is obtained from the Andreev amplitudes and results in an extremely simple form for any number of ferromagnetic layers. In the Matsubara summation it enters the denominator as a $\cos\phi$ plus a ϕ-independent term. The reduced formulae are amenable to efficient numerical computation. For a few cases we also give simple equations for the numerical determination of the bound states, obtained with algebraic matrix multiplication and numerical results are discussed.

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(Some figures in this article are in colour only in the electronic version)

1. Introduction

Hybrid systems containing superconducting and ferromagnetic elements are actively studied experimentally with advances in junction preparation techniques. The effort is for well-characterized interfaces between clean ferromagnet and superconductors to study spin-dependent transport properties. Spin polarized tunnelling can probe the electronic spectrum near the Fermi energy [1] as has been established with point contact spectroscopy by using the Andreev spectroscopy of magnetic materials in contact with superconductor [2, 3]. These hybrid systems could well find applications in magnetoelectronics [4], quantum information etc. Here we limit ourselves to Josephson junctions where the intermediate layer is an array of ferromagnets. In this case an interesting experimental observation is the π-junction behaviour which was predicted long time ago for the case of paramagnetic impurities [5] and recently observed experimentally [6–8]. The π-junction has also been proposed along with the 0-junction in a superconducting loop as a quantum bit [9]. In the case of a normal-superconductor (NS) system [10] the flow occurs by means of the Andreev reflection [11] mechanism, where an electron incident from the metal side with energy in the superconducting gap is reflected from the NS interface as a hole which has opposite charge velocity and spin, while at the same time a pair is transmitted in the superconductor. In the case of a perfect interface the probability of electron to hole scattering goes to unity when the energy of the electron is in the gap [10], if one assumes also that there is no mismatch of band parameters across the interface. If the energy of the incident electron is at the Fermi level then the hole is exactly retroreflected, while for energy E from the Fermi level there is a momentum mismatch $\Delta p = 2E/v_f$, where v_f is the Fermi velocity. When the normal metal is sandwiched between two superconductors forming an SNS junction, there are current carrying Andreev bound states localized in the intermediate layer, via which the transmission of supercurrent is possible [12, 13]. While this gives the dominant contribution, at higher temperatures we must also consider the contribution from the continuum spectrum [14].

In the case of a ferromagnet in contact with an s-superconductor, the electrons and reflected holes in the ferromagnet, due to the opposite spins, get a Zeemann splitting from the exchange field E_{ex}. Thus even for an incident electron at the Fermi energy we have a momentum mismatch $\Delta p = 2E_{\mathrm{ex}}/v_f$, which can be significant since in general $E_{\mathrm{ex}} \gg \Delta$. Thus, in an SFS junction, the relative phase increases with width of the ferromagnet d as $\Delta\Phi \sim 2E_{\mathrm{ex}}d/\hbar v_f$ for the ballistic case. This loss of coherence will affect phase sensitive quantities like the spectrum of Andreev bound states and the supercurrent.

Several analytic approximations can be obtained using the Andreev approximation [15, 16] for a single ferromagnetic layer if we neglect misfit between the bands in the layers, since we can neglect normal scattering. Due to the inhomogeneity in the superconducting gap, we have reflections at the boundary superconductor/ferromagnet with crossing channels, like the Andreev reflection of an electron to a hole. Recently there has been strong interest in the study of the effect of more than one layer [15, 18–20] and in particular if the polarization of the exchange field in two layers is antiparallel. This is to see the effect on the dephasing and the conditions under which π-junction behaviour is observed.

In this paper we extend this to the possibility of having several ferromagnetic layers with variable exchange fields with interface scattering. Normal metal intermediate layers are also easily included but will not be considered here. On the other hand, we exclude the case of superconducting intermediate layers due to the extra channel of scattering due to the Andreev reflection, at internal superconducting layer interfaces. For simplicity we consider the problem in one dimension and derive simple equations for the determination of the Andreev bound states and the supercurrent in ballistic junctions. The final results are given in terms of determinant products all of which involve 2×2 matrices which are given analytically. Some numerical evaluation is needed for the determination of the Andreev spectrum and the current, but the computational time is greatly reduced from that required from direct numerical evaluation of the determinant obtained from the matching condition. For special cases we will also give simple expressions. The model can also include the case where the left and right superconductors are different materials with different gaps and critical temperature. In this case Andreev bound states can be missing for some phase differences between the two superconductors, and for this range the current is carried entirely by continuum states. In section 2 we present the model for the hybrid junction, the Bogoliubov–de Gennes equations for this inhomogeneous structure and the matching conditions at the interfaces. In section 3 we derive a simplified expression for the determinant which will give us the Andreev spectrum, and in section 4 we derive an expression for the supercurrent. In section 5 we present some simple cases for the Andreev bound state equation, and in the final section we give some numerical results which we discuss.

2. Scattering problem

To calculate the supercurrent we first solve the Bogoliubov–de Gennes (BdG) equations to compute the state vectors that describe the possible quasiparticle scattering states and then construct Green's function using the method introduced by Furusaki [17] and derive the supercurrent formula using the relation from Green's function.

2.1. The $S_L I_L F_1 I_1 F_2 \ldots I_{n-1} F_n I_L S_R$ model

We consider a hybrid superconducting junction consisting of two bulk superconductors which are in contact with two thin insulating (oxide) layers and are separated by a nonsuperconducting region of total length d, which consists of several ferromagnetic layers F_i, $i = 1, \ldots, n$, of thicknesses d_i correspondingly, with $d = \sum_{i=1}^{n} d_i$. The two superconductors can be different with zero temperature gaps equal to $\Delta_{0L}(\Delta_{0R})$ for the left (right) superconductor. The ferromagnetic layers have different (in both magnitude and direction) exchange energies equal to $E_{\mathrm{ex},i}$ with polarization which can be parallel or antiparallel to the junction interface and with each other, while in their interface there is misfit in general due to the different exchange field. We assume a simple step-like spatial dependence of the order parameter, although in general it must be computed self-consistently, because it has spatial variations near the interfaces and in the intermediate region due to the proximity effect. The analytical expression that we use is

$$\Delta(z) = \begin{cases} \Delta_L\, \mathrm{e}^{\mathrm{i}\phi_L}, & z < 0 \\ 0, & 0 < z < d \\ \Delta_R\, \mathrm{e}^{\mathrm{i}\phi_R}, & z > d, \end{cases} \tag{1}$$

where ϕ_L, ϕ_R are the phases of the left (L) and right (R) superconductor respectively, and $\Delta_{L,R}(T)$ are the bulk superconducting gaps whose temperature dependence are given by

$$\Delta(T) = \Delta(0) \tanh\left(1.74\sqrt{T_c/T - 1}\right). \tag{2}$$

In the case of different superconductors we can introduce the corresponding zero temperature gaps and the critical temperatures.

The Ferromagnets are described within the effective exchange Stoner model by the one-body potential $V_\sigma(z) = -\sigma E_{\mathrm{ex}}$ and depends on the spin direction. The index $\sigma = \pm 1$ denotes spin up or down. The exchange fields shift the Fermi levels of the two spin sub-bands and also cause ordinary reflections at the SF interfaces due to the Fermi energy mismatch. In the superconducting banks $V_\sigma(z) = 0$, i.e. we neglect the effect of the ferromagnet, which can be the case if the insulating layer is relatively strong.

In order to model different bandwidths in the layers, the diagonal terms of the BdG equations are written in the effective mass approximation

$$h_0 = -\hbar^2 \nabla \frac{1}{2m(z)} \nabla + V(z) \tag{3}$$

with piecewise constant effective masses. The total potential consists of three terms

$$V(z) = W(z) + U(z) - \mu, \tag{4}$$

where $U(z)$ and μ are the electrostatic and the chemical potential, respectively. We allow these quantities to have different but constant values in the layers of the junction. The quantities $\mu - U_i(z)$ ($i = S, F_i$) are the Fermi energies of the appropriate regions.

Scattering processes which are caused by the S/F and F/F' interface insulating layers are modelled by the interface potential

$$W(z) = \hat{W}_L \delta(z) + \sum_{i=1}^{n-1} \hat{W}_i \delta(z - d_i) + \hat{W}_R \delta(z - d), \tag{5}$$

where we assume that scattering only takes place in the vicinity of the interfaces (delta-barrier potential). Since we examine the behaviour of this junction in the ballistic limit no other scattering processes take place in the bulk of the layers due to disorder or spin-flip processes. The parameters that model the band structure misfit are the ratios

$$m_{rj} = m_{F_j} \big/ m_S, \qquad f_{rj} = E_F^{(F_j)} \big/ E_F^{(S)}, \qquad k_{rj} = q_F^{(F_j)} \big/ k_F^{(S)}, \tag{6}$$

i.e. correspondingly the ratios of the effective masses in the ferromagnet $\left(m_{F_j}\right)$ to the one in the superconductor (m_S), the ratio of the Fermi energies in the ferromagnets $\left(E_F^{(F_j)}\right)$ to the one in the superconductor $\left(E_F^{(S)}\right)$ and the Fermi wavevector in the ferromagnet $\left(q_F^{(F_j)}\right)$ to $k_F^{(S)}$. From the definitions of the Fermi wavevectors

$$q_F^{(F_j)} = \left(\frac{2m_{F_j} E_F^{(F_j)}}{\hbar^2}\right)^{1/2}, \qquad k_F^{(S)} = \left(\frac{2m_S E_F^{(S)}}{\hbar^2}\right)^{1/2}, \tag{7}$$

it follows that

$$k_{rj} = \sqrt{f_{rj} m_{rj}}. \tag{8}$$

2.2. *Bogoliubov–de Gennes equations*

In the absence of spin-flip processes the two spin channels are decoupled and for each set of solutions $(u_\sigma(z), v_{-\sigma}(z))$ the BdG equations

$$\begin{pmatrix} h_0 + V_\sigma(z) & \Delta(z) \\ \Delta^*(z) & -h_0 + V_\sigma(z) \end{pmatrix} \begin{pmatrix} u_\sigma(z) \\ v_{-\sigma}(z) \end{pmatrix} = E \begin{pmatrix} u_\sigma(z) \\ v_{-\sigma}(z) \end{pmatrix} \tag{9}$$

can be solved easily.

We construct the solution of the inhomogeneous problem by solving the set of equations for each region and subsequently applying the boundary conditions at the interfaces [21]. For the superconducting regions the solutions are

$$\psi_{L,R}^{\pm e}(z) = \exp\left(\pm \mathrm{i} k_{L,R}^{+} z\right) \begin{pmatrix} u_{L,R}\, \mathrm{e}^{+\mathrm{i}\phi_{L,R}/2} \\ v_{L,R}\, \mathrm{e}^{-\mathrm{i}\phi_{L,R}/2} \end{pmatrix}, \tag{10}$$

$$\psi_{L,R}^{\pm h}(z) = \exp\left(\mp \mathrm{i} k_{L,R}^{-} z\right) \begin{pmatrix} v_{L,R}\, \mathrm{e}^{+\mathrm{i}\phi_{L,R}/2} \\ u_{L,R}\, \mathrm{e}^{-\mathrm{i}\phi_{L,R}/2} \end{pmatrix}. \tag{11}$$

Here $\pm e(h)$ indicates the electron(hole)-like quasiparticle moving to the right(+) or left(−), $u_{L,R} = \sqrt{(1+\Omega_{L,R}/E)/2}$ and $v_{L,R} = \sqrt{(1-\Omega_{L,R}/E)/2}$ are the BCS amplitudes, and $\Omega_{L,R} = \sqrt{E^2 - \Delta_{L,R}^2}$. The wavevectors are

$$k_{L,R}^{\pm} = k_F^{(S)} \left[1 \pm \mathrm{sign}(E) \frac{\Omega_{L,R}}{E_F^{(S)}}\right]^{1/2}, \tag{12}$$

where the sign(E) ensures us that in the limit $\Delta_{L,R} \to 0 (\Omega_{L,R} \to |E|)$ the solutions reduce to the normal state solutions with E being either positive or negative.

When $\Delta = 0$ the solutions in the ith ferromagnetic region have the simple plane wave spatial dependence:

$$\psi_{F_i}^{\pm e}(z) = \exp(\pm \mathrm{i} q_{ei,\sigma} z) \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad \psi_{F_i}^{\pm h}(z) = \exp(\mp \mathrm{i} q_{hi,-\sigma} z) \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \tag{13}$$

Again $\pm e(h)$ indicates the electron(hole) quasiparticle moving to the right or left. The wavevectors $q_{ei,\sigma}$ and $q_{hi,-\sigma}$ obey

$$q_{ei,\sigma} = q_F^{(F_i)}\left[1 + \left(\frac{E}{E_F^{(F_i)}} + \sigma\eta_i\right)\right]^{1/2} \tag{14}$$

$$q_{hi,-\sigma} = q_F^{(F_i)}\left[1 - \left(\frac{E}{E_F^{(F_i)}} + \sigma\eta_i\right)\right]^{1/2}, \tag{15}$$

where we have defined the normalized exchange field $\eta_i = E_{\mathrm{ex},i}\big/E_F^{(F_i)}$.

The scattering problem for the inhomogeneous structure has eight solutions when $E > \Delta$, which can be built up by combining the fundamental solutions in the different layers for a homogeneous material. They correspond to the cases: electron-like quasiparticle (ELQ) injection from the left (Ψ_1), hole-like quasiparticle (HLQ) injection from the left (Ψ_2), ELQ injection from the right (Ψ_3) and HLQ injection from the right (Ψ_4), plus the same injection processes with opposite spin (for the electron part) of the injected quasiparticles. For example the first process has the explicit form

$$\Psi_1(z) = \begin{cases} \psi_L^{+e}(z) + a_1\psi_L^{-h}(z) + b_1\psi_L^{-e}(z), & z < 0 \\ c_1\psi_R^{+e}(z-d) + d_1\psi_R^{+h}(z-d), & z > d, \end{cases} \tag{16}$$

where a_1, b_1, c_1 and d_1 are the Andreev amplitude, the normal reflection amplitude, the normal transmission amplitude and the transmission amplitude with branch crossing, respectively. The solution in the ith Ferromagnetic layer is

$$\begin{aligned}\Psi_{Fi}(z) = {} & c_{i,\sigma}^{+}\psi_{Fi}^{+e}(z - z_{i-1}) + c_{i,\sigma}^{-}\psi_{Fi}^{-e}(z - z_{i-1}) \\ & + d_{i,-\sigma}^{+}\psi_{Fi}^{+h}(z - z_{i-1}) + d_{i,-\sigma}^{-}\psi_{Fi}^{-h}(z - z_{i-1}),\end{aligned} \tag{17}$$

where $z_{i-1} \leqslant z \leqslant z_i$, $i = 1, 2, \ldots,$ and $c_{i,\sigma}^{+}(c_{i,\sigma}^{-})$ are the amplitudes of the right (left) going electron with spin σ and $d_{i,-\sigma}^{+}(d_{i,-\sigma}^{-})$ the amplitudes of the corresponding holes with opposite spin in the ith layer. Note that the phase of the wave has reference point the left interface of the ith layer ($z = z_{i-1}$). The positions of the interfaces are taken at $z = z_i = \sum_{j=1}^{i} d_j$, $i = 1, 2, \ldots, n$, where the origin is $z_0 = 0$ at the left superconductor/ferromagnet interface. We can calculate the coefficients through the matching conditions at the interfaces at z_i:

$$\Psi(z)|_{z=z_{i-}} = \Psi(z)|_{z=z_{i+}}, \tag{18}$$

$$\frac{1}{m_r(z_{i-})}\frac{\mathrm{d}\Psi(z)}{\mathrm{d}z}\bigg|_{z=z_{i-}} = \frac{1}{m_r(z_{i+})}\frac{\mathrm{d}\Psi(z)}{\mathrm{d}z}\bigg|_{z=z_{i+}} - \frac{2m_S\hat{W}_i}{\hbar^2}\Psi(z_i), \tag{19}$$

with $m_r(z_{i-}) = m_{ri}$ and $m_r(z_{i+}) = m_{r,i+1}$. In the following we will not be concerned with the eigenfunctions of the Andreev bound states but only with their spectrum and the contribution to the supercurrent. In the rest of the paper we will normalize all wavevectors to k_F, but we will keep the same symbols. This means that we divide all the boundary condition equations by k_F. When the wavevectors are in exponentials we also normalize appropriately the length as will be stated below.

2.3. Matching conditions matrix (MCM)

The matching conditions for the scattering states can be written in terms of a matrix equation as follows: first the continuity of the wavefunction and the discontinuity of the derivative for the electron part of the wavefunction, and then the same for the hole part at the first interface.

This procedure is continued until the last interface. The coefficients for each scattering state are equal to $N = 4 + 4n$ and are arranged in the following way: first the outgoing hole-like and electron-like quasiparticles in the left superconductor, then the coefficients for right- and left-moving electrons, left and right moving holes in the intermediate layers, and finally the outgoing electron-like and hole-like quasiparticles in the right superconductor.

The complete boundary condition equations are thus written in a matrix form

$$B_n \vec{e}_n = \vec{b}_n^{\mathrm{inc}}, \tag{20}$$

where for one layer the coefficient vector is

$$\vec{e}_1 = \left\{a, b, c_1^+, c_1^-, d_1^-, d_1^+, c, d\right\} \tag{21}$$

and for n layers

$$\vec{e}_n = \left\{a, b, c_1^+, c_1^-, d_1^-, d_1^+, \ldots, c_n^+, c_n^-, d_n^-, d_n^+, c, d\right\}, \tag{22}$$

with $N = 4 + 4n$ elements, where for simplicity we omit the spin index σ. The constant vector for the first process (incident electron quasiparticle from left) is

$$\left(\vec{b}_n^{\mathrm{inc}}\right)_1 = \left\{-u_L, -\mathrm{i}k_L^+ u_L, -v_L, -\mathrm{i}k_L^+ v_L, 0, \ldots, 0, \ldots, 0_N\right\}. \tag{23}$$

In the following we consider the normalized interface scattering potential parameters:

$$Z_j = \frac{2m_S \hat{W}_j}{\hbar^2 k_F}, \qquad j = 0, 1, \ldots, n. \tag{24}$$

Solution of this system gives the wavefunction everywhere. Of course here we are interested only in the coefficients a_1 and a_2, which enter the expression of the current, and their denominators from which the bound state spectrum is obtained. By this arrangement the matching condition matrix (MCM) takes the block form. For one layer

$$B_1 \equiv \left(\begin{array}{c|cc|c} (L_1) & (E_1) & & \\ \hline (L_2) & & (H_1) & \\ & (e_1) & & (R_1) \\ \hline & & (h_1) & (R_2) \end{array}\right), \tag{25}$$

for two layers

$$B_2 \equiv \left(\begin{array}{c|cccc|c} (L_1) & (E_1) & & & & \\ \hline (L_2) & & (H_1) & & & \\ & (e_1) & & (E_2) & & \\ & & (h_1) & & (H_2) & \\ & & & (e_2) & & (R_1) \\ \hline & & & & (h_2) & (R_2) \end{array}\right), \tag{26}$$

and for n layers

$$B_n \equiv \left(\begin{array}{c|cc|c} (L_1) & (E_1) & & \\ \hline (L_2) & & & \\ & & R_{4n} & \\ & & & (R_1) \\ \hline & & (h_n) & (R_2) \end{array}\right)_{N\times N}, \tag{27}$$

where R_{4n} is the $4n \times 4n$ matrix

$$R_{4n} = \begin{pmatrix} & (H_1) & & & & \\ (e_1) & & (E_2) & & & \\ & (h_1) & & \ddots & & \\ & & \ddots & & (E_n) & \\ & & & (h_{n-1}) & & (H_n) \\ & & & & (e_n) & \end{pmatrix}, \tag{28}$$

and N is the dimension of the MCM matrix, which is equal to $4(n+1)$.

The $L(R)$ blocks are

$$(L_1) = \begin{pmatrix} v_L & u_L \\ \mathrm{i}k_L^- v_L & -\mathrm{i}k_L^+ u_L \end{pmatrix}, \qquad (L_2) = \begin{pmatrix} u_L & v_L \\ \mathrm{i}k_L^- u_L & -\mathrm{i}k_L^+ v_L \end{pmatrix}, \tag{29}$$

and

$$(R_1) = \begin{pmatrix} -u_R & -v_R \\ -\left(\mathrm{i}k_R^+ - Z_R\right)u_R & \left(\mathrm{i}k_R^- + Z_R\right)v_R \end{pmatrix} \mathrm{e}^{\mathrm{i}\phi/2} \tag{30}$$

$$(R_2) = \begin{pmatrix} -v_R & -u_R \\ -\left(\mathrm{i}k_R^+ - Z_R\right)v_R & \left(\mathrm{i}k_R^- + Z_R\right)u_R \end{pmatrix} \mathrm{e}^{-\mathrm{i}\phi/2}. \tag{31}$$

The normal layer blocks are

$$(e_j) = \begin{pmatrix} \mathrm{e}^{\mathrm{i}\chi_{ej}} & \mathrm{e}^{-\mathrm{i}\chi_{ej}} \\ \mathrm{i}\tilde{q}_{ej}\,\mathrm{e}^{\mathrm{i}\chi_{ej}} & -\mathrm{i}\tilde{q}_{ej}\,\mathrm{e}^{-\mathrm{i}\chi_{ej}} \end{pmatrix} \tag{32}$$

$$(E_j) = \begin{pmatrix} -1 & -1 \\ -(\mathrm{i}\tilde{q}_{ej} - Z_{j-1}) & (\mathrm{i}\tilde{q}_{ej} + Z_{j-1}) \end{pmatrix} \tag{33}$$

$$(h_j) = \begin{pmatrix} \mathrm{e}^{\mathrm{i}\chi_{hj}} & \mathrm{e}^{-\mathrm{i}\chi_{hj}} \\ \mathrm{i}\tilde{q}_{hj}\,\mathrm{e}^{\mathrm{i}\chi_{hj}} & -\mathrm{i}\tilde{q}_{hj}\,\mathrm{e}^{-\mathrm{i}\chi_{hj}} \end{pmatrix} \tag{34}$$

$$(H_j) = \begin{pmatrix} -1 & -1 \\ -(\mathrm{i}\tilde{q}_{hj} - Z_{j-1}) & (\mathrm{i}\tilde{q}_{hj} + Z_{j-1}) \end{pmatrix}, \tag{35}$$

where in the pre-exponentials we use the normalized wavevectors

$$\tilde{q}_{ej} = q_{ej}/m_{rj}, \qquad \tilde{q}_{hj} = q_{hj}/m_{rj}. \tag{36}$$

The phases that occur in the above equations are

$$\chi_{ej} = \kappa q_{ej} d_j, \qquad \chi_{hj} = \kappa q_{hj} d_j, \qquad j = 1, \ldots, n, \tag{37}$$

which are the evolved phases of an electron (χ_e) or a hole (χ_h) respectively, traversing the jth ferromagnetic region forth or back (for the hole). Here q is normalized to k_F, the width of the jth layer d_j is normalized to the coherence length ξ_0 and the dimensionless parameter $\kappa = k_F\xi_0 = 2E_F/(\pi\Delta_0)$. In all cases we must evaluate the determinant of the MCM which enters the denominator of the coefficients and will determine the Andreev bound states. The determinants of the normal blocks which will be used later are

$$\det(e_j) = \det(E_j) = -2\mathrm{i}\tilde{q}_{ej}, \qquad \det(H_j) = \det(h_j) = -2\mathrm{i}\tilde{q}_{hj}, \tag{38}$$

while for the other matrices the determinants are given in appendix A.

3. Determinant of MCM

The localized Andreev states are determined from the vanishing of the determinant of B_n, defined as $\Gamma(E) \equiv \det(B_n)$. In the following we will show that the full denominator can be written as

$$\Gamma(E) = D[\cos(\phi) + \gamma(E)], \tag{39}$$

where $D\gamma(E)$ includes no ϕ-dependent term, and the only phase dependence is in the form $\cos\phi$ in the first term. First we will consider the ϕ-dependent term of the denominator. We expand the determinant of the MCM by 2×2 subdeterminants as follows:

$$\Gamma = \Delta_{N-1,N}|M_{N-1,N}| + \Delta_{N-3,N-2}|M_{N-3,N-2}| - \Delta_{N-2,N}|M_{N-2,N}| \\ + \Delta_{N-2,N-1}|M_{N-2,N-1}| + \Delta_{N-3,N}|M_{N-3,N}| - \Delta_{N-3,N-1}|M_{N-3,N-1}|, \quad (40)$$

where $\Delta_{i,j}$ are the 2×2 subdeterminants which contain the elements of the ith and jth rows of the last two columns of B_n, i.e. elements of (R_1) and (R_2). $|M_{i,j}|$ are the determinants of the complement matrices to the submatrices, whose determinants are $\Delta_{i,j}$ and the values of $\Delta_{i,j}$ do not depend on the number of the layers, since it involves only quantities related to the right superconductor, and are given explicitly in appendix A. Only the terms $\Delta_{N-1,N}$ and $\Delta_{N-3,N-2}$ involve the phase difference.

The ϕ dependence of Γ is calculated combining the ϕ-dependent terms $\Delta_{N-1,N}|M_{N-1,N}|$ and $\Delta_{N-3,N-2}|M_{N-3,N-2}|$. The derivation of the relevant complement submatrix determinants $|M_{N-1,N}|$ and $|M_{N-3,N-2}|$ is presented in appendix B and here we give the result.

The expansions of $|M_{N-1,N}|$ and $|M_{N-3,N-2}|$ for n layers are

$$|M_{N-1,N}| = \left(\prod_{i=1}^{n} \det(e_i)\det(H_i)\right)\det(L_1) \quad (41)$$

and

$$|M_{N-3,N-2}| = \left(\prod_{i=1}^{n} \det(h_i)\det(E_i)\right)\det(L_2), \quad (42)$$

where

$$\det(L_1) = -\mathrm{i}\left(k_L^+ + k_L^-\right)u_L v_L \quad (43)$$

$$\det(L_2) = -\mathrm{i}\left(k_L^+ + k_L^-\right)u_L v_L. \quad (44)$$

These are two of the possible determinants obtained from the first two columns of the MCM matrix by taking any two rows at a time. They are tabulated in appendix A, and they depend on the properties of the left superconductor. The other four are involved in the current determination.

Thus, the ϕ-dependent term of the denominator is written as

$$\Gamma_\phi \equiv D\cos(\phi) = Q\left(k_L^+ + k_L^-\right)\left(k_R^+ + k_R^-\right)u_L v_L u_R v_R(\mathrm{e}^{\mathrm{i}\phi} + \mathrm{e}^{-\mathrm{i}\phi}), \quad (45)$$

where we have defined Q as

$$Q \equiv \left(\prod_{i=1}^{n} \det(e_i)\det(H_i)\right) = \left(\prod_{i=1}^{n} \det(E_i)\det(h_i)\right) = \prod_{i=1}^{n}(-4\tilde{q}_{ei}\tilde{q}_{hi}). \quad (46)$$

3.1. Evaluation of γ

Above we derived a simple expression for the coefficient of the phase-dependent term D as a simple product of wavevectors. To complete the evaluation of the denominator we also need an expression for the phase-independent factor γ. We will derive in a similar manner a closed formula, which can be used for arithmetical calculation and under some circumstances for evaluation of analytical expressions for the denominator.

For n layers we have (see appendix B.2)

$$D\gamma = \sum_{\{l_{n+1}\},\{k_{n+1}\}} (-1)^{l_{n+1}+k_{n+1}+1} \det\begin{pmatrix}(L_1)_{\bar{k}_1}\\(L_2)_{\bar{l}_1}\end{pmatrix} \det\begin{pmatrix}(R_1)_{k_{n+1}}\\(R_2)_{l_{n+1}}\end{pmatrix} \times \left\{\prod_{j=1}^{n}(-1)^{l_j+k_j} \det\begin{pmatrix}(H_j)_{l_j}\\(h_j)_{\bar{l}_{j+1}}\end{pmatrix} \det\begin{pmatrix}(E_j)_{k_j}\\(e_j)_{\bar{k}_{j+1}}\end{pmatrix}\right\}, \tag{47}$$

where D is defined earlier and the subscripts i of $(S)_i$ take the values $i = 1, 2$ and stand for the ith row of the corresponding 2×2 submatrix (S). The sets of integers $\{l_{n+1}\}$, $\{k_{n+1}\}$ are the sets of indices $\{l_1, \ldots, l_{n+1}\}$ and $\{k_1, \ldots, k_{n+1}\}$, respectively, and take the values $1, 2$ and the complement indices $\bar{l}_1$ and $\bar{k}_1$ etc are defined as follows:

$$\bar{i} = \begin{cases} 2, & \text{for} \quad i = 1 \\ 1, & \text{for} \quad i = 2. \end{cases} \tag{48}$$

This formula is useful for numerical calculations because the calculations involved reduce to $2^{2(n+1)}$. Also the compactness achieved makes more efficient use of algebraic calculations and analytic simplifications by computer. To simplify this expression we assume that the superconductors are identical and that the electron-like and hole-like wavevectors are equal to their value at the Fermi sphere, i.e. $k^{\pm}_{L,R} = k_F$. Thus in normalized wavevectors

$$D\gamma = -(2\mathrm{i})^{2n} \sum_{\{l_{n+1}\},\{k_{n+1}\}} \mathcal{L}_{k_1,l_1} \left(\prod_{j=1}^{n} \mathcal{H}^{(j)}_{l_j,l_{j+1}} \mathcal{E}^{(j)}_{k_j,k_{j+1}}\right) \mathcal{R}_{k_{n+1},l_{n+1}}, \tag{49}$$

where

$$\mathcal{R} = \begin{pmatrix} \delta & -\mathrm{i}s - \delta Z_R \\ \mathrm{i}s - \delta Z_R & \delta\left(1 + Z_R^2\right) \end{pmatrix}, \qquad \mathcal{L} = \begin{pmatrix} -\delta & -\mathrm{i}s \\ \mathrm{i}s & -\delta \end{pmatrix},$$

with

$$\delta = u^2 - v^2, \qquad s = u^2 + v^2 \tag{50}$$

and

$$\mathcal{H}^{(j)} = \begin{pmatrix} \tilde{q}_{hj}\cos(\chi_{hj}) & -\sin(\chi_{hj}) \\ \tilde{q}^2_{hj}\sin(\chi_{hj}) - \tilde{q}_{hj}Z_{j-1}\cos(\chi_{hj}) & \tilde{q}_{hj}\cos(\chi_{hj}) + Z_{j-1}\sin(\chi_{hj}) \end{pmatrix} \tag{51}$$

$$\mathcal{E}^{(j)} = \begin{pmatrix} \tilde{q}_{ej}\cos(\chi_{ej}) & -\sin(\chi_{ej}) \\ \tilde{q}^2_{ej}\sin(\chi_{ej}) - \tilde{q}_{ej}Z_{j-1}\cos(\chi_{ej}) & \tilde{q}_{ej}\cos(\chi_{ej}) + Z_{j-1}\sin(\chi_{ej}) \end{pmatrix}. \tag{52}$$

The phases that occur in the above equations are defined earlier. So we get the remaining part of the denominator, γ, in terms of a summation of products of elements of 2×2 matrices.

One could also use the transfer matrix approach, starting from a product of 2×2 matrices. For numerical purposes we prefer the present form where the phase dependence appears simple. Expression (39) for the eigenspectrum determination and (49) for the γ term, which will also appear in (67) for the supercurrent determination, are well suited for efficient numerical computation. The ϕ dependence is explicitly shown, and especially for the current the formula will be efficient. For a single ferromagnetic layer starting from the transfer matrix, we can explicitly show to recover the same analytic form, but after lengthy term rearrangements. For many ferromagnetic layers the reduction is not obvious and the amount of analytical calculations to reduce in our simple form is prohibitive, except if one uses symbolic matrix multiplication. The large number of terms, however, makes symbolic simplification extremely difficult, time consuming and most likely impossible.

4. Andreev amplitudes and current

The main contribution to the supercurrent comes from the Andreev bound states and can be written from the free energy of the system as

$$I_b = \frac{2e}{\hbar}\sum_n \frac{\mathrm{d}E_n}{\mathrm{d}\phi} f(E_n), \tag{53}$$

where the sum is taken over all bound states $E_n(\phi)$ and the contribution is weighted by the Fermi distribution function. At low temperatures it is the negative energies that contribute. Thus from the spectrum $E_n(\phi)$ one has a good idea about the supercurrent. Thus the slope of the spectrum at negative energies also gives the sign of the maximum critical current and one can distinguish the situations of 0- or π-junction.

There is also a contribution from the continuum spectrum $E > \Delta$, which can be written as

$$I_c = \frac{2e}{\hbar}k_B T\left(\int_{-\infty}^{-\Delta} + \int_{\Delta}^{\infty}\right)\mathrm{d}E \ln\left[\cosh\left(\frac{E}{2k_b T}\right)\right]\frac{\mathrm{d}\rho}{\mathrm{d}\phi}, \tag{54}$$

where $\rho(E, \phi)$ is the density of quasiparticles as a function of energy which also depends on the relative phase of the superconductors. The density of states can be determined from the scattering matrix of the system. Here we will consider the formula obtained from Green's function approach given by Furusaki [17], which contains both the discrete and the continuum contribution in terms of the Andreev amplitudes:

$$I = \frac{e}{\hbar}k_B T\sum_{\omega_n,\sigma}\frac{\Delta_L}{\Omega_L}\left(k_L^+ + k_L^-\right)\left(\frac{a_1}{k_L^+} - \frac{a_2}{k_L^-}\right), \tag{55}$$

where the sum is over the Matsubara frequencies $\omega_n = (2n+1)\pi k_B T/\hbar$ for $n = 0, \pm 1, \pm 2, \ldots$, and the expression is evaluated using the analytic continuation $E + \mathrm{i}0^+ \to \mathrm{i}\hbar\omega_n$. The formula takes into account the degeneracy between left-going electron and right-going hole and the same for the opposite directions, while there is also a summation over spins, since the exchange field splits the energy levels.

To calculate the numerator of the Andreev coefficients $a_1(a_2)$ for left incident electron-like (hole-like) we interchange the first (second) column of the MCM by the corresponding constant vectors $\vec{b}_n^{\mathrm{inc}}$ due to the incident wave and obtain matrices A_1 (A_2) correspondingly. We can expand the determinant of these matrices by the first two columns as follows:

$$|A| = \delta'_{1,2}|M_{1,2}| - \delta'_{1,3}|M_{1,3}| + \delta'_{1,4}|M_{1,4}| + \delta'_{2,3}|M_{2,3}| - \delta'_{2,4}|M_{2,4}| + \delta'_{3,4}|M_{3,4}|, \tag{56}$$

where $\delta'_{i,j}$ are the 2×2 determinants obtained from the i and j rows of the first two columns in the numerator matrices. They are different from $\delta_{i,j}$ (as seen by the prime), since we have substituted the first or second column in the B matrices, and are also different for A_1 and A_2. The expressions for the numerator determinants of the Andreev amplitudes for the left-incident electron (A_1) and the left-incident hole (A_2) are

$$|A_1| = 2\mathrm{i}k_L^+\left\{u_L^2|M_{1,2}| + v_L^2|M_{3,4}| + u_L v_L(|M_{1,4}| - |M_{2,3}|)\right\} \tag{57}$$

$$|A_2| = 2\mathrm{i}k_L^-\left\{v_L^2|M_{1,2}| + u_L^2|M_{3,4}| + u_L v_L(|M_{1,4}| - |M_{2,3}|)\right\}. \tag{58}$$

The combination that occurs in the Josephson current takes the form

$$\frac{|A_1|}{k_L^+} - \frac{|A_2|}{k_L^-} = 2\mathrm{i}\left(u_L^2 - v_L^2\right)(|M_{1,2}| - |M_{3,4}|) \tag{59}$$

and

$$\frac{\Delta_L}{\Omega_L}\left(k_L^+ + k_L^-\right)\left(\frac{|A_1|}{k_L^+} - \frac{|A_2|}{k_L^-}\right) = 4\mathrm{i}\left(k_L^+ + k_L^-\right)u_L v_L(|M_{1,2}| - |M_{3,4}|), \tag{60}$$

while the analytic continuation of this at the Matsubara frequencies is summed in the calculation of the current.

Again we show explicitly $|M_{1,2}|$ and $|M_{3,4}|$ for the one layer:

$$|M_{1,2}| = \det\left(\begin{array}{cc|c} & (H_1) & \\ (e_1) & & (R_1) \\ \hline & (h_1) & (R_2)\end{array}\right) = \det(H_1)\det\left(\begin{array}{c|c}(e_1) & (R_1) \\ \hline & (R_2)\end{array}\right)$$
$$= \det(H_1)\det(e_1)\Delta_{N-1,N} \tag{61}$$

and

$$|M_{3,4}| = \det\left(\begin{array}{cc|c}(E_1) & & \\ \hline (e_1) & & (R_1) \\ \hline & (h_1) & (R_2)\end{array}\right) = \det(E_1)\det\left(\begin{array}{c|c} & (R_1) \\ \hline (h_1) & (R_2)\end{array}\right)$$
$$= \det(E_1)\det(h_1)\Delta_{N-3,N-2}, \tag{62}$$

where all the subdeterminants are defined earlier and involve terms that contain the phase in a simple way.

For the n layers we get by induction

$$|M_{1,2}| = Q\Delta_{N-1,N} \tag{63}$$

and

$$|M_{3,4}| = Q\Delta_{N-3,N-2}, \tag{64}$$

where the factor Q was defined in the evaluation of the denominator determinant, and will drop out since it also appears as a factor in the denominator matrix which is the same as before. The ϕ dependence is equally simple, so the expressions are

$$\frac{|A_1|}{k_L^+} - \frac{|A_2|}{k_L^-} = Q\left(u_L^2 - v_L^2\right)\left\{-\mathrm{i}u_R v_R\left(k_R^+ + k_R^-\right)(\mathrm{e}^{-\mathrm{i}\phi} - \mathrm{e}^{\mathrm{i}\phi})\right\}$$
$$= Q\left(u_L^2 - v_L^2\right)\left\{-2u_R v_R\left(k_R^+ + k_R^-\right)\sin(\phi)\right\}, \tag{65}$$

and dividing by Γ to obtain the Andreev amplitude, the contributing term in the Furusaki [17] formula for the Josephson current can be written as

$$\frac{\Delta_L}{\Omega_L}\left(k_L^+ + k_L^-\right)\left(\frac{a_1}{k_L^+} - \frac{a_2}{k_L^-}\right) = \frac{-2\sin(\phi)}{\cos(\phi) + \gamma(E(\phi))}. \tag{66}$$

So finally the current is given for the ballistic case by the formula

$$I = -\frac{e}{\hbar}\frac{1}{\beta}\sum_{\omega_n,\sigma}\frac{\sin(\phi)}{\cos(\phi) + \gamma(\omega_n)} \tag{67}$$

as the sum over the Matsubara frequencies ω_n and the spin, and $\gamma(\omega_n)$ is the analytic continuation of $\gamma(E)$. In this paper we considered the calculations of the Andreev bound state spectrum and the supercurrent. For this only the Andreev amplitudes (a_1, a_2) are needed. One can also calculate with the same difficulty the normal reflection amplitudes (b_1, b_2). Once this is done, one can calculate Green's function in the left superconductor and then other quantities such as density of states.

Expression (67) for the supercurrent is valid for arbitrary number of intermediate layers, which cannot be superconducting, but otherwise can be either metallic or aligned ferromagnet, and can also easily include the case of band misfits. The analytical form of the current is very convenient for numerical calculations. Since the quantities $\gamma(\omega_n)$ depend only on constant parameters and are independent of the phase difference, they can be tabulated as a vector with as many elements as the terms in the Matsubara summation. Actually because of the spin we need two vectors for each spin. Then they can be used for every value of the phase, in order to find the maximum current. Here we consider $I(\phi)$, but actually it is the supercurrent through the device that fixes the phase difference. So the question of what is the maximum supercurrent is of practical importance. The above simplification is due to the separation out of the determinants of the phase dependence. In fact one can avoid evaluating the current for all values of the phase to find the maximum current. What we need is to find from (67) the phase where

$$\frac{\mathrm{d}I}{\mathrm{d}\phi} = -\frac{e}{\hbar}\frac{1}{\beta}\sum_{\omega_n,\sigma}\frac{\gamma(\omega_n)\cos(\phi)+1}{[\cos\phi+\gamma(\omega_n)]^2} = 0. \tag{68}$$

Since the search routine for the roots needs about ten iterations for convergence it is more efficient than to scan over 200 points of $0 < \phi < 2\pi$. In our case we did not take this extra advantage, but we used a scan over the phase. In the following we will obtain some simple limits, where the analytic expressions are significantly simplified.

5. Simple cases

The phase-independent part of the denominator $\gamma(E)$ can be reduced to simple analytic expressions for cases which have not been treated previously. One such case is the $S/F/I/F/I/F/S$ structure with three intermediate layers, which are separated by interface potentials of equal normalized strength Z. There is no interface barrier potential between the superconductors and the normal region. The case of misfit in Fermi wavevector between the superconductor and the normal layer is also included. The intermediate layers can include normal metallic or ferromagnetic. The two superconductors are the same and also the exchange fields in the normal layers, which however can have different widths. This structure can be studied for the influence of the scattering barriers (positions and common strength) on the interplay between the Andreev bound states and the resonances of the double barrier potential. The phase-independent term in (39) is reduced to

$$\begin{aligned}
\frac{D\gamma}{(2\mathrm{i})^6} = u^4\,\mathrm{e}^{-\mathrm{i}(\chi_{e1}-\chi_{h1}+\chi_{e3}-\chi_{h3})}&\left\{\left[(Z-\mathrm{i})^2-q_e^2\right]\sin(\chi_{e2})+2q_e(Z-\mathrm{i})\cos(\chi_{e2})\right\}\\
&\times\left\{\left[(Z+\mathrm{i})^2-q_h^2\right]\sin(\chi_{h2})+2q_h(Z+\mathrm{i})\cos(\chi_{h2})\right\}+v^4\,\mathrm{e}^{\mathrm{i}(\chi_{e1}-\chi_{h1})}\,\mathrm{e}^{\mathrm{i}(\chi_{e3}-\chi_{h3})}\\
&\times\left\{\left[(Z+\mathrm{i})^2-q_e^2\right]\sin(\chi_{e2})+2q_e(Z+\mathrm{i})\cos(\chi_{e2})\right\}\\
&\times\left\{\left[(Z-\mathrm{i})^2-q_h^2\right]\sin(\chi_{h2})+2q_h(Z-\mathrm{i})\cos(\chi_{h2})\right\}\\
&-u^2v^2\cos[((\chi_{e1}-\chi_{h1})-(\chi_{e3}-\chi_{h3}))]\\
&\times\left\{\left[(1+Z^2)-q_e^2\right]\sin(\chi_{e2})+2q_eZ\cos(\chi_{e2})\right\}\\
&\times\left\{\left[(1+Z^2)-q_h^2\right]\sin(\chi_{h2})+2q_hZ\cos(\chi_{h2})\right\}.
\end{aligned} \tag{69}$$

Since we are interested for states within the superconducting gap, we can use

$$\left.\begin{matrix}u\\ v\end{matrix}\right\} = \frac{1}{\sqrt{2}}\,\mathrm{e}^{(\pm\mathrm{i}\varphi_E/2)}, \qquad \text{with} \quad \varphi_E = \cos^{-1}\frac{E}{\Delta} \tag{70}$$

so that u and v are complex conjugate and the expression for γ is real as expected. The above expression was obtained by algebraic computer simplification using the result of (49).

A special case of the previous structure is when the exchange field is weak so that in all pre-exponential terms we have $q_e = q_h = 1$ for the case of no misfit between superconductor and normal layer. The exact wavevectors are kept, however, in the exponential terms. If we also impose vanishing interface potential ($Z = 0$) we get from the vanishing of the denominator for the bound state energies the well-known result

$$\cos(S_e - S_h - 2\phi_\epsilon) - \cos(\phi) = 0, \tag{71}$$

which can be re-expressed as a condition of the total phase shift $(S_e - S_h)$ as the electron–hole pair traverses the normal region of width d, i.e. is the phase shift of the electron traversing the total distance d, and the reflected hole traversing backwards the distance d. The term $2\varphi_E$ is the phase shift at the electron to hole (and hole to electron) reflection due to the fact that the wavefunctions decay exponentially in the superconducting layers. The last equation shows that at $S_e - S_h = \pi$, we have a π-junction spectrum for different layers with weak inhomogeneity and no interface potential. It is the interface potential which adds more interference paths.

6. Numerical results and discussion

The analytical results obtained for the eigenvalue determinant and the supercurrent are exact within the approximations explicitly stated. The saving in computational time is significant, since the direct numerical evaluation of the eigenvalue determinant is lengthy due to the search in energy and similarly for the Andreev amplitudes, which involve several matrices, due to the many terms required at low temperatures in the Matsubara summation.

In the following we will limit ourselves to a few numerical results by varying only a few of the parameters in the structure. Thus we will keep the intermediate layer widths fixed and equal to 0.05 which is about $30A$, for which a ballistic approach could be justified. The case of band parameter misfit can also be treated but will not be discussed here. There is no barrier at the interfaces with the superconducting layers, while the interfacial barriers between all FIF' interfaces are taken equal to $Z_{NN} = 0$ or 0.5 corresponding to no or weak barriers. There is still, however, the Andreev reflection and some normal reflection due to misfit from the exchange field. The exchange fields are interchanged between h_1 and h_2 for consecutive layers with $h_1 = 0.15$ fixed and variation of the exchange field in the even layers, h_2. For the parameters chosen, the exchange field has opposite direction in the even layers.

We present the critical supercurrent for different number of ferromagnetic layers as a function of the phase shift due to the propagation of the electron across the ferromagnetic layers and the reflected hole backwards, $S_e - S_h$. We use this parameter instead of h_2, because it seems to be a useful parameter to characterize the possibility of π-junction [15, 16]. This phase shift is defined as

$$S_e - S_h = \sum_{i=1}^{n} [\chi_{ei} + \chi_{hi}] = \sum_{i=1}^{n} \kappa [q_{ei} d_i + q_{hi} d_i], \tag{72}$$

and the only variable quantity on the rhs is h_2. We should remark that the calculation of the maximum current requires first the calculation for every set of material parameters of $I(\phi)$ for all phases and then determine the maximum current. This procedure has to be repeated for every change in geometry or material parameters. Thus the saving in computational time in every following plot is significant.

In figure 1, we give the maximum supercurrent for the case of three layers ($n = 3$) and two values of the interfacial barrier parameter taken to be the same between all F/F' interfaces and equal to $Z_{NN} = 0, 0.5$, while there is no barrier between the superconducting layers and their neighbouring ferromagnetic layers. We see that for no interface barrier the

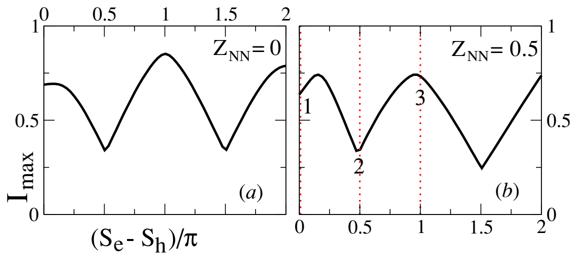

Figure 1. Plot of the maximum supercurrent I_{max} versus the phase shift $S_e - S_h$ in (72), for $n = 3$ ferromagnetic layers and two values of $Z_{NN} = 0$ and 0.5. $d_1 = d_2 = d_3 = 0.05$. The corresponding exchange fields are $h_1 = h_3 = 0.15$. h_2 is determined from $S_e - S_h$. $T = 0.1T_c$ and $Z_{SN} = 0$.

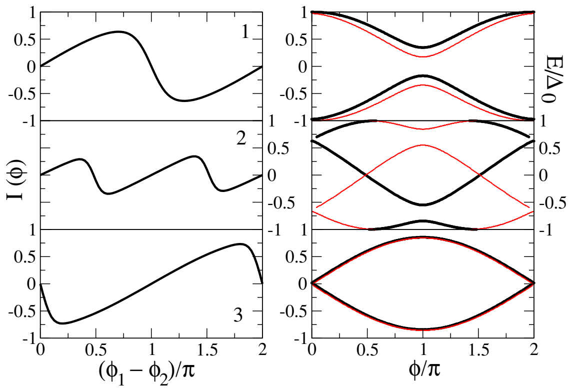

Figure 2. Plots of $I(\phi)$ and $E(\phi)$ for $n = 3$ layers from figure 1(b) corresponding to the three numbered lines.

maximum current shows the characteristic behaviour of a single layer [16], with the region of π-junction behaviour around the $S_e - S_h = \pi$ point, while at the two dips we have the transition between 0- and π-junctions. The pattern is almost independent of other geometries examined (which in this case is symmetric), implying that the total electron–hole phase shift across the ferromagnetic layers ($S_e - S_h$) is the important phase shift in this case. For the case $Z_{NN} = 0.5$, we see that the pattern develops more asymmetry, which is more important for different width layers. Still, however, we can distinguish the three peaks with 0, π, 0 behaviour correspondingly. This implies that while $S_e - S_h$ is still a determining factor, the phase shifts within each layer are also contributing factors, which can introduce new substructure.

For the range shown in figure 1, h_2 varies between -0.297 and -0.1022 in the opposite direction to h_1. To verify the $0 - \pi$ transition, we check the supercurrent versus phase difference $I(\phi)$ and the Andreev spectrum $E(\phi)$ curves for three points (numbered) in figure 1, which correspond to approximately $S_e - S_h = 0$ and π and the left dip. This is shown in figure 2. We see that the $I(\phi)$ curves for the two points present the characteristic signature for 0 (curve 1), π (curve 3) and in curve 2 the transition point where the second harmonic in the supercurrent is evident. The Andreev bound spectrum shows an almost coincidence of spin-up and spin-down states for $S_e - S_h = 0$ and π, while the degeneracy is broken at the transition point. Of course, there is still the degeneracy between electrons and holes of the same spin but moving in opposite directions and the symmetry $E(\downarrow) = -E(\uparrow)$.

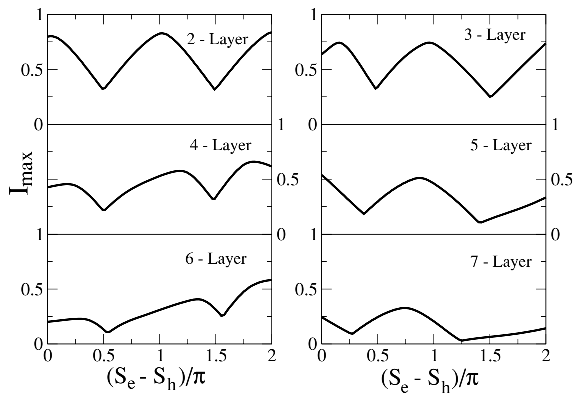

Figure 3. Plot of the maximum supercurrent I_{max} versus the phase shift $S_e - S_h$ in (72), for $n = 2$–7 ferromagnetic layers of equal width $d = 0.05$ and $Z_{NN} = 0.5$. The corresponding exchange fields are $h_1 = 0.15$ for odd layers. h_2 is determined from $S_e - S_h$. $T = 0.1T_c$ and $Z_{SN} = 0$.

Finally in figure 3 we plot the maximum supercurrent versus $S_e - S_h$ for $n = 2$–7 layers with the same parameters as in figure 1, with $Z_{NN} = 0.5$. Of course, in this case except the misfit, we also have the interface scattering which seems to be more important with increasing number of layers and asymmetry, and should create not only a change in the phase shift for the path described but also extra reflections that can influence coherence. We still see however that the phase shift parameter is still a good indicator of the π-junction behaviour. There is always a significant region of π-junction. While the region persists there is some assymetry which increases with interface scattering. We also see that the asymmetry is tilted oppositely for odd or even number of layers.

In this work we have not included at all disorder in the S and F layers. The treatment of disorder requires a diffusive approach, with the introduction of a characteristic scattering time in the linearized Usadel equations for the quasiclassical Green's function [22, 23]. In our approach, however, we can include easily important factors such as strong band misfits and spatial variation of the exchange field. We should remark that disorder will lead to a strong decay with the junction width, but similar effects can be due to misfit in three-dimensional junctions. We also hope that with the improvement of junction preparation techniques we will approach the region of quasiclean junctions.

7. Summary

In summary we considered a multilayer ferromagnetic clean Josephson junction with interfacial barriers. We developed analytical expressions in the form of products and summations of elements of 2×2 matrices for the determinant that gives the Andreev spectrum. The supercurrent is given in the summation over the Matsubara frequencies and in each term the ϕ dependence is isolated. This leads to an efficient algorithm for numerical calculations, especially when one is interested for the critical current.

The numerical results have concentrated in an intermediate region of several layers and consecutively opposite exchange fields. The goal was to check whether for a reasonable range of parameters the phase shift $S_e - S_h$ is a useful quantity to characterize the junction as 0 or π for a range of reasonable widths and exchange fields. From the results of I_{max} versus $(S_e - S_h)$ and the spectrum, we see that $S_e - S_h$ can give us an indication of π-junction behaviour.

Appendix A. The S-block determinants

For the right (R) superconductor the determinants of the submatrices $\Delta_{i,j}$ are

$$
\begin{aligned}
\Delta_{N-3,N-2} &= \det\begin{pmatrix}(R_1)_1\\(R_1)_2\end{pmatrix} = -\mathrm{i}u_R v_R\left(k_R^+ + k_R^-\right)\mathrm{e}^{\mathrm{i}\phi}\\
\Delta_{N-3,N-1} &= \det\begin{pmatrix}(R_1)_1\\(R_2)_1\end{pmatrix} = \left(u_R^2 - v_R^2\right)\\
\Delta_{N-3,N} &= \det\begin{pmatrix}(R_1)_1\\(R_2)_2\end{pmatrix} = \left(-\mathrm{i}\left(k_R^- u_R^2 + k_R^+ v_R^2\right) - Z_R\left(u_R^2 - v_R^2\right)\right)\\
\Delta_{N-2,N-1} &= \det\begin{pmatrix}(R_1)_2\\(R_2)_1\end{pmatrix} = \left(\mathrm{i}\left(k_R^- v_R^2 + k_R^+ u_R^2\right) - Z_R\left(u_R^2 - v_R^2\right)\right)\\
\Delta_{N-2,N} &= \det\begin{pmatrix}(R_1)_2\\(R_2)_2\end{pmatrix} = \left(u_R^2 - v_R^2\right)\left(k_R^+ k_R^- + Z_R^2 - \mathrm{i}\left(k_R^+ - k_R^-\right)Z_R\right)\\
\Delta_{N-1,N} &= \det\begin{pmatrix}(R_2)_1\\(R_2)_2\end{pmatrix} = -\mathrm{i}u_R v_R\left(k_R^+ + k_R^-\right)\mathrm{e}^{-\mathrm{i}\phi}
\end{aligned}
\qquad \text{(A.1)}
$$

and

$$
\begin{aligned}
\Delta_{N-3,N-2} &= \det(R_1), & \Delta_{N-1,N} &= \det(R_2)\\
\Delta_{N-3,N-1} &= \mathcal{R}_{11}, & \Delta_{N-2,N} &= \mathcal{R}_{22}\\
\Delta_{N-3,N} &= \mathcal{R}_{12}, & \Delta_{N-2,N-1} &= \mathcal{R}_{21}.
\end{aligned}
\qquad \text{(A.2)}
$$

For the left (L) superconductor, we give all the possible determinants obtained from the first two columns of the MCM matrix by taking any two rows i and j at a time and denoted as $\delta_{i,j}$ with $i < j$. They are used in the evaluation of the determinant. Two of them $\delta_{1,2} = \det(L_1)$ and $\delta_{3,4} = \det(L_2)$ enter the ϕ-dependent term in the denominator determinant and the other four, which enter the ϕ-independent term, are defined as elements of the 2×2 matrix $\mathcal{L}$.

$$
\begin{aligned}
\delta_{1,2} &= \det\begin{pmatrix}(L_1)_1\\(L_1)_2\end{pmatrix} = -\mathrm{i}u_L v_L\left(k_L^+ + k_L^-\right) \equiv \det L_1\\
\delta_{1,3} &= \det\begin{pmatrix}(L_1)_1\\(L_2)_1\end{pmatrix} = -\left(u_L^2 - v_L^2\right) \longrightarrow \mathcal{L}_{22}\\
\delta_{1,4} &= \det\begin{pmatrix}(L_1)_1\\(L_2)_2\end{pmatrix} = -\mathrm{i}\left(k_L^- u_L^2 + k_L^+ v_L^2\right) \longrightarrow -\mathcal{L}_{21}\\
\delta_{2,3} &= \det\begin{pmatrix}(L_1)_2\\(L_2)_1\end{pmatrix} = \mathrm{i}\left(k_L^- v_L^2 + k_L^+ u_L^2\right) \longrightarrow -\mathcal{L}_{12}\\
\delta_{2,4} &= \det\begin{pmatrix}(L_1)_2\\(L_2)_2\end{pmatrix} = -k_L^+ k_L^-\left(u_L^2 - v_L^2\right) \longrightarrow \mathcal{L}_{11}\\
\delta_{3,4} &= \det\begin{pmatrix}(L_2)_1\\(L_2)_2\end{pmatrix} = -\mathrm{i}u_L v_L\left(k_L^+ + k_L^-\right) \equiv \det L_2.
\end{aligned}
\qquad \text{(A.3)}
$$

For the normal (N) blocks we have the determinants

$$\begin{aligned}
&\det\begin{pmatrix}(E_j)_1\\(e_j)_1\end{pmatrix} = 2\mathrm{i}\sin(\chi_{ej}) = -2\mathrm{i}\mathcal{E}_{12}^{(j)}\\
&\det\begin{pmatrix}(E_j)_1\\(e_j)_2\end{pmatrix} = 2\mathrm{i}q_{ej}\cos(\chi_{ej}) = 2\mathrm{i}\mathcal{E}_{11}^{(j)}\\
&\det\begin{pmatrix}(E_j)_2\\(e_j)_1\end{pmatrix} = -2\mathrm{i}(q_{ej}\cos(\chi_{ej}) + Z_{j-1}\sin(\chi_{ej})) = -2\mathrm{i}\mathcal{E}_{22}^{(j)}\\
&\det\begin{pmatrix}(E_j)_2\\(e_j)_2\end{pmatrix} = 2\mathrm{i}\big(q_{ej}^2\sin(\chi_{ej}) - Z_{j-1}\cos(\chi_{ej})\big) = 2\mathrm{i}\mathcal{E}_{21}^{(j)},
\end{aligned} \tag{A.4}$$

which correspond to the electron part and are related to the elements of a matrix

$$(E_j)(e_j)^{-1} = \frac{2\mathrm{i}}{\det(e_j)}(\mathcal{E}^{(j)}). \tag{A.5}$$

The corresponding matrices for the holes are

$$\begin{aligned}
&\det\begin{pmatrix}(H_j)_1\\(h_j)_1\end{pmatrix} = 2\mathrm{i}\sin(\chi_{hj}) = -2\mathrm{i}\mathcal{H}_{12}^{(j)}\\
&\det\begin{pmatrix}(H_j)_1\\(h_j)_2\end{pmatrix} = 2\mathrm{i}q_{hj}\cos(\chi_{hj}) = 2\mathrm{i}\mathcal{H}_{11}^{(j)}\\
&\det\begin{pmatrix}(H_j)_2\\(h_j)_1\end{pmatrix} = -2\mathrm{i}(q_{hj}\cos(\chi_{hj}) + Z_{j-1}\sin(\chi_{hj})) = -2\mathrm{i}\mathcal{H}_{22}^{(j)}\\
&\det\begin{pmatrix}(H_j)_2\\(h_j)_2\end{pmatrix} = 2\mathrm{i}\big(q_{hj}^2\sin(\chi_{hj}) - Z_{j-1}\cos(\chi_{hj})\big) = 2\mathrm{i}\mathcal{H}_{21}^{(j)},
\end{aligned} \tag{A.6}$$

which are related to the elements of the matrix

$$(H_j)(h_j)^{-1} = \frac{2\mathrm{i}}{\det(h_j)}(\mathcal{H}^{(j)}). \tag{A.7}$$

Appendix B. The evaluation of the $|M_{N-1,N}|$ and $|M_{N-3,N-2}|$ determinants

As an example we calculate explicitly $|M_{N-1,N}|$ for the one-layer and two-layer cases and $|M_{N-3,N-2}|$ for the one-layer case. So for one layer we have

$$\begin{aligned}
|M_{N-1,N}| \rightarrow |M_{7,8}| &= \det\left(\begin{array}{c|c} (L_1) & (E_1) \\ \hline (L_2) & \quad\quad (H_1) \\ & (e_1) \end{array}\right)\\
&= \det(e_1)\det\left(\begin{array}{c|c} (L_1) & \\ \hline (L_2) & (H_1) \end{array}\right)\\
&= \det(e_1)\det(H_1)\delta_{1,2},
\end{aligned} \tag{B.1}$$

where $\delta_{1,2}$ is defined in appendix A and is the determinant of L_1. In a similar manner we calculate $|M_{N-3,N-2}|$. For one layer we have

$$\begin{aligned}
|M_{N-3,N-2}| \rightarrow |M_{5,6}| &= \det\left(\begin{array}{c|c} (L_1) & (E_1) \\ \hline (L_2) & \quad\quad (H_1) \\ & \quad\quad (h_1) \end{array}\right)\\
&= \det(h_1)\det\left(\begin{array}{c|c} (L_1) & (E_1) \\ \hline (L_2) & \end{array}\right)\\
&= \det(h_1)\det(E_1)\delta_{3,4}.
\end{aligned} \tag{B.2}$$

The determinants that occur in the above expressions are $\delta_{i,j}$, which contain the elements of the ith and jth rows of the first two columns. They are

$$\delta_{1,2} = -\mathrm{i}\big(k_L^+ + k_L^-\big)u_L v_L \equiv \det(L_1) \tag{B.3}$$

$$\delta_{3,4} = -\mathrm{i}\big(k_L^+ + k_L^-\big)u_L v_L \equiv \det(L_2). \tag{B.4}$$

For the two-layer case we have $N = 12$

$$\begin{aligned}
|M_{N-1,N}| \to |M_{11,12}| &= \det\left(\begin{array}{c|cccc}
(L_1) & (E_1) & & & \\ \hline
(L_2) & & (H_1) & & \\
 & (e_1) & & (E_2) & \\
 & & (h_1) & & (H_2) \\
 & & & (e_2) &
\end{array}\right) \\
&= \det(e_2)\det\left(\begin{array}{c|ccc}
(L_1) & (E_1) & & \\ \hline
(L_2) & & (H_1) & \\
 & (e_1) & & \\
 & & (h_1) & (H_2)
\end{array}\right) \\
&= \det(e_2)\det(H_2)\det\left(\begin{array}{c|cc}
(L_1) & (E_1) & \\ \hline
(L_2) & & (H_1) \\
 & (e_1) &
\end{array}\right) \\
&= \det(e_2)\det(H_2)\det(e_1)\det\left(\begin{array}{c|c}
(L_1) & \\ \hline
(L_2) & (H_1)
\end{array}\right) \\
&= \det(e_2)\det(H_2)\det(e_1)\det(H_1)\delta_{1,2}.
\end{aligned} \tag{B.5}$$

The expansions of $|M_{N-1,N}|$ and $|M_{N-3,N-2}|$ for n layers are obtained by induction and are

$$|M_{N-1,N}| = \left(\prod_{i=1}^{n}\det(e_i)\det(H_i)\right)\delta_{1,2} \tag{B.6}$$

and

$$|M_{N-3,N-2}| = \left(\prod_{i=1}^{n}\det(h_i)\det(E_i)\right)\delta_{3,4}. \tag{B.7}$$

Appendix C. Evaluation of γ

First we calculate γ for the one-layer case. Therefore we rewrite the matrix B_1 in a slightly different way, by displaying the two rows for each 2×2 submatrix, i.e.

$$B_1 \equiv \left(\begin{array}{c|cc|c}
(L_1)_1 & (E_1)_1 & & \\
(L_1)_2 & (E_1)_2 & & \\ \hline
(L_2)_1 & & (H_1)_1 & \\
(L_2)_2 & & (H_1)_2 & \\
 & (e_1)_1 & & (R_1)_1 \\
 & (e_1)_2 & & (R_1)_2 \\ \hline
 & & (h_1)_1 & (R_2)_1 \\
 & & (h_1)_2 & (R_2)_2
\end{array}\right), \tag{C.1}$$

where the subscripts $i = 1, 2$ of $(S)_i$ stand for the ith row of the corresponding 2×2 submatrix (S). We will calculate the determinants of the complement matrices in (C.1) that enter equation (40) for $N = 8$.

First we calculate $|M_{N-2,N}| \rightarrow |M_{6,8}|$,

$$
|M_{6,8}| = \det \left(\begin{array}{c|cc} (L_1)_1 & (E_1)_1 & \\ (L_1)_2 & (E_1)_2 & \\ \hline (L_2)_1 & & (H_1)_1 \\ (L_2)_2 & & (H_1)_2 \\ & (e_1)_1 & \\ \hline & & (h_1)_1 \end{array} \right)
$$

$$
= \det \begin{pmatrix} (H_1)_1 \\ (h_1)_1 \end{pmatrix} \det \left(\begin{array}{c|c} (L_1)_1 & (E_1)_1 \\ (L_1)_2 & (E_1)_2 \\ \hline (L_2)_2 & \\ & (e_1)_1 \end{array} \right) - \det \begin{pmatrix} (H_1)_2 \\ (h_1)_1 \end{pmatrix} \det \left(\begin{array}{c|c} (L_1)_1 & (E_1)_1 \\ (L_1)_2 & (E_1)_2 \\ \hline (L_2)_1 & \\ & (e_1)_1 \end{array} \right)
$$

$$
= \det \begin{pmatrix} (H_1)_1 \\ (h_1)_1 \end{pmatrix} \left\{ \det \begin{pmatrix} (E_1)_1 \\ (e_1)_1 \end{pmatrix} \det \begin{pmatrix} (L_1)_2 \\ (L_2)_2 \end{pmatrix} - \det \begin{pmatrix} (E_1)_2 \\ (e_1)_1 \end{pmatrix} \det \begin{pmatrix} (L_1)_1 \\ (L_2)_2 \end{pmatrix} \right\}
$$

$$
- \det \begin{pmatrix} (H_1)_2 \\ (h_1)_1 \end{pmatrix} \left\{ \det \begin{pmatrix} (E_1)_1 \\ (e_1)_1 \end{pmatrix} \det \begin{pmatrix} (L_1)_2 \\ (L_2)_1 \end{pmatrix} - \det \begin{pmatrix} (E_1)_2 \\ (e_1)_1 \end{pmatrix} \det \begin{pmatrix} (L_1)_1 \\ (L_2)_1 \end{pmatrix} \right\}
$$

$$
= \sum_{l_1,k_1} (-1)^{l_1+k_1} \det \begin{pmatrix} (H_1)_{l_1} \\ (h_1)_1 \end{pmatrix} \det \begin{pmatrix} (E_1)_{k_1} \\ (e_1)_1 \end{pmatrix} \det \begin{pmatrix} (L_1)_{\bar{k}_1} \\ (L_2)_{\bar{l}_1} \end{pmatrix}, \tag{C.2}
$$

where the indices $l_1, k_1 = 1, 2$ and the complement indices $\bar{l}_1$ and $\bar{k}_1$ are defined as follows:

$$
\bar{i} = \begin{cases} 2, & \text{for} \quad i = 1 \\ 1, & \text{for} \quad i = 2. \end{cases} \tag{C.3}
$$

In a similar manner we calculate the other subdeterminants. We have

$$
|M_{5,8}| = \sum_{l_1,k_1} (-1)^{l_1+k_1} \det \begin{pmatrix} (H_1)_{l_1} \\ (h_1)_1 \end{pmatrix} \det \begin{pmatrix} (E_1)_{k_1} \\ (e_1)_2 \end{pmatrix} \det \begin{pmatrix} (L_1)_{\bar{k}_1} \\ (L_2)_{\bar{l}_1} \end{pmatrix}, \tag{C.4}
$$

$$
|M_{6,7}| = \sum_{l_1,k_1} (-1)^{l_1+k_1} \det \begin{pmatrix} (H_1)_{l_1} \\ (h_1)_2 \end{pmatrix} \det \begin{pmatrix} (E_1)_{k_1} \\ (e_1)_1 \end{pmatrix} \det \begin{pmatrix} (L_1)_{\bar{k}_1} \\ (L_2)_{\bar{l}_1} \end{pmatrix}, \tag{C.5}
$$

$$
|M_{5,7}| = \sum_{l_1,k_1} (-1)^{l_1+k_1} \det \begin{pmatrix} (H_1)_{l_1} \\ (h_1)_2 \end{pmatrix} \det \begin{pmatrix} (E_1)_{k_1} \\ (e_1)_2 \end{pmatrix} \det \begin{pmatrix} (L_1)_{\bar{k}_1} \\ (L_2)_{\bar{l}_1} \end{pmatrix}. \tag{C.6}
$$

To write the γ term in a compact form, we rewrite the Δ subdeterminants in terms of the lines of (R_1) and (R_2) matrices given in appendix A.1. So from the determinant of (B_1) we obtain for a single layer our final form after reordering the determinant product

$$
\begin{aligned}
D\gamma = \sum_{l_1,l_2,k_1,k_2} & (-1)^{l_2+k_2+1} \det \begin{pmatrix} (L_1)_{\bar{k}_1} \\ (L_2)_{\bar{l}_1} \end{pmatrix} \det \begin{pmatrix} (R_1)_{k_2} \\ (R_2)_{l_2} \end{pmatrix} \\
& \times \left\{ (-1)^{l_1+k_1} \det \begin{pmatrix} (H_1)_{l_1} \\ (h_1)_{\bar{l}_2} \end{pmatrix} \det \begin{pmatrix} (E_1)_{k_1} \\ (e_1)_{\bar{k}_2} \end{pmatrix} \right\}.
\end{aligned} \tag{C.7}
$$

For n layers we have by induction

$$D\gamma = \sum_{\{l_{n+1}\},\{k_{n+1}\}} (-1)^{l_{n+1}+k_{n+1}+1} \det\begin{pmatrix}(L_1)_{\bar{k}_1}\\(L_2)_{\bar{l}_1}\end{pmatrix} \det\begin{pmatrix}(R_1)_{k_{n+1}}\\(R_2)_{l_{n+1}}\end{pmatrix} \tag{C.8}$$

$$\times\left\{\prod_{j=1}^{n}(-1)^{l_j+k_j} \det\begin{pmatrix}(H_j)_{l_j}\\(h_j)_{\bar{l}_{j+1}}\end{pmatrix} \det\begin{pmatrix}(E_j)_{k_j}\\(e_j)_{\bar{k}_{j+1}}\end{pmatrix}\right\}, \tag{C.9}$$

where $\{l_{n+1}\}$, $\{k_{n+1}\}$ are the sets of indices $\{l_1,\ldots,l_{n+1}\}$ and $\{k_1,\ldots,k_{n+1}\}$, respectively. We simplify this expression by using short symbols for the determinants as elements of matrices to be given in appendix A.2 and the main text, to obtain

$$D\gamma = -(2\mathrm{i})^{2n} \sum_{\{l_{n+1}\},\{k_{n+1}\}} \mathcal{L}_{k_1,l_1}\left(\prod_{j=1}^{n}\mathcal{H}^{(j)}_{l_j,l_{j+1}}\mathcal{E}^{(j)}_{k_j,k_{j+1}}\right)\mathcal{R}_{k_{n+1},l_{n+1}}. \tag{C.10}$$

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