Minigap in superconductor–ferromagnet junctions with inhomogeneous magnetization

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We consider the minigap in a disordered ferromagnet (F) in contact with a superconductor (S) in the situation when the magnetization of the F layer is inhomogeneous in space and noncollinear. If the magnetization is strongly inhomogeneous, it effectively averages out, and the minigap survives up to the exchange field $h_c \sim (L/a)E_{Th}$, where $L$ is the thickness of the F layer, $a$ is the scale on which the magnetization varies, and $E_{Th}$ is the Thouless energy. Technically, we use the “triplet” version of the Usadel equations, including both singlet and triplet components of the Green’s functions. In many cases, the effect of disordered magnetization may be effectively included in the conventional Usadel equations as the spin-flip scattering term. In the case of low-dimensional magnetic inhomogeneities (we consider spiral magnetization as an example), however, the full set of “triplet” equations must be solved.

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I. INTRODUCTION

A normal metal in contact with a superconductor acquires some superconductive properties; this phenomenon is known as the proximity effect. One of the most prominent manifestations of the proximity effect is the (mini)gap in the single-electron spectrum of the normal metal. While the density of states in the normal metal is spatially dependent, the minigap is a property of the normal part as a whole. In the diffusive limit, if the thickness of the normal metal $L$ is larger than the coherence length, the characteristic scale of the minigap $E_g$ is set by the Thouless energy $E_{Th} = D/L^2$, where $D$ is the diffusion constant (we put $\hbar = 1$). Experimentally, the minigap can be directly probed by a scanning tunneling microscope (see, e.g., Ref.\textsuperscript{2} and references therein).

Nowadays, the proximity effect in more complicated superconductor–ferromagnet (SF) structures is actively studied (see Ref.\textsuperscript{3} for a recent review of theoretical and experimental progress). While the majority of earlier theoretical studies treated the case of single-domain ferromagnets, one of the open questions is the influence of a domain structure. For example, in some setups, inhomogeneous magnetization may generate long-range triplet superconducting correlations\textsuperscript{4}.

In a single-domain ferromagnet, the exchange field $h$ (measured in energy units) shifts the densities of states for the two spin subbands in the opposite directions, therefore the minigap in the spectrum closes at $h \sim E_{Th}\textsuperscript{2}$. A domain structure would effectively lead to averaging the nonuniform field $\mathbf{h}(\mathbf{r})$ acting on electrons; hence one can expect that the minigap would survive even at $h \gg E_{Th}$. In previous studies, the influence of inhomogeneous magnetization on the density of states was considered only in situations where the minigap was absent\textsuperscript{6,7} while the influence of a domain structure on the minigap has not been investigated.

In this paper, we study the minigap in SF junctions in the presence of inhomogeneous magnetization with the help of the Usadel equations in the form allowing for the triplet superconducting component\textsuperscript{8} We introduce a generalization of the well-known $\theta$ parametrization\textsuperscript{9} which involves, in addition to $\theta$, a complex vector function $\mathbf{M}$ with the same number of components as for the exchange field $\mathbf{h}$ (three in the general case).

The problem has three relevant energy scales: $E_{Th}$, $h$, and the energy $E_d = D/a^2$ associated with the length scale $a$ over which the magnetization varies (typically, of the order of the domain size). Note that the superconducting gap $\Delta$ will not play any role, as it is taken to be much larger than $E_{Th}$ and $h$. Throughout the paper we assume that the domains are small and that the ferromagnetic exchange field is weak,

$$E_d \gg h, \quad E_d \gg E_{Th},$$

making no assumption on the relative scale of $h$ and $E_{Th}$.

First we consider a SF (or SFS) system with randomly oriented magnetization [Fig. I(a)] described by the pair correlation function

$$\mathbf{h}(\mathbf{r})\mathbf{h}(\mathbf{r'}) = F(\mathbf{r} - \mathbf{r'}) ,$$

where the averaging is over an ensemble. We assume that the integral of the correlation function $F(\mathbf{r} - \mathbf{r'})$ vanishes,

$$\int F(\mathbf{r})\, d\mathbf{r} = 0,$$

and take $a$ to be the corresponding length scale. Physically, it means that the field $\mathbf{h}$ averages out on the scale $a$ (of the order of several domain sizes). This assumption appears necessary for the smallness of the triplet superconducting correlations and for the possibility to take them into account as an additional effective local term in the Usadel equation on the singlet component. Such a reduction is possible for the three-dimensional disorder (in the whole range of parameters, except at very low exchange fields and at energies near the minigap edge,
where $\hat{\tau}$ and $\hat{\sigma}$ are the Pauli matrices in the Nambu and spin spaces, respectively; $E$ is the energy; $h$ is the exchange field; and $\Delta$ is the superconducting order parameter. For simplicity, we choose $\Delta$ to be real and do not consider systems with a phase difference.

The solution has the form

$$
\hat{g} = \hat{\tau}_3 (g_0 \hat{\sigma}_0 + g \hat{\sigma}) + \hat{\tau}_1 (f_0 \hat{\sigma}_0 + f \hat{\sigma}).
$$

The normalization condition can be resolved by the parametrization

$$
g_0 = M_0 \cos \theta, \quad g = iM \sin \theta, \quad f_0 = M_0 \sin \theta, \quad f = -iM \cos \theta,
$$

with complex functions $\theta$, $M_0$, and $M$, and with the constraint

$$M_0^2 - M^2 = 1.
$$

The Usadel equation (6) then yields one scalar and one vector equation:

$$
\frac{D}{2} \nabla^2 \theta + M_0 (iE \sin \theta + \Delta \cos \theta) - (hM) \cos \theta = 0,
$$

$$
\frac{D}{2} \left( M \nabla^2 M_0 - M_0 \nabla^2 M \right) - M (iE \cos \theta - \Delta \sin \theta)
- hM_0 \sin \theta = 0.
$$

We may note the following general properties of Eqs. (10) and (11):

(i) In the absence of ferromagnetism, $h = 0$, $M_0 = 1$, $M = 0$, and Eqs. (10) and (11) reduce to the conventional Usadel equation.

(ii) For the uniform nonzero magnetization $h = \text{const}$, Eqs. (10) and (11) imply the triplet vector $M$ directed along the field $h$. 

(iii) A convenient feature of the parametrization is that in the Matsubara representation [with $-iE$ replaced by the Matsubara frequency $\omega_n$ in Eqs. (10) and (11)] the functions $\theta$, $M_0$, and $M$ are real.

The density of states (summed over spin projections and normalized to the normal-metallic value) is standardly expressed via the retarded and advanced Green’s functions, $\nu = \text{Tr} \left[ \hat{\tau}_3 \hat{\sigma}_0 \left( \hat{g}^R - \hat{g}^A \right) \right] / 8$, which yields

$$
\nu = \text{Re} \, g_0 = \text{Re} \left( M_0 \cos \theta \right).
$$

Below we consider SF and SFS systems and employ the rigid boundary conditions, which imply that the bulk solution in the superconductor with constant $\Delta$ is valid up to the SF interface, and the Green’s function is continuous. The rigid boundary conditions are applicable if the SF interface is transparent and the F material is much more disordered than the S one. Thus at SF interfaces

$$
\theta = \frac{\pi}{2}, \quad M_0 = 1, \quad M = 0,
$$
where the first condition is justified since $h \ll \Delta$ and we consider energies $E \lesssim E_{\mathrm{Th}}$, hence $E \ll \Delta$. The boundary conditions at the free surface of the F layer in the SF system are
\[
\frac{d\theta}{dz} = 0, \quad \frac{dM_0}{dz} = 0, \quad \frac{dM}{dz} = 0. \tag{14}
\]
Below we consider Eqs. (10) and (11) in the F part where $\Delta = 0$; the superconducting correlations are induced due to the boundary conditions $\Gamma_{\text{sf}}$.

III. DISORDERED MAGNETIZATION

We start our analysis with the disordered system [Fig. 1(a)]. To reduce the effect of the inhomogeneous field $h$ to a spin-flip term, we use the self-consistent scheme for determining the spin-flip rate $\Gamma_{\text{sf}}$: We first solve the conventional “spin-flip” Usadel equation,
\[
\frac{D}{2}\nabla^2 \theta + iE \sin \theta - 2\Gamma_{\text{sf}} \sin \theta \cos \theta = 0. \tag{15}
\]
We expect that variations of $h$ in space lead to the effective averaging of the magnetization, hence the vector part $\mathbf{M}$ of the Green’s function is small. Thus we substitute the solution of Eq. (15) into the linearized version of the vector Usadel equation (11) to obtain
\[
\left(\frac{D}{2}\nabla^2 + iE \cos \theta\right) \mathbf{M} = -h \sin \theta. \tag{16}
\]
This equation is solved for $\mathbf{M}$ with the appropriate boundary conditions, and further $\Gamma_{\text{sf}}$ is found self-consistently as
\[
\Gamma_{\text{sf}} = \left\langle \frac{hM \cos \theta}{2\sin \theta} \right\rangle, \tag{17}
\]
where the average is taken over a region much larger than the characteristic scale of variation of the field $h$.

For this scheme to work, not only must we require $|\mathbf{M}| \ll 1$, but the (typically stronger) condition
\[
|\mathbf{M}|^2 \ll \frac{\Gamma_{\text{sf}}}{E_{\text{Th}}} \tag{18}
\]
[since in the scalar Usadel equation (10) we neglect the term quadratic in $\mathbf{M}$, while keeping $\Gamma_{\text{sf}}$].

Equation (10) is an inhomogeneous linear equation on $\mathbf{M}$. We consider energies $E \lesssim E_{\text{Th}}$, hence $|\theta| \sim 1$, and the $(iE \cos \theta)$ term affects the Green’s function of the linear operator in the left-hand side at a length scale of order $L$. It can be neglected if it produces a small relative correction to $\mathbf{M}$, which in turn depends on the number of dimensions in which $h(r)$ varies. While we always consider three-dimensional (3D) samples, $h$ can either depend on all the three coordinates or be a function of only two (quasi-2D films) or one (quasi-1D wires) coordinate. Without the $(iE \cos \theta)$ term, the Green’s function of Eq. (10) is $G \propto 1/r$ in 3D, $G \propto \ln r$ in 2D, and $G \propto r$ in 1D. The inaccuracy introduced due to neglecting the $(iE \cos \theta)$ term is
\[
\delta \mathbf{M}(\mathbf{r}) = - \int \frac{\delta G(\mathbf{r} - \mathbf{r}_1)h(\mathbf{r}_1) \sin \theta(\mathbf{r}_1)d^3\mathbf{r}_1}{\mathbf{M} \sin \theta}. \tag{19}
\]
where the correction $\delta G$ is negligible at length scales smaller than $L$. A straightforward estimate using the correlation function (2) with the vanishing integral (3) gives $|\delta \mathbf{M}|^2 \sim a^2 + d^2L^2 - d^2h^2/D^2$ and $|\mathbf{M}|^2 \sim a^2h^2/D^2$, hence
\[
\frac{|\delta \mathbf{M}|^2}{|\mathbf{M}|^2} \sim \left(\frac{a}{D}\right)^{-2} \tag{20}
\]
Therefore we can neglect the $(iE \cos \theta)$ term in 3D, can obtain order-of-magnitude estimates in this way in 2D, and cannot do it in 1D. Note that we have also neglected the effect of boundaries. It can be taken into account via “mirror charges” (of the same or opposite sign for the “Hamiltonian” on the left-hand side of Eq. (16), we find that the effective spin-flip approximation breaks down. In this region, the zero mode becomes a low-energy mode with a small contribution of the low-energy mode is determined by
\[
c_0 = \frac{1}{E_0} \int d^3\mathbf{r}(h\mathbf{M}_0) \sin \theta. \tag{22}
\]
Using the correlation function \( \langle \overline{c_0^2} \rangle \sim a^{2+d}L^{-2h^2/E_2^2} \). Finally, the condition \( \overline{c_0M_0}\overline{c} \ll \Gamma_{sf}/E_{Th} \) that the contribution from the low-energy mode is small, yields

\[
\frac{E_0}{E_{Th}} \gg \left( \frac{a}{L} \right)^{d/2} .
\] (23)

The energy \( E_0 \) grows as we go away from the gap-closing point at \( \Gamma_{sf} = 0, E = E_g \). The perturbation theory yields

\[
\frac{E_0}{E_{Th}} \sim \max \left( \sqrt{\frac{|E - E_g|}{E_{Th}}}, \frac{\Gamma_{sf}}{E_{Th}} \right) .
\] (24)

The combination of Eqs. (23) and (24) determines a small region near the \( \Gamma_{sf} = 0, E = E_g \) point [shown as the shaded region in Fig. 1(b)], where the spin-flip approximation (with the effective rate \( \Gamma_{sf} \)) breaks down due to the noninvertibility of the linear operator in Eq. (16).

Summarizing, the Usadel equations (10) and (11) in the 3D problem reduce to the conventional Usadel equation (16) with the spin-flip rate (4) if the conditions (11) and (23) are satisfied. Then the results of Ref. 11 for the \( E_g(\Gamma_{sf}) \) dependence apply. The critical value of the exchange field, at which the minigap closes, is given by Eq. (4) and is much larger than \( h_c \) in the case of a homogeneous ferromagnet.

\section*{IV. SPIRAL MAGNETIZATION}

The above discussion in terms of the spin-flip approximation applies to the 3D case and should give an order-of-magnitude estimate in the 2D case. In 1D setups (with the field \( h \) depending only on one of the coordinates), one generally needs to solve the full nonlinear set of Eqs. (10) and (11). Below we present an analysis of the two examples [SFS and SF systems, see Figs. 1(c) and 1(d), respectively] with the regular spiral magnetic structure:

\[
h = h(\cos kz, \sin kz, 0),
\] (25)

where the \( z \) direction is perpendicular to the SF interface(s). In both the examples we are unable to analytically find the full dependence of the minigap on the strength of the field \( h \), but we calculate the critical value \( h_c \) at which the minigap closes.

Technically, the SF case turns out to be more complicated, because the linearization over \( M \) does not work in this situation (while it is still applicable in the SFS system).

\subsection*{A. SFS case}

We consider the spiral ferromagnet of length \( 2L \) [Fig. 1(c)] with the rigid boundary conditions (13) at the

\[
\text{FIG. 2: Effective quantum-mechanical potentials for (a) SFS and (b) SF junctions. The minigap vanishes when the Hamiltonian with the corresponding potential has the ground state with zero energy. In both cases, the impenetrable walls are at \( z = 0 \) and \( z = 2L \). (a) Rectangular potential well. (b) Potential well with a \( \delta \)-functional contribution in the middle.}
\]

SF interfaces. With these boundary conditions and at zero energy it is possible to perform a derivation similar to that in the disordered 3D case. To find the gap-closing point, we find the minimal value of \( h \) at which the \( E = 0 \) solution with \( \theta = \pi/2 \) has a bifurcation (a gapless solution forks out). Linearizing in \( (\theta - \pi/2) \) and in \( M \) at \( E = 0 \), we solve Eq. (10), without taking into account boundary conditions, by the oscillating function

\[
M_{osc} = \frac{2h}{Dk^2} .
\] (26)

The boundary conditions \( M(0) = M(2L) = 0 \) are easily satisfied by adding a smooth (nonoscillating) term linear in \( z \) of the same order of magnitude: \( M = M_{osc} + M_{sm} \). On substituting this solution into the linearized scalar Usadel equation, we find the effective equation for the smooth part of \( \theta(z) \) [the oscillating part of \( \theta(z) \) has a smaller order of magnitude and is neglected; only \( M_{osc} \) needs to be taken into account at this step]:

\[
\left( \nabla_z^2 + \frac{4h^2}{D^2k^2} \right) \left( \theta - \frac{\pi}{2} \right) = 0
\] (27)

with the boundary conditions

\[
\theta(0) = \theta(2L) = \frac{\pi}{2} .
\] (28)

Equation (27) can be viewed as the Schrödinger equation at zero energy with \( h = 1 \), mass \( 1/2 \), and the constant potential \( -4h^2/(D^2k^2) \), while \( (\theta - \pi/2) \) plays the role of the eigenfunction. The boundary conditions (28) correspond to the impenetrable walls at \( z = 0 \) and \( z = 2L \), see Fig. 2(a).

Therefore, the bifurcation of a nontrivial solution for the problem (27) and (28) (i.e., closing of the minigap) with increasing \( h \) corresponds to the ground-state energy crossing zero. This immediately leads to the result

\[
h_{c}^{SFS} = \left( \frac{\pi}{4} \right) \frac{Dk}{L} .
\] (29)
We verify that the linearization over $M$ is justified under the conditions (11) (with $E_d = Dk^2$) which, in turn, reduce to the single requirement $kL \gg 1$ at $\hbar \sim \hbar_{c}^{SFS}$. Note that Eq. (29) formally coincides with the expression (11) in combination with the critical value of $\Gamma_{sf}$ from Ref. 11. The critical value of the exchange field is, as in the previous example, much larger than the Thouless energy: $\hbar_{c}^{SFS} \sim (kL)E_{Th}$.

### B. SF case

Another example we consider is one half of the above SFS junction: the SF junction with the ferromagnet of length $L$ [Fig. 1(d)]. In this case, the open boundary conditions cannot be satisfied at small $M$ and the linearization over $M$ does not work. Physically, $M$ is enhanced because electrons incident on the outer F surface through the field $h(z)$, feel the same $h(z)$ after reflection, hence the effective average of $h$ is nonzero. Thus we need to solve the full nonlinear Eq. (11) at $E = 0$. Below the gap, $M$ is real, and it is convenient to introduce the new complex function

$$m(z) = M_1 + iM_2$$

(30)

(where $M_1$ and $M_2$ are the two components of the vector $M$). Then in the new complex notation Eq. (11) takes the form

$$\frac{D}{2} \left[ m'' - \left( \frac{M''}{M_0} \right) m \right] + h e^{ikz} = 0, \quad M_0 = \sqrt{1 + mm^*},$$

(31)

with the boundary conditions $m(0) = 0$ and $m'(L) = 0$.

We separate rapidly oscillating modes,

$$m = b_0 + b_1 e^{ikz} + b_{-1} e^{-ikz} + \ldots,$$

(32)

and keep only the leading ones (the amplitudes $b_n$ are slow functions of $z$ and decrease in magnitude with increasing $|n|$, as we verify below). The equations for different modes are coupled, and after a straightforward algebra, we express the amplitudes $b_1$ and $b_{-1}$ via the smooth part $b_0$:

$$b_1 = \frac{h}{Dk^2} \left( 2 + |b_0|^2 \right), \quad b_{-1} = \frac{h}{Dk^2} \overline{b_0^*}.$$  

(33)

Substituting these amplitudes in Eq. (31) and parametrizing $b_0 = -i e^{ikL} \sinh \varphi$, we arrive at the effective equation on $\varphi(z)$:

$$\varphi'' + \frac{\varphi^2}{2} \sinh \varphi \cosh \varphi = 0,$$

(34)

with the boundary conditions

$$\varphi(0) = 0, \quad \varphi'(L) = \kappa \cosh \varphi(L),$$

(35)

where $\kappa = 2h/(Dk)$. The solution to this equation must be substituted back into the scalar Usadel equation (10) to find the bifurcation point of the solution $\theta = \pi/2$. Linearizing the equation in the vicinity of the bifurcation point, we obtain

$$\left[ \nabla_{z}^2 + \varphi^2 \left( 1 + \frac{\sinh^2 \varphi}{2} \right) - (k \varphi \sinh \varphi) \sin k(z - L) - \left( \frac{\varphi^2 \sinh^2 \varphi}{2} \right) \cos 2k(z - L) + \ldots \right] \left( \theta - \frac{\pi}{2} \right) = 0.$$  

(36)

Again, we need to take into account not only the smooth part of $\theta$, but also the oscillating modes at $\pm k$:

$$\theta - \frac{\pi}{2} = t_0 + t_1 \sin k(z - L) + \ldots$$

(37)

Solving coupled equations for the amplitudes $t_n$ (which are slow functions of $z$ and decrease in magnitude with increasing the order of the harmonic), we find, to the leading order in $\varphi/k$,

$$t_1 = - \left( \frac{\varphi}{k} \sinh \varphi \right) t_0,$$

(38)

and finally obtain the equation for the smooth component $t_0$:

$$\left( \nabla_{z}^2 + \varphi^2 \cosh^2 \varphi \right) t_0 = 0,$$

(39)

with the boundary conditions

$$t_0(0) = 0, \quad t_0'(L) = \left[ \kappa \sinh \varphi(L) \right] t_0(L).$$

(40)

At the bifurcation point (i.e., when the minigap closes), this homogeneous linear equation acquires a nonzero solution. The resulting problem again has a quantum-mechanical analogy if we symmetrically continue the potential $-\varphi^2 \cosh^2 \varphi(z)$ in the Schrödinger equation (39) from the $(0, L)$ interval to $(L, 2L)$; see Fig. 2(b). As a result, we obtain the Schrödinger equation at zero energy with $h = 1$ and mass $1/2$, while $t_0$ plays the role of the eigenfunction. At $z = 0$ and $z = 2L$, we obtain the impenetrable walls, while the boundary condition (40) at $z = L$ corresponds to the following $\delta$-functional contribution to the potential: $-2 \left[ \kappa \sinh \varphi(L) \right] \delta(x - L)$.

Therefore, the appearance of a nontrivial solution for the problem (39) and (40) at the bifurcation point with increasing $h$ corresponds to the situation, in which the ground state of the Schrödinger equation has zero energy. Numerically, we find that this happens at $\varphi = 0.5955/L$, which translates into the critical value of the exchange field

$$\hbar_{c}^{SF} = 0.2977 \frac{Dk}{L}.$$  

(41)

Having found $\hbar_{c}^{SF}$, we can check that $b_0 \sim 1$, $b_{\pm 1} \sim 1/(kL)$, $b_{\pm 2} \sim 1/(kL)^2$, $t_1 \sim t_0/kL$, etc., confirming the validity of the expansions (42) and (57). Note that the critical strength of $h$ has the same order of magnitude as in the SFS case [and thus also agrees with the estimate (5)], but it has a smaller numerical prefactor.
V. CONCLUSIONS

In conclusion, we have shown that SF and SFS systems with random three-dimensional domain disorder admit an effective description in terms of the spin-flip rate $\Gamma_{sf}$. We have also considered SF and SFS junctions with spiral magnetic order, where the spin-flip approximation does not hold. In all the systems considered, the minigap survives up to the exchange fields of the order $E_{Th}$, i.e., much larger than $E_{Th}$. For an experimental observation of the effects described in the present paper, it is crucial to use weak ferromagnets with a very fine domain structure, so that the main constraints are satisfied.

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12. Our Green’s function is related to the one used in Ref. 2, $\hat{g}_{BVE}$, via a rotation $\hat{g} = \hat{U} \hat{g}_{BVE} \hat{U}^\dagger$ with $\hat{U} = (1 + i\hat{\tau}_3 \hat{\sigma}_3)(1 - i\hat{\sigma}_3)/2$ (plus inessential change of sign of $\vec{h}$). We prefer this definition because then the Usadel equation possesses explicit symmetry with respect to rotations of the exchange field $\vec{h}$.
13. Note that, in a uniform ferromagnet, $\textbf{M}$ parallel to $\vec{h}$ does not produce a “long-range triplet proximity effect” in the terminology of Ref. 14. For the long-range effect described in Ref. 14, one needs to generate a component of $\textbf{M}$ perpendicular to $\vec{h}$. For example, long-range triplet correlations are absent in Ref. 15 in that particular configuration of the inhomogeneous field, $\textbf{M}$ follows the direction of $\vec{h}$.
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