Atomic thickness hybrid F/S/F structures

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Abstract

We propose an exactly solvable model to describe the properties of atomic thickness hybrid ferromagnet-superconductor-ferromagnet (F/S/F) structures. We show that the superconducting critical temperature is always higher for antiparallel orientation of the ferromagnetic moments. However at low temperature the superconducting gap occurs to be larger for parallel orientation of the ferromagnetic moments. This leads to a peculiar temperature dependence of the proximity effect in (F/S/F) structures.

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I. INTRODUCTION

In recent years the superconductor-ferromagnet (S/F) hybrid structures attract a steadily growing interest. The actual progress in the preparation of S/F/S junctions permits to observe the transition from normal 0-junction to the so-called $\pi$-junction with the change of the thickness of the ferromagnetic layer [1,2]. Such a behavior has been predicted in [3,4] and it is related to the oscillations of a superconducting order parameter in the ferromagnetic layer. Another manifestation of the spin-dependent transport in S/F hybrid structures is the dependence of the critical temperature of metallic F/S/F sandwiches on the mutual orientation of ferromagnetic moments of the outer layers. On the basis of Usadel equations, applicable in the dirty limit, it has been demonstrated in [5–8], that the antiparallel orientation of the ferromagnetic moments is more favorable for superconductivity, i.e. it corresponds to the higher superconducting transition temperature and to the larger amplitude of the superconducting order parameter. Recently this effect has been observed on experiment [9]. Note also that for the first time the coupling between ferromagnets through a superconducting layer has been treated theoretically in [10] for the case of ferromagnetic insulators and observed on experiment in [11,12].

At the same time in [13,14], a microscopic multiterminal model for S-F hybrid structure at $T = 0$ has been proposed, where the ferromagnet was described by different density of states for opposite orientations of the magnetic moment. Then, it has been deduced that the superconducting gap is less influenced by the ferromagnetism for the case of parallel orientation of the F electrodes. Hence at $T = 0$, the parallel orientation of the ferromagnetic moments appears more favorable for superconductivity.
In the present work we analyze the properties of the microscopic model system comprising three coupled atomic-scale layers: one superconducting layer in between of two ferromagnetic layers, which can have parallel or antiparallel orientation of the magnetic moments. This model may be relevant for the description of layered superconductors like RuSr$_2$GdCu$_8$, where superconducting and magnetic layers alternate [15] as well as artificial S/F structures obtained by molecular beam epitaxy. Such a model can be solved exactly and so we may verify that the results for the critical temperature for a diffusive regime of electrons motion, obtained in [5–8], are also qualitatively applicable for a clean atomic layered system. We demonstrate that in all cases the antiparallel alignment of ferromagnetic moments corresponds to the higher transition temperature to the superconducting state. However at low temperature the situation may be different and as it follows from our analysis, the superconducting gap for parallel alignments of ferromagnetic moments increases faster with the decrease of the temperature comparing with the antiparallel alignment. At some temperature $T^*$ the gaps for parallel and antiparallel alignment coincides and at $T < T^*$ the gap is higher for parallel alignment. So at $T = 0$ the parallel alignment is more favorable for superconductivity while near $T_c$ the situation is inverse. This result is in accordance with [13,14], where the superconducting gap have been calculated at $T = 0$ in the framework of quite different model of bulk superconductor in the contact with small ferromagnetic electrodes.

II. SPIN-ORIENTATION-DEPENDENCE OF SUPERCONDUCTING TRANSITION TEMPERATURE

Adopting the model of [16], we consider a three layers system with one superconducting layer between two ferromagnetic layers, see Fig. 1. It is supposed that the coupling between layers is realized via the transfer integral $t$, which is relatively small ($t \ll T_c$), so the superconductivity can coexist with ferromagnetism in the adjacent layers. Introducing the notations $\varphi^{\dagger}_{\sigma}$ and $\eta^{\dagger}_{\sigma}$ for electrons creation operators in F layers and $\psi^{\dagger}_{\sigma}$ in S layer, the Hamiltonian of the system can be written as

$$H = H_0 + H_\psi + H_{\varphi\psi} + H_{\psi\eta}$$

$$H_0 = \sum_{p,\sigma} \left[ \xi^{\varphi}_{\sigma}(p)\varphi^{\dagger}_{\sigma}(p)\varphi_{\sigma}(p) + \xi(p)\psi^{\dagger}_{\sigma}(p)\psi_{\sigma}(p) + \xi^{\eta}_{\sigma}(p)\eta^{\dagger}_{\sigma}(p)\eta_{\sigma}(p) \right],$$

$$H_\psi = \sum_p \left[ \Delta^* \psi^\dagger_p(p)\psi_p(-p) + \Delta \psi^\dagger_p(p)\psi_p(-p) \right],$$

$$H_{\varphi\psi} = t \sum_{p,\sigma} \left[ \psi^\dagger_{\sigma}(p)\varphi_{\sigma}(p) + \varphi^\dagger_{\sigma}(p)\psi_{\sigma}(p) \right],$$

$$H_{\psi\eta} = t \sum_{p,\sigma} \left[ \psi^\dagger_{\sigma}(p)\eta_{\sigma}(p) + \eta^\dagger_{\sigma}(p)\psi_{\sigma}(p) \right],$$

where $H_0$ describes the free electrons motion in F layers with the spectra $\xi^{\varphi}_{\sigma}(p)$ and $\xi^{\eta}_{\sigma}(p)$ respectively, and with the spin-independent spectrum $\xi(p)$ in S layer. The BCS pairing in the middle S layer is treated in $H_\psi$ in the mean field approximation [17] and the coupling...
between neighboring layers via the transfer integral $t$ is described by $H_{\varphi\psi}$ and $H_{\psi\eta}$. Note that the electrons spectra in (1) are calculated from the Fermi energy. The superconducting order parameter satisfies the usual self-consistency equation

$$\Delta^* = |\lambda| \int \langle \psi_\uparrow^+(p)\psi_\uparrow^+(-p) \rangle \frac{d^2p}{(2\pi)^2},$$

(2)

where, $\lambda$ is the Cooper pairing constant which is assumed to be non zero in $S$ layers only.

Introducing in the usual way [17] the Green functions

$$G_{\alpha\beta} = - <T_\tau(\varphi_\alpha\psi_\beta^+)>, \ F_{\alpha\beta} = <T_\tau(\varphi_\alpha\psi_\beta^+)>, \ G_{\alpha\beta} = - <T_\tau(\psi_\alpha\psi_\beta^+)>, \ F_{\alpha\beta} = <T_\tau(\psi_\alpha\psi_\beta^+)>,$$

and writing the corresponding equations for the Green functions, we finally obtain the following exact expressions for the Green functions in $S$ layer:

$$G_{\uparrow\uparrow} = \frac{b^*}{a^* a + |\Delta|^2}; \ G_{\downarrow\downarrow} = \frac{a^*}{a^* b + |\Delta|^2};$$

$$F_{\downarrow\uparrow} = \frac{\Delta^*}{a^* a + |\Delta|^2}; \ F_{\uparrow\downarrow} = - \frac{\Delta^*}{a^* b + |\Delta|^2},$$

(3)

where

$$a = i\omega - \xi - t^2 \left[ \frac{1}{i\omega - \xi_\uparrow^*} + \frac{1}{i\omega - \xi_\uparrow^\eta} \right],$$

$$b = i\omega - \xi - t^2 \left[ \frac{1}{i\omega - \xi_\downarrow^*} + \frac{1}{i\omega - \xi_\downarrow^\eta} \right].$$

The self-consistency equation for superconducting order parameter is now written as

$$\Delta^* = |\lambda| T \sum_\omega \int F_{\downarrow\uparrow} \frac{d^2p}{(2\pi)^2}. $$

To calculate the critical temperature of the superconducting transition it is sufficient to know the anomalous Green function $F_{\downarrow\uparrow}$ in the linear approximation on $\Delta^*$. Then it is convenient to write the linearized self-consistency equation for $T_c$ in the following form [17]

$$\ln \left( \frac{T_c}{T_c^0} \right) = 2T_c \sum_\omega > 0 \left[ \frac{\pi}{\omega} - \int \text{Re}(f) \ d\xi \right],$$

(4)

where we have defined a reduced function $f = 1/(a^* b)$ and $T_c^0$ is the bare mean-field critical temperature of the central $S$ layer in the absence of the proximity effect (i.e. for $t = 0$).

In the case when both ferromagnetic layers are equivalent we may distinguish two different situations

either the parallel (P) orientation of the magnetic moments, where $\xi_\uparrow \equiv \xi_\uparrow^\varphi = \xi_\uparrow^\eta$ and $\xi_\downarrow \equiv \xi_\downarrow^\varphi = \xi_\downarrow^\eta$. 

3
or the anti-parallel (AP) orientation, where $\xi^\uparrow \equiv \xi^\uparrow_0$ and $\xi^\downarrow \equiv \xi^\downarrow_0$.

Firstly we consider the situation when the electron dispersion spectra in the ferromagnet differs only by the exchange field $h$ from the electron spectrum in S layer i.e. $\xi^\uparrow = \xi - h$ and $\xi^\downarrow = \xi + h$

Performing in (4) the integration over energy $\xi$ and summation over Matsubara’s frequencies $\omega = (2k + 1)\pi T_c$, we finally obtain

$$\ln \frac{T_{c0}}{T_{cP}} = \frac{1}{\pi^2 T_{cP}^2} \frac{2t^2}{8t^2 + h^2} \left\{ h^2 \Phi_1 \left( \frac{h}{2\pi T_{cP}} \right) + 4t^2 \left[ \Phi_1 \left( \frac{\sqrt{8t^2 + h^2} + h}{2\pi T_{cP}} \right) + \Phi_1 \left( \frac{\sqrt{8t^2 + h^2} - h}{2\pi T_{cP}} \right) \right] \right\},$$

where $T_{cP}$ ($T_{cAP}$) is the superconducting transition temperature for parallel (antiparallel) orientation of the F-layers magnetic moments and we define the function $\Phi_1$ through the Digamma function $\Psi$ as ($\gamma$ is Euler constant)

$$\Phi_1(x) = \frac{1}{2x^2} \left\{ \gamma + 2\ln(2) + \frac{1}{2} \left[ \Psi \left( \frac{1+ix}{2} \right) + \Psi \left( \frac{1-ix}{2} \right) \right] \right\}.$$  

Using (5) we can determine the relative variation of critical temperature $\delta T = (T_c - T_{c0})/T_{c0}$ in the two following limits:

**i)** in the limit $\sqrt{\frac{2t^2 + h^2}{T_c}} \to 0$ up to the fourth order over $t$ we have:

$$\delta T_P \simeq -\frac{7\zeta(3)}{(2\pi T_{c0})^2} t^2 + \frac{1}{(2\pi T_{c0})^4} \left[ \left( 62\zeta(5) - \frac{147}{2}\zeta(3)^2 \right) t^4 + \frac{31}{4}\zeta(5)t^2h^2 \right] +$$

$$+ \frac{1}{(2\pi T_{c0})^6} \left[ \left( \frac{1085}{16}\zeta(3)\zeta(5) - \frac{889}{8}\zeta(7) \right) t^4h^2 - \frac{127}{16}\zeta(7)t^2h^4 \right],$$

$$\delta T_P - \delta T_{AP} \simeq -\frac{1397\zeta(7)}{512\pi^6} t^4h^2 \frac{T_{c0}^6}{T_{c0}^6} \simeq -0.0029 \frac{t^4h^2}{T_{c0}^2}. \quad (6)$$

The last result, the difference $\delta T_P - \delta T_{AP}$, was already found for S/F multilayer in [7] (after correcting a sign mistake).

**ii)** in the limit $\sqrt{\frac{2t^2 + h^2}{T_c}} \to \infty$ and for $t << h$ we obtain:

$$\delta T_P \simeq -\frac{4t^2}{h^2} \left[ \gamma + \ln \left( \frac{h}{\pi T_{c0}} \right) + \frac{7\zeta(3)}{4\pi^2} \frac{t^2}{T_{c0}^2} \right],$$

$$\delta T_A \simeq -\frac{4t^2}{h^2} \left[ \gamma + \ln \left( \frac{h}{\pi T_{c0}} \right) \right],$$

4
\[ \delta T_P - \delta T_{AP} \simeq -\frac{7\zeta(3)}{4\pi^2} \frac{t^4}{h^2 T_{c0}^2} \simeq -0.21 \frac{t^4}{h^2 T_{c0}^2}. \]  

Also the difference of the critical temperatures \( \delta T_P - \delta T_{AP} \) coincides with that of the S/F multilayer [7].

We see that in all cases the difference between critical temperatures for parallel and antiparallel alignment is proportional to \( t^4 \), while the decrease of the critical temperature itself is proportional to \( t^2 \). This fact demonstrates that the spin-orientation dependence of \( T_c \) is related with a rather subtle interference effect between electrons coming from ferromagnetic layers.

Now we consider the case of a ferromagnetic half-metal, which we may model in (3) by \( \xi_\downarrow = \xi + h \) and \( \xi_\uparrow \to \infty \), that corresponds to a zero density of sates for the electrons with spin orientation along magnetic moment in ferromagnetic layers. Note that the limit \( \xi_\uparrow \to \infty \) is equivalent to take the transfer integral for electrons with spin up orientation equal to zero. This may be simply demonstrated from the initial equations for the Green functions. Performing integration over \( \xi \) and summation over Matsubara frequencies in the self-consistency equation, we can deduce the relative temperature variation \( \delta T = (T_c - T_{c0})/T_{c0} \) at the order up to \( t^4 \), in terms of the dimensionless field \( \hat{h} = h/(2\pi T_{c0}) \)

\[ \delta T_P = -\Phi_1(\hat{h}) \frac{t^2}{\pi^2 T_{c0}^2} \]
\[ + \left\{ \frac{1}{2} \Phi_1(\hat{h})^2 - 2\Phi_1(\hat{h}) \Phi_2(\hat{h}) - \frac{1}{\hat{h}^2} \left[ \frac{7}{16} \zeta(3) - \frac{3}{2} \Phi_1(\hat{h}) + \Phi_2(\hat{h}) \right] \right\} \frac{t^4}{\pi^4 T_{c0}^4}, \]

and

\[ \delta T_P - \delta T_{AP} = -\frac{1}{2\hat{h}^2} \left[ \frac{7}{8} \zeta(3) - \Phi_1(\hat{h}) \right] \frac{t^4}{\pi^4 T_{c0}^4}, \]

where the function \( \Phi_1 \) was defined before and the function \( \Phi_2 \) is

\[ \Phi_2(x) = \frac{1}{16i} \left[ \Psi'(\frac{1-ix}{2}) - \Psi'(\frac{1+ix}{2}) \right]. \]

In the limiting case \( h \to 0 \), which corresponds to the situation \( h \ll T_{c0} \), or simply \( \xi_\uparrow = \xi \), we have

\[ \delta T_P = -\left[ \frac{7}{8} \zeta(3) \right] \frac{t^2}{\pi^2 T_{c0}^2} + \left\{ \frac{31}{64} \zeta(5) - \frac{3}{2} \left( \frac{7}{8} \zeta(3) \right)^2 \right\} \frac{t^4}{\pi^4 T_{c0}^4}, \]

and the critical temperature difference is

\[ \delta T_P - \delta T_{AP} = -\frac{31}{64} \zeta(5) \frac{t^4}{\pi^4 T_{c0}^4} \simeq -0.50 \frac{t^4}{\pi^4 T_{c0}^4}. \]

In the opposite limit \( h \gg T_{c0} \), we find

\[ \delta T_P = -\frac{1}{2\hat{h}^2} \ln(\hat{h}) \frac{t^2}{\pi^2 T_{c0}^2} - \frac{7}{16} \zeta(3) \frac{t^4}{\hat{h}^2 \pi^4 T_{c0}^4}, \]
\[ \delta T_P - \delta T_{AP} = -4t^4 \ln \left( \frac{h}{2\pi T_{c0}} \right). \]  

(10)

Then we may conclude that in all cases the critical temperature is higher for the antiparallel alignment of the ferromagnetic moments.

### III. SUPERCONDUCTING GAP AT LOW TEMPERATURES

In this section we demonstrate that the proximity effect at low temperature is very special and that the superconducting gap at \( T = 0 \), for half-metal and for usual ferromagnet with small exchange field, is higher for parallel orientation in accordance with [13,14].

Firstly we consider the model of a half-metal with \( \xi_\uparrow \to \infty \) and \( \xi_\downarrow = \xi \). So the self consistency equations for parallel and antiparallel orientations may be written as

\[
\frac{1}{|\lambda| N(0)} = T \sum_\omega \frac{d\xi}{\omega^2 + \xi^2 + 2t^2 \frac{i\omega - \xi}{i\omega + \xi} + \Delta_P^2},
\]

\[ = T \sum_\omega \frac{d\xi}{\omega^2 + \xi^2 + 2t^2 \frac{\omega^2 - \xi^2}{\omega^2 + \xi^2} + \frac{t^4}{\omega^2 + \xi^2} + \Delta_{AP}^2} \]

(11)

where \( N(0) \) is the electron density of state.

In the limit of weak interlayer coupling \( t \ll T_{c0} \) and at \( T = 0 \), we obtain the following expression for the superconducting gap for parallel orientation \( \Delta_P \)

\[
\ln \left( \frac{\Delta_0}{\Delta_P} \right) = \frac{\pi}{2} \int_0^{2\pi} \ln \left[ 1 + 2 \frac{t^2}{\Delta_P^2} \exp(2i\theta) \right] d\theta,
\]

(12)

where \( \Delta_0 \) is the gap of an isolated S layer. Performing expansion over \( t \), it may be demonstrated that at all order over \( t^2 \) the corrections to \( \Delta_P \) disappear, and \( \Delta_P = \Delta_0 \). So the proximity effect for the case of half-metal vanishes. It may be understood as an impossibility of Cooper pair destruction. Indeed at \( T = 0 \), the disappearance of the Cooper pair in S layer means that two electrons with opposite spins must leave it. Due to the insulating character of neighboring F layer for some one spin orientation it becomes impossible and so, the Cooper pair is not destroyed at all.

On the other hand, for the antiparallel alignment this argument does not works and the proximity effect leads to a decrease of the gap \( \Delta_{AP} \)

\[
\ln \left( \frac{\Delta_0}{\Delta_{AP}} \right) = \frac{t^4}{\Delta_{AP}^4} \left( 1 + 2 \ln \frac{\Delta_{AP}}{t} \right).
\]

(13)

Therefore the superconducting gap variation is \( (\Delta_0 - \Delta_{AP}) / \Delta_0 \approx 2 (t/\Delta_0)^4 \ln (\Delta_0/t) \). As the superconducting transition temperature is higher for the AP case, it means that above some temperature \( T^* \) the gap for parallel orientation becomes smaller than that for antiparallel orientation.
To find this temperature $T^*$ in the limit $t << T_{c0}$ we perform an expansion over $t$ in the self-consistency equations for $\Delta_{AP} = \Delta_P = \Delta^*$. After integration over energy $\xi$ we have the following equation for the ratio $X = \Delta^*/(\pi T^*)$

$$\sum_{k} \frac{2(2k+1)^3 + 5(2k+1)X^2 - 2[5(2k+1)^2 - X^2][2k+1]^2 + X^2]}{(2k+1)([(2k+1)^2 + X^2]^{3/2}[(2k+1) + \sqrt{(2k+1)^2 + X^2}]^4)} = 0,$$  

(14)

from what we find $\Delta^*/T^* = 4.22$. Taking into account that in the limit $t << T_{c0}$ the temperature dependence of the superconducting gap in the first approximation is the same as that for an isolated S layer $\Delta_0(T)$, we directly find the temperature of gap inversion $T^* = 0.41T_{c0}$.

Similar calculations can be performed for the standard ferromagnetic case with $\xi_\uparrow = \xi - h$ and $\xi_\downarrow = \xi + h$ in the limit $t, h \ll T_{c0}$. In the result we obtain the following equation for the ratio $X = \Delta^*/(\pi T^*)$

$$\sum_{k} \left\{ \frac{-2(2k+1)^4 - 16(2k+1)^2X^2 - 6X^4}{(2k+1)^2[(2k+1)^2 + X^2]^{3/2}[(2k+1) + \sqrt{(2k+1)^2 + X^2}]^6} + \frac{+38(2k+1)^4 - 11(2k+1)^2X^2 - X^4}{(2k+1)^3[(2k+1)^2 + X^2]^{3/2}[(2k+1) + \sqrt{(2k+1)^2 + X^2}]^6} \right\} = 0,$$  

(15)

which gives $\Delta^*/T^* = 3.61$, and the temperature $T^*$ of the gap inversion is $T^* = 0.47T_{c0}$.

IV. CONCLUSION

In the present work we have demonstrated that, in the framework of the considered microscopic model, in all cases the superconducting transition temperature is higher for antiparallel orientation of the ferromagnetic moments. This is consistent with the predictions made in [5–8], on the basis of the diffusive dirty limit model and recent experimental results [9]. We may consider this result as a quite general one and model independent. On the other hand the superconducting gap at low temperature for the case of half-metal and for usual ferromagnet with small exchange field occurs to be larger for parallel orientation. This is in opposite with the diffusive model prediction [8], but in accordance with the $T = 0$ result [13,14] obtained in the framework of the multiterminal model for S-F hybrid structures. It may be interesting to calculate the superconducting critical temperature in the model [13,14] to compare with our predictions.

Finally we conclude that the spin-orientation dependence of the superconductivity in F/S/F atomic layers structure may be quite different at high and low temperature regimes. Note also that the condition of small interlayer coupling $t << T_{c0}$, may be crucial for the conclusion that there is a gap inversion for parallel and antiparallel orientation with temperature decrease. Indeed, it has been demonstrated in [18], that the strength of interlayer coupling may qualitatively change the critical temperature dependence via the exchange field.

Note also, that strictly speaking, the superconductivity is impossible in atomic 2D system. However, our results must be qualitatively applicable for systems consisting of several
consecutive S and F layers, as well as for S/F multilayered systems, where the fluctuations are strongly suppressed.

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Figure caption

FIG. 1. Geometry of three layers F-S-F system, one superconducting layer is between two ferromagnetic layers.
Figure 1