

## Effect of spin-triplet correlations on Josephson transport in atomically thin superconductor/half-metal/superconductor structures

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We study the effect of the triplet proximity effect on Josephson transport in superconductor/half-metal/superconductor structures of atomic thickness beyond the quasiclassical approximation. Using the combination of microscopic Gor'kov formalism and tight-binding model we show that the full spin polarization inside the half-metal give rise to nonmonotonic temperature dependence of the critical current in S/HM/S Josephson junction with two spin active S/HM interfaces. We also calculate the magnetic moment inside the S<sub>2</sub> layer in S<sub>1</sub>/HM/S<sub>2</sub> structure with spin-active S<sub>1</sub>/HM interface, which is induced by the spin-triplet superconducting correlations. Finally, we analyze the second-harmonic generation in S<sub>1</sub>/HM/S<sub>2</sub> structure with one spin-active interface.

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### I. INTRODUCTION

Spin-polarized superconducting states are the subject of intense research since they are promising for application in the devices of superconducting spintronics combining the spin and current degrees of freedom [1]. The basic system that supports such states consists of *s*-wave superconductor (S) and several ferromagnets (F) [2–4]. The magnetization inside ferromagnets transforms spin-singlet Cooper pairs with total spin  $s = 0$  to the spin-triplet ones with  $s = 1$ . Note that collinear magnetic configuration produces only superconducting correlations with spin projection  $s_z = 0$ , while the spin polarized equal spin triplet correlations ( $s_z = \pm 1$ ) are produced by noncollinear magnetization distribution [2]. An important feature of these spin-triplet correlations is their insensitivity to the exchange field parallel to spin-quantization axes [2,5]. As a result, they become long-ranged and decay at distances of the order of the superconducting coherence length in a normal metal  $\xi_n = \sqrt{D_n/2\pi T}$ , while the correlations with  $s_z = 0$  decay faster, namely, at the scale of the superconducting coherence length in a ferromagnet  $\xi_f = \sqrt{D_f/\hbar}$ , where  $D_n$  and  $D_f$  are diffusion coefficients in a normal metal and a ferromagnet, respectively, and  $\hbar$  is the exchange field.

During the past decade the focus of research of long-ranged triplet superconducting correlations is moving towards heterostructures containing half-metals (HM)—strong ferromagnets, in which the exchange field is of the order of the Fermi energy [6,7]. As a result, the electron density of states is large for spin-up band, while for spin-down one it is almost zero. Thus, only the spin-triplet correlations can penetrate into half-metals, while the amplitude of another correlations should tend to zero at the interface with HM [8]. This makes

the superconducting hybrid structures containing HMs very convenient platforms for studying long-ranged triplet superconducting correlations separately from other effects. The recent advances in fabrication of the structures containing a half-metal resulted in the breakthrough experiments, where the long-ranged Josephson transport [9,10] and the triplet spin-valve effect [11] were observed. Moreover, the experimental evidence of triplet-proximity effect were reported in vertical heterostructures with the high- $T_c$  superconductor YBCO and half-metallic LSMO [12,13], which strongly suggest the triplet generation due to the spin-active interfaces [14,15].

The theoretical description of proximity effect with half-metals meets the fundamental problem due to inapplicability of the quasiclassical approximation, which is widely used for the “weak” ferromagnets both in dirty and clean limits [3,4]. This approximation is justified when the density of states in all layers is basically the same. Such assumption is fulfilled in the heterostructures containing “weak” ferromagnets (e.g., CuNi and PdFe), but fails when one deals with strong ferromagnets, where the density of states for spin-up electrons is much larger than for the spin-down ones. To overcome this difficulty one may introduced the quasiclassical Green functions separately inside and outside of half-metal and then match them with some sort of boundary conditions. The generic form of such boundary conditions for the Usadel Green functions in the dirty limit strongly depends on the number of phenomenological parameters controlling the spin-dependent electron tunneling at the HM boundaries and the results appear to be rather cumbersome [16]. The application of the so-called adiabatic approximation allows to make the boundary conditions more transparent [17]. However, the

applicability of the resulting theory is restricted to the case of the slowly varying exchange field, which is not the case of the wide range of superconducting heterostructures containing half-metals where the exchange field reveals the jumps at the atomic length scales. Similar variants of the boundary conditions were derived in the frames of the Keldysh theory [18,19]. Another approach is based on Bogolubov-De Gennes [20–27] or Blonder-Tinkham-Klapwick [1,28–30] equations. However, the analysis of these models typically requires numerical simulations, and allows one to obtain the exact results only for the specific system parameters. Thus, up to now there is no commonly accepted theory for the proximity effect with half-metals providing an analytical description of this phenomenon.

While the spin-singlet superconducting correlations are well studied, the spin-triplet ones can demonstrate unexpected behavior. For example, in the recent experimental studies of spin-triplet S/F<sub>L</sub>/S'/F<sub>R</sub>/S device it was observed that the emergence of singlet superconductivity in the central S' layer leads to the decrease of the Josephson current [31]. This situation is very different from one in spin-singlet S/S'/S structures, where the emergence of superconductivity in the S' layer increases the spin-singlet Josephson current. To explain this puzzling experiment we have calculated the Josephson current in atomically thin S/HM<sub>L</sub>/S'/HM<sub>R</sub>/S structure with spin-active S/HM<sub>L,R</sub> interfaces in the framework of microscopic Gor'kov formalism and tight-binding model. We managed to show that the singlet superconducting gap in the S' layer indeed suppresses the triplet Josephson current [31] contrary to the case of singlet current in S/S'/S structure. One can expect that the spin-triplet superconducting correlations would manifest themselves in other observable properties even in simpler structures. Note that some aspects of the interplay between triplet and singlet correlations were studied theoretically in Refs. [4,32–34].

In the present paper, we study the peculiarities of superconducting spin-triplet correlations in atomically thin S<sub>1</sub>/HM/S<sub>2</sub> structures with spin-active S/HM interfaces. We use the combination of the microscopic Gor'kov formalism and tight-binding model allowing to obtain exact analytical results, which are valid beyond the quasiclassical approximation [35–39]. In particular, we show that the spin-triplet Josephson critical current in S<sub>1</sub>/HM/S<sub>2</sub> junction with two spin-active S/HM interfaces nonmonotonically depends on temperature. Note that this peculiar temperature dependence of the critical current has nothing to do with the temperature anomalies of the critical current in the vicinity of 0 – π transition in S/F/S systems. We also calculate the induced magnetic moment inside S<sub>2</sub> superconductor in the S<sub>1</sub>/HM/S<sub>2</sub> structure with strong ferromagnet as an insulating layer and spin-active S<sub>1</sub>/HM interface, which supports spin-triplet superconducting correlations. We show that the induced magnetic moment contains the components perpendicular to the spin-quantization axis (z axis) in HM. Moreover, the magnetic moment depends on the phase difference across the junction φ as  $M_x = m \cos \varphi$ ,  $M_y = m \sin \varphi$ . Previously, the magnetic moment induced in the superconductor was calculated for various S/F hybrids with “weak” ferromagnets (the exchange field is much smaller than the Fermi energy) and collinear magnetic configuration producing only the superconducting correlations with

spin-singlet and triplet spin states with zero-spin projection [40–46]. In these cases, obviously, the induced magnetic moment appeared to be collinear to the exchange field in the F layer. Contrary to our results ( $M_x = m \cos \varphi$ ,  $M_y = m \sin \varphi$ ), in Refs. [44,45] *nonsinusoidal* dependence  $M_z(\varphi)$  in S/F hybrids with “weak” ferromagnets was obtained. The induced magnetic moment in hybrids with spin-triplet superconducting correlations was studied in Refs. [32,47] in the framework of Usadel and BdG equations, respectively. Contrary to our study, in Ref. [47] it was obtained that the component of the induced magnetic moment perpendicular to S/F interfaces is absent. We believe that it could be related with the fact that we consider the situation that is outside of the range of the applicability of the quasiclassical Usadel approach used in this paper for the calculation of the induced magnetic moment. At the same time, in Ref. [32], S/F/S/F/S structure was considered and the *nonsinusoidal* dependence of the magnetic moment induced on the central S layer on the phase difference across the structure was obtained. Since the magnetic moment appeared in S<sub>1</sub> layer is not collinear to the spin-quantization axis in HM and depends on the phase difference across the junction, one can expect the emergence of the second harmonic of the spin-triplet superconducting current in the structure. However, we show that it is not the case and the second harmonic does not appear. We may speculate that some Fermi-liquid effects [48,49] (for example, the electron-electron interaction) and/or multiband character of superconductivity should restore the second-harmonic triplet current. The electron band not involved in superconductivity could acquire a magnetic moment due to the interband interaction, which can serve as a source of “external” magnetism for superconductivity.

The paper is organized as follows. In Sec. II, we introduce the model and calculate the critical current in S<sub>1</sub>/HM/S<sub>2</sub> Josephson junction with both spin-active interfaces. In Sec. III, we calculate the induced magnetic moment of S<sub>2</sub> layer the structure with spin-active S<sub>1</sub>/HM interface and analyze the possibility of the second-harmonic generation. In Sec. IV, we summarize our results.

## II. NONMONOTONIC TEMPERATURE DEPENDENCE OF JOSEPHSON CURRENT IN S/HM/S STRUCTURE

We consider S<sub>1</sub>/HM/S<sub>2</sub> Josephson junction consisting of atomically thin superconducting layers separated by the half-metal, see Fig. 1. We assume both S/HM interfaces to be spin-active and model it by introducing the superconducting ferromagnets (SF<sub>*i*</sub>), in which both the superconducting gap and the exchange field  $\mathbf{h}_i$  ( $i = 1, 2$ ) are nonzero. We assume noncollinear magnetization configuration in the system, which gives rise to the emergence of the spin-triplet superconducting correlations. Due to the strong spin polarization in half-metals, spin-singlet Cooper pairs cannot penetrate through them and only the spin-triplet correlations are responsible for Josephson transport.

We denote the superconducting gaps in SF<sub>1</sub> and SF<sub>2</sub> layers as  $\Delta_1 = \Delta_0 e^{i\varphi/2}$ ,  $\Delta_2 = \Delta_0 e^{-i\varphi/2}$ . Thus, the phase difference across the junction equals to φ. We choose y axis to be perpendicular to the layers. The spin-quantization axes in the half-metal coincides with the z axis, while the exchange field

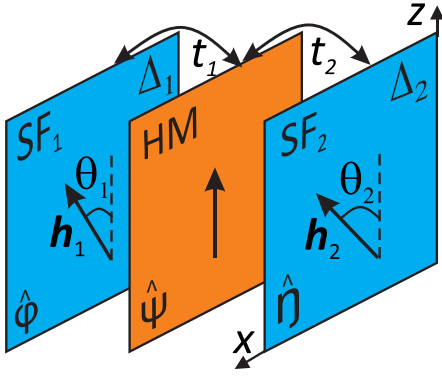


FIG. 1. The sketch of  $S_1/HM/S_2$  stricture of atomic thickness with the spin-active  $S_i/HM$  interfaces, which are modeled by introducing the superconducting ferromagnets  $SF_1$  and  $SF_2$ . The layers are coupled by the transfer integrals  $t_1$  and  $t_2$  of the tight-binding model.

in  $SF_i$  layer forms the angle  $\theta_i$  with  $z$  axis:  $\mathbf{h}_i = h_i(\cos \theta_i \mathbf{z} + \sin \theta_i \mathbf{x})$ . The quasiparticle motion inside the layers is characterized by the momentum  $\mathbf{p}$ , while the layers are coupled by the transfer integrals  $t_i$ ,  $i = 1, 2$  of tight-binding model. We assume that  $t_i \ll T_{c1}$ . In addition, we assume that the interlayer tunneling conserves the momentum. The energy spectrum in the superconductors is  $\xi(\mathbf{p})$ , while in the half-metals it is spin-dependant:  $\xi_\uparrow = \xi(\mathbf{p})$  and  $\xi_\downarrow = +\infty$ .

Let us denote the electron annihilation operators in  $SF_1$ ,  $HM$ , and  $SF_2$  layers as  $\hat{\phi}$ ,  $\hat{\psi}$ , and  $\hat{\eta}$ , respectively. The Hamiltonian of the system under consideration consists of three parts:

$$\hat{H} = \hat{H}_0 + \hat{H}_{BSC} + \hat{H}_t. \quad (1)$$

The first term  $\hat{H}_0$  describes the electron motion in each isolated layer:

$$\hat{H}_0 = \sum_{\mathbf{p}; \beta, \gamma = \uparrow, \downarrow} \hat{A}_{\beta\gamma}^{(1)} \hat{\phi}_{\mathbf{p}, \beta}^\dagger \hat{\phi}_{\mathbf{p}, \gamma} + \hat{B}_{\beta\gamma} \hat{\psi}_{\mathbf{p}, \beta}^\dagger \hat{\psi}_{\mathbf{p}, \gamma} + \hat{A}_{\beta\gamma}^{(2)} \hat{\eta}_{\mathbf{p}, \beta}^\dagger \hat{\eta}_{\mathbf{p}, \gamma}. \quad (2)$$

The second term is the Bardeen-Cooper-Schrieffer Hamiltonian of two superconductors:

$$\begin{aligned} \hat{H}_{BSC} = & \sum_{\mathbf{p}} \Delta_1 \hat{\phi}_{\mathbf{p}, \uparrow}^\dagger \hat{\phi}_{-\mathbf{p}, \downarrow}^\dagger + \Delta_1^* \hat{\phi}_{-\mathbf{p}, \downarrow} \hat{\phi}_{\mathbf{p}, \uparrow} \\ & + \Delta_2 \hat{\eta}_{\mathbf{p}, \uparrow}^\dagger \hat{\eta}_{-\mathbf{p}, \downarrow}^\dagger + \Delta_2^* \hat{\eta}_{-\mathbf{p}, \downarrow} \hat{\eta}_{\mathbf{p}, \uparrow}. \end{aligned} \quad (3)$$

The last term in Eq. (2) describes the tunneling between the neighboring layers:

$$\hat{H}_t = \sum_{\mathbf{p}; \beta} t_1 (\hat{\psi}_{\mathbf{p}, \beta}^\dagger \hat{\phi}_{\mathbf{p}, \beta} + \hat{\phi}_{\mathbf{p}, \beta}^\dagger \hat{\psi}_{\mathbf{p}, \beta}) + t_2 (\hat{\eta}_{\mathbf{p}, \beta}^\dagger \hat{\psi}_{\mathbf{p}, \beta} + \hat{\psi}_{\mathbf{p}, \beta}^\dagger \hat{\eta}_{\mathbf{p}, \beta}). \quad (4)$$

We introduce the matrices

$$\begin{aligned} \hat{A}^{(i)} &= \begin{pmatrix} \xi - h_i \cos \theta_i & -h_i \sin \theta_i \\ -h_i \sin \theta_i & \xi + h_i \cos \theta_i \end{pmatrix}, \\ \hat{P} &= \begin{pmatrix} \xi & 0 \\ 0 & \infty \end{pmatrix}. \end{aligned} \quad (5)$$

In the model under consideration with the transfer integrals between the layers, the current density  $j_y$  is proportional to the time derivative of the averaged particle number operator in  $SF_1$ ,  $HM$ , or  $SF_2$  layer. Thus,  $j_y$  can be expressed via the Fourier component of the off-diagonal Matsubara Green function [50]. Note that since the current through the structure is conserved we can use any of off-diagonal Green functions. Without loss of generality, let us consider the function  $E_{\alpha\beta}^\phi(\mathbf{p}; \tau_1, \tau_2) = -\langle T_\tau \hat{\phi}_{\mathbf{p}, \alpha}(\tau_1) \hat{\psi}_{\mathbf{p}, \beta}^\dagger(\tau_2) \rangle$ . Then the currents reads:

$$j_y = -2e\nu_0 t_1 T \text{Im} \sum_{\omega=-\infty}^{\infty} \int_{-\infty}^{\infty} d\xi E_{\alpha\alpha}^\phi(\mathbf{p}; \omega). \quad (6)$$

Here  $e > 0$  is the electron charge and  $\nu_0$  is the electron density of states at the Fermi level.

To find  $E^\phi$ , we introduce the following set of the Green functions in the imaginary-time representation:

$$\begin{aligned} G_{\alpha\beta}(\mathbf{p}; \tau_1, \tau_2) &= -\langle T_\tau \hat{\psi}_{\mathbf{p}, \alpha}(\tau_1) \hat{\psi}_{\mathbf{p}, \beta}^\dagger(\tau_2) \rangle, \\ F_{\alpha\beta}^\dagger(\mathbf{p}; \tau_1, \tau_2) &= \langle T_\tau \hat{\psi}_{-\mathbf{p}, \alpha}^\dagger(\tau_1) \hat{\psi}_{\mathbf{p}, \beta}^\dagger(\tau_2) \rangle, \\ E_{\alpha\beta}^\phi &= -\langle T_\tau \hat{\phi}_{\mathbf{p}, \alpha} \hat{\psi}_{\mathbf{p}, \beta}^\dagger \rangle, \quad F_{\alpha\beta}^{\psi^\dagger} = \langle T_\tau \hat{\phi}_{-\mathbf{p}, \alpha}^\dagger \hat{\psi}_{\mathbf{p}, \beta}^\dagger \rangle, \\ E_{\alpha\beta}^\eta &= -\langle T_\tau \hat{\eta}_{\mathbf{p}, \alpha} \hat{\psi}_{\mathbf{p}, \beta}^\dagger \rangle, \quad F_{\alpha\beta}^{\eta^\dagger} = \langle T_\tau \hat{\eta}_{-\mathbf{p}, \alpha}^\dagger \hat{\psi}_{\mathbf{p}, \beta}^\dagger \rangle. \end{aligned}$$

Following the usual procedure (see Ref. [51]), we write down the system of the matrix Gor'kov equations in the frequency representation:

$$\begin{aligned} (i\omega - \hat{P})G - t_1 E^\phi - t_2 E^\eta &= \hat{1}, \\ (i\omega + \hat{P})F + t_1 F^{\phi^\dagger} + t_2 F^{\eta^\dagger} &= 0, \\ [i\omega - \hat{A}^{(1)}]E^\phi + \Delta_1 \hat{I} F^{\phi^\dagger} - t_1 G &= 0, \\ [i\omega + \hat{A}^{(1)}]F^{\phi^\dagger} - \Delta_1^* \hat{I} E^\phi + t_1 F^\dagger &= 0, \\ [i\omega - \hat{A}^{(2)}]E^\eta + \Delta_2 \hat{I} F^{\eta^\dagger} - t_2 G &= 0, \\ [i\omega + \hat{A}^{(2)}]F^{\eta^\dagger} - \Delta_2^* \hat{I} E^\eta + t_2 F^\dagger &= 0, \end{aligned}$$

where  $\hat{I} = i\sigma_y$ .

Solving the above system of equations one can find the exact expression for  $E^\phi$  (see Appendix A). Making the expansion up to third order over  $t \ll T$ , we find (for details see Appendix A)  $E_{22}^\psi(\mathbf{p}; \omega) = 0$  and

$$\begin{aligned} \text{Im}[E_{11}^\phi(\mathbf{p}; \omega)] = & \text{Im} \left\{ -\frac{\Delta_1 \Delta_2^* t_1 t_2^2}{(i\omega + \xi)(i\omega - \xi)} \left[ ((i\omega + A^{(2)}) + \Delta_0^2 \hat{I} (i\omega - A^{(2)})^{-1} \hat{I})^{-1} \hat{I} (i\omega - A^{(2)})^{-1} \right]_{11} \right. \\ & \left. \times \left[ ((i\omega - A^{(1)}) + \Delta_0^2 \hat{I} (i\omega + A^{(1)})^{-1} \hat{I})^{-1} \hat{I} (i\omega + A^{(1)})^{-1} \right]_{11} \right\}. \end{aligned} \quad (7)$$

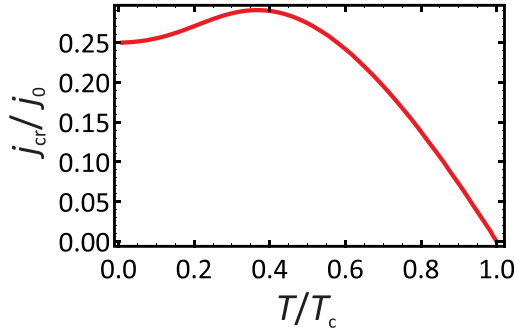


FIG. 2. The dependence of the spin-triplet critical current  $j_{cr}$  on the temperature. Here  $j_0 = -8ev_0t_1^2t_2^2h^2\sin\theta_1\sin\theta_2$ .

As a result, we obtain

$$\begin{aligned} \text{Im} \sum_{\omega=-\infty}^{\infty} \int_{-\infty}^{\infty} d\xi E_{11}^{\phi}(\mathbf{p}; \omega) \\ = \sum_{\omega>0} \frac{4\pi t_1 t_2^2 h^2 \omega^2 \sin\varphi \sin\theta_1 \sin\theta_2}{\Delta_0^2} \left[ \frac{2}{\omega} - \frac{2\omega^2 + 3\Delta_0^2}{(\omega^2 + \Delta_0^2)^{3/2}} \right]. \end{aligned} \quad (8)$$

Substituting Eq. (8) into Eq. (6) we finally find  $j_y = j_{cr} \sin\varphi$ , where

$$\begin{aligned} j_{cr} = \sum_{\omega>0} \frac{-8\pi ev_0 t_1^2 t_2^2 h^2 T \omega^2}{\Delta_0^2} \left[ \frac{2}{\omega} - \frac{2\omega^2 + 3\Delta_0^2}{(\omega^2 + \Delta_0^2)^{3/2}} \right] \\ \times \sin\theta_1 \sin\theta_2. \end{aligned} \quad (9)$$

The spin-polarized triplet critical current nonmonotonically depends on the temperature, as shown in Fig. 2. This situation is different from the one in Josephson junctions with normal metal or weak ferromagnets as an insulating layer, where the current is not spin polarized and monotonically increases with decrease of temperature. Similar nonmonotonic dependence was obtained in Refs. [52–55] for the triplet supercurrent although the half-metallic Josephson junction with spin-active interfaces in the framework of Usadel equations. Thus, it seems that the nonmonotonic dependence of the critical current is inherent for Josephson junctions with spin-polarized triplet supercurrents and does not depend on the model.

For  $T \sim T_c$  and  $t_1 = t_2 = t$  we obtain the following critical current:

$$\begin{aligned} j_{cr} = -j \left( \frac{t}{T_c} \right)^4 \left( \frac{h}{T_c} \right)^2 \left( \frac{\Delta_0}{T_c} \right)^2 \left( \frac{T_c}{T} \right)^2 \\ \times \sin\theta_1 \sin\theta_2, \end{aligned} \quad (10)$$

where  $j = [-21\zeta(3)ev_0T_c^6]/\pi^2$ .

At the same time, for  $T \ll T_c$ , where  $\Delta_0 \gg T$  we find

$$j_{cr} = -4ev_0t^4h^2\sin\theta_1\sin\theta_2. \quad (11)$$

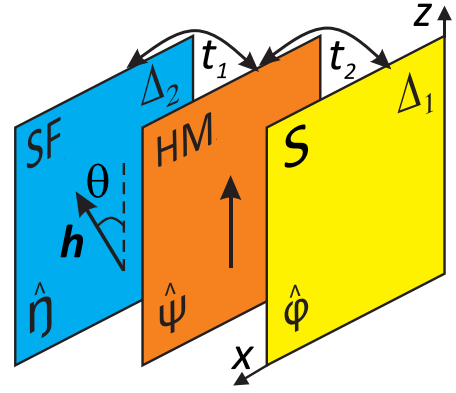


FIG. 3. The sketch of atomically thin SF/HM/S structure.

### III. MAGNETIC MOMENT OF SUPERCONDUCTING LAYER

In  $S_1$ /HM/ $S_2$  structure of atomic thickness with the spin-active HM/ $S_2$  interface (see Fig. 3) the induced magnetic moment appears in  $S_1$  layer. This magnetic moment depends on the phase difference  $\varphi$  across the junction and has the out-of-plane component  $M_y$ ; below we calculate it. The magnetic moment  $\mathbf{M}$  is expressed via the Fourier component of diagonal Green function  $\tilde{G}_{\alpha\beta} = -\langle T_{\tau} \hat{\phi}_{\mathbf{p},\alpha} \hat{\phi}_{\mathbf{p},\beta}^{\dagger} \rangle$  in S layer as

$$M_x = \mu_B v_0 T \sum_{\omega=-\infty}^{\infty} \int_{-\infty}^{\infty} d\xi (\tilde{G}_{21} + \tilde{G}_{12}), \quad (12)$$

$$M_y = -i\mu_B v_0 T \sum_{\omega=-\infty}^{\infty} \int_{-\infty}^{\infty} d\xi (\tilde{G}_{21} - \tilde{G}_{12}), \quad (13)$$

$$M_z = \mu_B v_0 T \sum_{\omega=-\infty}^{\infty} \int_{-\infty}^{\infty} d\xi (\tilde{G}_{11} + \tilde{G}_{22}), \quad (14)$$

where  $\mu_B$  is the Bohr magneton.

To find  $\tilde{G}_{\alpha\beta}$  we introduce the set of imaginary time Green functions:

$$\begin{aligned} \tilde{G}_{\alpha\beta} &= -\langle T_{\tau} \hat{\phi}_{\mathbf{p},\alpha} \hat{\phi}_{\mathbf{p},\beta}^{\dagger} \rangle, & \tilde{F}_{\alpha\beta}^{\dagger} &= \langle T_{\tau} \hat{\phi}_{-\mathbf{p},\alpha}^{\dagger} \hat{\phi}_{\mathbf{p},\beta} \rangle \\ \tilde{E}_{\alpha\beta}^{\psi} &= -\langle T_{\tau} \hat{\psi}_{\mathbf{p},\alpha} \hat{\phi}_{\mathbf{p},\beta}^{\dagger} \rangle, & \tilde{F}_{\alpha\beta}^{\psi\dagger} &= \langle T_{\tau} \hat{\psi}_{-\mathbf{p},\alpha}^{\dagger} \hat{\phi}_{\mathbf{p},\beta} \rangle, \\ \tilde{E}_{\alpha\beta}^{\eta} &= -\langle T_{\tau} \hat{\eta}_{\mathbf{p},\alpha} \hat{\phi}_{\mathbf{p},\beta}^{\dagger} \rangle, & \tilde{F}_{\alpha\beta}^{\eta\dagger} &= \langle T_{\tau} \hat{\eta}_{-\mathbf{p},\alpha}^{\dagger} \hat{\phi}_{\mathbf{p},\beta} \rangle. \end{aligned}$$

Following the usual procedure we write down the system of matrix Gor'kov equations in the frequency representation:

$$\begin{aligned} (i\omega - \xi)\tilde{G} + \Delta_1 \hat{I} \tilde{F}^{\dagger} - t_1 \tilde{E}^{\psi} &= \hat{1}, \\ (i\omega + \xi)\tilde{F}^{\dagger} - \Delta_1^* \hat{I} \tilde{G} + t_1 \tilde{F}^{\psi\dagger} &= 0, \\ (i\omega - \hat{P})\tilde{E}^{\psi} - t_1 \tilde{G} - t_2 \tilde{E}^{\eta} &= 0, \\ (i\omega + \hat{P})\tilde{F}^{\psi\dagger} + t_1 \tilde{F}^{\dagger} + t_2 \tilde{F}^{\eta\dagger} &= 0, \\ (i\omega - \hat{A})\tilde{E}^{\eta} + \Delta_2 \hat{I} \tilde{F}^{\eta\dagger} - t_2 \tilde{E}^{\psi} &= 0, \\ (i\omega + \hat{A})\tilde{F}^{\eta\dagger} - \Delta_2^* \hat{I} \tilde{E}^{\eta} + t_2 \tilde{F}^{\psi\dagger} &= 0, \end{aligned}$$

where

$$\hat{A} = \begin{pmatrix} \xi - h \cos\theta & -h \sin\theta \\ -h \sin\theta & \xi + h \cos\theta \end{pmatrix}. \quad (15)$$

As a result, we find the sought-for Green function  $\tilde{G}_{\alpha,\beta}$  (for details see Appendix B):

$$\tilde{G}_{11} = -\frac{i\omega + \xi}{\omega^2 + \xi^2 + \Delta_0^2 + t_1^2(i\omega + \xi)\gamma}, \quad (16)$$

$$\tilde{G}_{22} = -\frac{i\omega + \xi - t_1^2\delta}{\omega^2 + \xi^2 + \Delta_0^2 + t_1^2(i\omega - \xi)\delta}, \quad (17)$$

$$\tilde{G}_{12} = -\frac{\Delta_1^* \Delta_2 \alpha_2 t_1^2 t_2^2 (i\omega + \xi)}{(\omega^2 + \xi^2 + \Delta_0^2)^2}, \quad (18)$$

$$\tilde{G}_{21} = \frac{\Delta_1 \Delta_2^* \alpha_1 t_1^2 t_2^2 (i\omega + \xi)}{(\omega^2 + \xi^2 + \Delta_0^2)^2}. \quad (19)$$

Here we introduce the notations:  $\alpha_{1,2} = d_{1,2}/[(i\omega - \xi)(i\omega + \xi)]$ ,  $d_1 = [\hat{D}\hat{I}(i\omega - \hat{A})^{-1}]_{11}$ ,  $d_2 = [(i\omega - \hat{A})^{-1}\hat{I}\hat{D}]_{11}$ ,  $\gamma = (i\omega - \xi - t_2^2 b_1)^{-1}$ ,  $\delta = (i\omega + \xi - t_2^2 a_1)^{-1}$ ,  $a_1 = \hat{D}_{11}$ ,  $b_1 = [(i\omega - \hat{A})^{-1}\hat{B}]_{11}$ ,

$$\hat{D} = [(i\omega + \hat{A}) + \Delta_0^2 \hat{f}(i\omega - \hat{A})^{-1} \hat{f}]^{-1},$$

$$\hat{B} = \hat{I} + \Delta_0^2 \hat{f} \hat{D} \hat{f}(i\omega - \hat{A})^{-1}.$$

Calculating the magnetic moment, we obtain that  $M_z \propto O(\Delta_0^2)$ , while  $M_x$  and  $M_y$  depend on the phase difference across the junction,

$$M_x = m \cos \varphi, \quad M_y = -m \sin \varphi, \quad (20)$$

$$m = \sum_{\omega>0} \frac{-\pi \mu_B v_0 T t_1^2 t_2^2 \Delta_0^2 h (3h^4 + 35h^2 \omega^2 + 140\omega^4) \sin \theta}{8\omega^3 (h^2 + \omega^2)(h^2 + 4\omega^2)^3}. \quad (21)$$

The magnetic moment induced by the long-ranged triplet correlations in S/F/F/S junctions was studied in Ref. [47] in the framework of quasiclassical Usadel equations. Similarly to our results, Eq. (20), the induced moment  $M_x \sim \cos \varphi$  was predicted, but not the component  $M_y$ . We believe that this circumstance may be related with the inaccuracy of the Usadel approach for the calculation of the induced electron magnetization.

The appearance of the phase-sensitive magnetization in the absence of the Josephson current may be considered as a presence of the long-range spin current [56] due to spin-triplet superconducting correlations.

To control the applied phase difference we could use the usual Josephson junction, connected at parallel. Changing the applied Josephson phase (or the Josephson current through this junction), one may vary the magnetization of S layer. In such a way, it would be possible to couple the phase oscillations of the Josephson current with the oscillations of the electron's magnetization. For  $h \sim T_c$  and  $t \sim T_c$  we may estimate the phase-dependent electron polarization as  $m \sim \mu_B v_0 h$ . If some part of the S electrode contains the magnetic atoms, the induced electron's magnetization should polarize them. Assuming the typical value of the exchange interaction between electron spin and the localized moment  $I \sim 10^3$  K and taking  $h \sim T_c \sim 10$  K, we may estimate that the electron's magnetization is equivalent to the magnetic field of 0.1 T.

Note that since triplet superconducting correlation produces the magnetic moment  $\mathbf{M}$  with nonzero  $M_x$  and  $M_y$

projections in the S layer, one can expect the emergence of triplet superharmonic Josephson current in the SF/HM/S structure through the mechanism similar that discussed in Ref. [57]. Indeed, the calculations performed in the previous section show that in SF<sub>1</sub>/HM/SF<sub>2</sub> structure the Josephson current has the form  $j_y \propto h_{1x} h_{2x} \sin \varphi$ . At the same time, in SF/HM/S structure one can assume  $h_x \propto M_x \propto \cos \varphi$ . As a result, one obtains  $j_y \propto \sin 2\varphi$ , i.e., one can expect the generation of the Josephson current on the second harmonic. However, careful analysis shows that it is not the case and Josephson current is absent (for details see Appendix B). We expect that Fermi-liquid effects [48,49] (for example, the electron-electron interaction) and/or multiband character of superconductivity should restore the second harmonic of triplet current.

#### IV. CONCLUSIONS

To sum up, we have studied the properties of spin-triplet superconducting correlations in atomically thin S<sub>1</sub>/HM/S<sub>2</sub> structures with one or two spin-active interfaces. We used the combination of microscopic Gor'kov formalism and tight-binding model, which allows to obtain analytical results beyond the quasiclassical approximation. We have shown that in S<sub>1</sub>/HM/S<sub>2</sub> structure with two spin-active interfaces (see Fig. 1), the triplet Josephson current nonmonotonically depends on the temperature (see Fig. 2). We expect that this property is inherent to triplet current and does not depend on the specific model. In S<sub>1</sub>/HM/S<sub>2</sub> structure with one spin-active S<sub>1</sub>/HM interface (see Fig. 1) we have calculated the magnetic moment induced by the triplet superconducting correlations in S layer and show that it is noncollinear to the spin-quantization axis in HM and depends on the phase difference across the junction. The emergence of this magnetic moment does not cause the appearance of the Josephson current on the second harmonic in the framework of standard BCS theory.

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#### APPENDIX A: GREEN FUNCTIONS IN SF<sub>1</sub>/HM/SF<sub>2</sub> STRUCTURE

In this Appendix we present the details of the derivation of Eq. (7). Solving the system of matrix Gor'kov equations presented in the main text we obtain the following exact expressions for the Green functions:

$$E^\phi = t_1 Q_1^{-1} [G + \Delta_1 I (i\omega + A_1)^{-1} F^\dagger], \quad (A1)$$

$$G = [1 + S_1^{-1} S_2 S_4^{-1} S_3]^{-1} S_1^{-1}, \quad (A2)$$

$$F^\dagger = -S_4^{-1} S_3 G. \quad (A3)$$

Here we introduce the following notations:

$$Q_{1,2} = (i\omega - A_{1,2}) + \Delta_0 I (i\omega + A_{1,2})^{-1} I,$$

$$M_{1,2} = (i\omega + A_{1,2}) + \Delta_0 I (i\omega - A_{1,2})^{-1} I,$$

$$S_1 = (i\omega - P) - t_1^2 Q_1^{-1} - t_2^2 Q_2^{-1},$$

$$S_4 = (i\omega + P) - t_1^2 M_1^{-1} - t_2^2 M_2^{-1},$$

$$S_2 = t_1^2 \Delta_1 Q_1^{-1} I (i\omega + A_1)^{-1} + t_2^2 \Delta_2 Q_2^{-1} I (i\omega + A_2)^{-1},$$

$$S_3 = t_1^2 \Delta_1^* M_1^{-1} I (i\omega - A_1)^{-1} + t_2^2 \Delta_2 M_2^{-1} I (i\omega - A_2)^{-1}.$$

Making the expansion up to the fourth order over  $t_1, t_2$  we obtain the following expressions for the Green functions  $\tilde{G}, \tilde{F}^\dagger$ :

$$G = \frac{1}{i\omega - \xi - t_1^2 [Q_1^{-1}]_{11} - t_2^2 [Q_2^{-1}]_{11}} \times \left( 1 - \frac{[S_2]_{11} [S_3]_{11}}{(i\omega - \xi)(i\omega + \xi)} \right) \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad (\text{A4})$$

$$F^\dagger = - \frac{[S_3]_{11}}{(i\omega + \xi - t_1^2 [M_1^{-1}]_{11}) - t_2^2 [M_2^{-1}]_{11}} \times \frac{1}{(i\omega - \xi - t_1^2 [Q_1^{-1}]_{11}) - t_2^2 [Q_2^{-1}]_{11}} \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}. \quad (\text{A5})$$

Next we substitute Eqs. (A4) and (A5) into Eq. (A1) and obtain  $E^\phi$  up to the third order over  $t_1, t_2$ . The part of  $E^\phi$  depending on the phase difference across the junction has the form of Eq. (7).

## APPENDIX B: ABSENCE OF SECOND HARMONIC OF JOSEPHSON CURRENT IN S/HM/SF STRUCTURE

In this Appendix we show that in SF/HM/S structure the Josephson current is absent, in spite of the induced magnetic moment in S layer is nonzero. Solving the system of matrix

Gor'kov equations presented in Sec. III we obtain the anomalous and normal Green functions in S layer:

$$\tilde{F}^\dagger = \left\{ [(i\omega - \xi) - t_1^2 V] [\Delta_1^* I + t_1^2 t_2^2 \Delta_2^* Q D I (i\omega - A)^{-1} V]^{-1} \times [(i\omega + \xi) - t_1^2 Q W] + \Delta_1 I + t_1^2 t_2^2 \Delta_2 V I (i\omega - A)^{-1} I D Q \right\}^{-1}, \quad (\text{B1})$$

$$\tilde{G} = [\Delta_1^* I + t_1^2 t_2^2 \Delta_2^* Q D I (i\omega - A)^{-1} V]^{-1} \times [(i\omega + \xi) - t_1^2 Q W] \tilde{F}^\dagger. \quad (\text{B2})$$

Here we introduced the following matrices:

$$Q = [(i\omega + P) - t_2^2 D]^{-1}, \quad (\text{B3})$$

$$V = [(i\omega - P) - t_2^2 \tilde{B}]^{-1}, \quad (\text{B4})$$

$$\tilde{B} = (i\omega - A)^{-1} [B - |\Delta_2|^2 t_2^2 I D Q D I (i\omega - A)^{-1}], \quad (\text{B5})$$

$$W = 1 - t_2^4 |\Delta_2|^2 D I (i\omega - A)^{-1} V (i\omega - A)^{-1} I D Q. \quad (\text{B6})$$

The matrices  $I, A, P, D,$  and  $B$  are presented in the main text.

Next we find the exact expressions for the following matrices:

$$Q = \frac{1}{i\omega + \xi - t_2^2 a_1} \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad (\text{B7})$$

$$V = \frac{1}{i\omega - \xi - t_2^2 \tilde{b}_1} \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad (\text{B8})$$

$$i\omega + \xi - t_1^2 Q W = \begin{pmatrix} i\omega + \xi - t_1^2 \delta & 0 \\ 0 & i\omega + \xi \end{pmatrix}, \quad (\text{B9})$$

where  $a_1 = D_{11}, \tilde{b}_1 = \tilde{B}_{11},$

$$\delta = \frac{1 - p t_2^4 |\Delta_2|^2 d_1 d_2}{i\omega + \xi - t_2^2 a_1}, \quad (\text{B10})$$

$$p = \frac{1}{(i\omega + \xi - t_2^2 a_1)(i\omega - \xi - t_2^2 \tilde{b}_1)}. \quad (\text{B11})$$

The parameters  $d_1$  and  $d_2$  are presented in the main text.

Substituting Eqs. (B7), (B8), and (B9) into  $\tilde{F}^\dagger$  after some transformation we obtain

$$\tilde{F}^\dagger = \left[ \frac{1}{\Delta_1^{*2}} \begin{pmatrix} t_1^2 t_2^2 \tilde{\alpha}_2 \Delta_1^{*2} \Delta_2 & -\Delta_1^* (i\omega - \xi - t_1^2 \tilde{\gamma})(i\omega + \xi) + \Delta_1^* |\Delta_1|^2 \\ \Delta_1^* (i\omega + \xi - t_1^2 \delta)(i\omega - \xi) - \Delta_1^* |\Delta_1|^2 & t_1^2 t_2^2 \tilde{\alpha}_1 \Delta_2^* (i\omega - \xi)(i\omega + \xi) \end{pmatrix} \right]^{-1}, \quad (\text{B12})$$

where  $\tilde{\gamma} = (i\omega - \xi - t_2^2 \tilde{b}_1)^{-1}, \tilde{\alpha}_1 = d_1 p, \tilde{\alpha}_2 = d_2 p.$  Substituting Eq. (B12) into Eq. (B2), we obtain all components of the normal Green function Eqs. (16)–(19), presented in the main text.

Next we can calculate  $\tilde{F}_{11}^\dagger, \tilde{G}_{11}$  and obtain the following expressions:

$$\tilde{F}_{11}^\dagger = \frac{t_1^2 t_2^2 \tilde{\alpha}_1 (i\omega + \xi)(i\omega - \xi) \Delta_2^*}{[\omega^2 + \xi^2 + |\Delta_1|^2 + t_1^2 (i\omega + \xi) \tilde{\gamma}] [\omega^2 + \xi^2 + |\Delta_1|^2 + t_1^2 (i\omega - \xi) \delta] - t_1^4 t_2^4 \tilde{\alpha}_1 \tilde{\alpha}_2 |\Delta_2|^2 (\omega^2 + \xi^2)}, \quad (\text{B13})$$

$$\tilde{G}_{11} = - \frac{(i\omega + \xi) [\omega^2 + \xi^2 + t_1^2 (i\omega - \xi) \delta]}{[\omega^2 + \xi^2 + |\Delta_1|^2 + t_1^2 (i\omega + \xi) \tilde{\gamma}] [\omega^2 + \xi^2 + |\Delta_1|^2 + t_1^2 (i\omega - \xi) \delta] - t_1^4 t_2^4 \tilde{\alpha}_1 \tilde{\alpha}_2 |\Delta_2|^2 (\omega^2 + \xi^2)}. \quad (\text{B14})$$

At the same time, from the system of matrix Gor'kov equations, presented in the main text, we find the off-diagonal Green function  $\tilde{E}^\psi$ :

$$\tilde{E}^\psi = t_1 V [G - t_2^2 \Delta_2 (i\omega - A) I D Q F^\dagger]. \quad (\text{B15})$$

As the result, we obtain

$$\tilde{E}_{11}^{\psi} = \frac{t_1 \tilde{G}_{11}}{(i\omega - \xi - t_2^2 \tilde{b}_1)} - \frac{t_1 t_2^2 d_2 \Delta_2 \tilde{F}_{11}^{\dagger}}{(i\omega + \xi - t_2^2 a_1)}, \quad (\text{B16})$$

$\tilde{E}_{22}^{\psi} = 0$ . Note that  $\tilde{E}_{11}^{\psi}$  does not depend on the phase difference across the junction  $\varphi$ , see Eqs. (B13), (B14), and (B16). Substituting Eqs. (B13), (B14), and (B16) for  $\tilde{E}_{11}^{\psi}$  and  $\tilde{E}_{22}^{\psi} = 0$  into Eq. (6), we obtain that the Josephson current is absent, i.e.,  $j_y = 0$ .

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