Crossover between standard and inverse spin-valve effect in atomically thin superconductor/half-metal structures

Zh. Devizorova[1,2,3] and S. Mironov[3]

[1]*Moscow Institute of Physics and Technology, 141700 Dolgoprudny, Russia*

[2]*Kotelnikov Institute of Radio-engineering and Electronics, RAS, 125009 Moscow, Russia*

[3]*Institute for Physics of Microstructures, Russian Academy of Sciences, 603950 Nizhny Novgorod, GSP-105, Russia*

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Spin-singlet Cooper pairs consisting of two electrons with opposite spins cannot directly penetrate from a superconductor to a half-metal (fully spin polarized ferromagnets) which blocks the superconducting proximity effect between these materials. In this paper we demonstrate that, nevertheless, two half-metallic layers electrically coupled to the superconducting film substantially affect its critical temperature and produce the spin-valve effect. Within the tight-binding model for the atomically thin multilayered spin valves we show that depending on the details of the electron energy spectra in half-metals, the critical temperature as a function of the angle between the spin quantization axes in half-metals can be either monotonically increasing or decreasing. This finding highlights the crucial role of the band structure details in the proximity effect with half-metals which cannot be adequately treated in the quasiclassical theories.

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I. INTRODUCTION

The phenomena originating from the exchange of electrons between superconductors and multilayered ferromagnets have great potential for application in superconducting spintronics [1,2] since they provide an efficient tool for the control of the charge and spin transport by changing the magnetic state of the ferromagnet. The basic control element (the so-called superconducting spin valve) consisting of a thin superconducting (S) film and two ferromagnets (F) performs as the superconducting analog of a transistor controlled by an external magnetic field [3–5]. The critical temperature T_c of such a structure strongly depends on the angle θ between the magnetic moments in the ferromagnets. Thus, fixing the system temperature between the minimum $T_c^{\min}$ and the maximum $T_c^{\max}$ of the critical temperature and changing the mutual orientation of the magnetic moment of the F layers by the external magnetic field, one can significantly vary the resistivity of the spin valve by switching it from the normal to the superconducting state (spin-valve effect).

The physics behind the strong dependence $T_c(\theta)$ is related to the superconducting proximity effect [6,7]. The exchange field in the ferromagnet destroys the Cooper pairs and changes their spin structure. This results in the peculiar damped oscillatory behavior of the Cooper pair wave function inside the F layers and damping of the superconductor critical temperature. If the thickness of the ferromagnets is small compared to the coherence length ξ_f characterizing the oscillations period, then the critical temperature is determined simply by the average exchange field, and therefore, the function $T_c(\theta)$ is monotonically increasing, and $T_c(\pi) > T_c(0)$ (the so-called standard spin-valve effect) [4,5,8–15]. For the F layers with thickness $\sim\xi_f$ the interference phenomena coming from the oscillations of the wave function make $T_c(\pi) < T_c(0)$ for a certain range of parameters (inverse spin-valve effect) [6,16,17]. Moreover, the noncollinearity of the magnetic moment orientation in the F layers produces the long-range spin-triplet correlations [18] which form an additional channel for the Cooper pair leakage from the superconductor and thus increase the damping of T_c. As a result, for certain parameters the minimum of T_c corresponds to $\theta \neq 0, \pi$ (the so-called triplet spin-valve effect) [16,17,19,20].

Experimentally, the spin-valve effect was observed in a wide class of $F_1/S/F_2$ [21–37] and $S/F_1/F_2$ [37–42] structures. The magnitude of the effect appears to be very sensitive to the choice of ferromagnetic materials. Indeed, the typical scale of the Cooper pair wave function decay in ferromagnets tends to decrease with the increase in the exchange field. Therefore, the vast majority of spin valves are based on ferromagnetic alloys (e.g., CuNi and PdFe) with small exchange field compared to the Fermi energy. However, such structures are hardly applicable for devices of superconducting spintronics since the variation of their critical temperature $\Delta T_c = T_c^{\max} - T_c^{\min}$ does not exceed several percent.

Recently, it was demonstrated that the magnitude of the spin-valve effect can be significantly increased [43], provided one of the ferromagnetic layers is made of a half-metal (HM), a material with an exchange field comparable to the Fermi energy (e.g., Co, CrO_2) [44,45]. The full spin polarization of electrons in half-metals makes them extremely promising materials for superconducting spintronics. However, the quantitative theoretical description of the proximity effect in S/HM structures appears to be challenging due to the breakdown of the quasiclassical approximation, which requires small exchange fields and energy shifts between electron energy bands in different layers compared to the Fermi energy. Despite several attempts to develop quasiclassical theory of the superconducting proximity effect with half-metals [46–49], the quantitative quasiclassical description of such materials is still lacking. An alternative numerical solution of the

Bogoliubov–de Gennes equations supports the experimentally observed increase of the spin-valve effect in HM-based systems [50,51]. At the same time, the exact analytical solutions of the Gor'kov equations for the atomically thin S/F/HM heterostructures beyond the quasiclassical approximation additionally demonstrate the strong sensitivity of the spin-valve effect to the details of the electronic energy band structure inside each of the layers [20]. Specifically, depending on the relative shift in the electron bands in different layers, the dependence $T_c(\theta)$ approaches its minimum at $\theta = 0$ or $\theta = \pi$, which corresponds to the standard or inverse spin-valve effect. Thus, an adequate theoretical description of the spin-valve effect in superconducting hybrids containing half-metals requires an accurate account of the band structure effects which cannot be done within the quasiclassical approaches.

Since half-metals can host only spin-1 triplet superconducting correlations, their direct contact with a singlet s-wave superconductor should not give rise to the proximity effect. As a result, the conventional design of the HM-based spin valve contains an additional ferromagnetic layer with a small exchange field or other type of spin-active interface. Such an additional layer modifies the spin structure of the Cooper pairs and generates spin-triplet correlations which can penetrate the half-metallic layer [43,52]. Interestingly, even if the superconductor is placed between two half-metals, its critical temperature depends on the mutual orientation of the spin quantization axes in the HM layers due to nonlocal effects [53]. The exact solution of the Gor'kov equations for the atomically thin HM/S/HM structure with two identical HM layers predicts both standard and inverse spin-valve effects, depending on the shift between the bottom of the energy bands in each half-metal and the one in the S layer. Remarkably, the situation $T_c(0) > T_c(\pi)$ was found only for the very specific case when the electron spectrum in one of two HM layers is holelike.

In the present paper we analyze the possible types of the spin-valve effect in atomically thin $HM_1/S/HM_2$ and $S/HM_1/HM_2$ structures. We assume an electronlike spectrum in each of the HM layers and take into account the dispersion of the only occupied energy band (in contrast to Ref. [53]). We find that the details of the electron band structure in the half-metallic layers have a major influence on the type of spin-valve effect. Specifically, the relative shift between these bands in two HM layers can lead to the inversion of the spin-valve effect [which corresponds to the situation $T_c(0) > T_c(\pi)$] even without a sign change in the electron effective mass. Our finding shows that combining different half-metals in the spin valve, one can tune the dependence $T_c(\theta)$, making it either increasing or decreasing.

This paper is organized as follows. In Sec. II we consider the $S/HM_1/HM_2$ structure in which the occupied spin band in the HM_1 or HM_2 layer is shifted with respect to the electron energy band in the S layer and analyze the effect of this shift on the behavior of the critical temperature. Section III is devoted to the spin-valve effect in the $HM_1/S/HM_2$ structure. In Sec. IV we summarize our results.

II. SPIN-VALVE EFFECT IN S/HM1/HM2 STRUCTURES

In this section we analyze the spin-valve effect in $S/HM_1/HM_2$ structures [see Fig. 1(a)] and calculate how

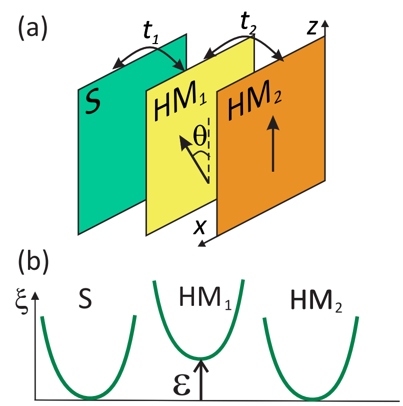

FIG. 1. (a) Atomically thin $S/HM_1/HM_2$ spin valve. The spin quantization axis in the central half-metal forms the angle θ with the z axis, while the one in the HM_2 layer coincides with the z axis. The transfer integrals t_1 and t_2 couple the adjacent layers. (b) The electron energy band structure in each layer. The parameter ε is the energy shift between the spin-up band of the HM_1 layer and the electron energy band in the superconductor.

the critical temperature T_c depends on the angle θ between the spin quantization axes in two half-metals. The y axis is chosen to be perpendicular to the layer interfaces. The spin quantization axis in the HM_2 layer is parallel to the z axis, while the spin quantization axis in the HM_1 layer is assumed to lie in the xz plane and form an angle θ with the z axis. We assume that each layer has atomic thickness and the in-plane electron motion is ballistic. For simplicity we consider the limit of coherent electron tunneling between the layers which conserves the in-plane momentum. Moreover, the transfer integrals t_1 and t_2 coupling the superconductor with the HM_1 and HM_2 layers, respectively, are assumed to be much smaller than the superconducting critical temperature T_c. Such a tight-binding model should be adequate for the description of the superconducting spin valves based, e.g., on $La_{0.7}Ca_{0.3}MnO_3$, a half-metallic compound [54] which has been shown to have a significant effect on the properties of an adjacent superconductor [55–58].

To calculate the dependence $T_c(\theta)$ we use the Gor'kov formalism (see, e.g., Refs. [10,11,59,60]). The system Hamiltonian consists of three terms:

$$\hat{H} = \hat{H}_0 + \hat{H}_S + \hat{H}_t. \tag{1}$$

The first term,

$$\hat{H}_0 = \sum_{\mathbf{p};\alpha,\beta=\{1,2\}} [\xi(\mathbf{p})\phi_\alpha^+\phi_\beta\delta_{\alpha\beta} + \hat{V}_{\alpha\beta}\psi_\alpha^+\psi_\beta + \hat{W}_{\alpha\beta}\eta_\alpha^+\eta_\beta], \tag{2}$$

describes the quasiparticle motion in the normal state in each isolated layer; the second term,

$$\hat{H}_S = \sum_{\mathbf{p}} (\Delta^*\phi_{\mathbf{p},2}\phi_{-\mathbf{p},1} + \Delta\phi_{\mathbf{p},1}^+\phi_{-\mathbf{p},2}^+), \tag{3}$$

describes the s-wave Cooper pairing in the S layer, and the last term,

$$\hat{H}_t = \sum_{\mathbf{p};\alpha=\{1,2\}} [t_1(\phi_\alpha^+\psi_\alpha + \psi_\alpha^+\phi_\alpha) + t_2(\psi_\alpha^+\eta_\alpha + \eta_\alpha^+\psi_\alpha)], \tag{4}$$

characterizes the tunneling between the layers. In Eqs. (2)–(4) ϕ, ψ, and η are the electron annihilation operators in the S, HM_1, and HM_2 layers, respectively, $\mathbf{p}$ is the quasiparticle momentum in the plane of the layers, $\xi(\mathbf{p})$ is the electron energy spectrum in the S layer, α and β are the spin indexes, and Δ is the superconducting gap function. The matrices $\hat{V}$ and $\hat{W}$ describe the spin-dependent single-particle spectra in the HM_1 and HM_2 layers, respectively. Let us denote $\xi_\uparrow$ and $\xi_\downarrow$ as the energy spectra for the electrons with spin parallel (spin up) and antiparallel (spin down) to the spin quantization axis in the corresponding half-metallic layer. To take into consideration only the most important features of the band structure we assume that in the HM_2 layer the energy spectrum for the spin-up electrons is the same as in the S layer $\xi_\uparrow = \xi(\mathbf{p})$, while the spin-down energy band is not occupied ($\xi_\downarrow = +\infty$). The corresponding matrix $\hat{W}$ reads

$$\hat{W} = \begin{pmatrix} \xi(\mathbf{p}) & 0 \\ 0 & \infty \end{pmatrix}. \tag{5}$$

In the HM_1 layer it is convenient to assume a finite value of the exchange field h and a possible energy band shift ξ_0 with respect to the superconductor. This gives the matrix $\hat{V}$ in the form

$$\hat{V} = \begin{pmatrix} \xi(\mathbf{p}) + \xi_0 - h\cos\theta & -h\sin\theta \\ -h\sin\theta & \xi(\mathbf{p}) + \xi_0 + h\cos\theta \end{pmatrix}, \tag{6}$$

where θ is the angle between $\mathbf{h}$ and the z axis. To approach the limit of the half-metal one should set simultaneously $h = +\infty$, $\xi_0 = +\infty$, and $\xi_0 - h = \varepsilon$. The resulting energy spectrum will contain only one band shifted by the value ε with respect to the one in the superconductor [see Fig. 1(b)].

In the limit of weak tunneling the critical temperature of the spin valve slightly differs from the critical temperature T_{c0} of the isolated superconductor. Then it is convenient to represent the expression for $T_c(\theta)$ coming from the self-consistency equation in the following form:

$$T_c(\theta) = T_c(0) - T_{c0}^2 \sum_{\omega_n=-\infty}^{+\infty} \int_{\xi=-\infty}^{+\infty} d\xi \, \frac{\hat{F}_{12}^+(\theta) - \hat{F}_{12}^+(0)}{\Delta^*}. \tag{7}$$

Here $\hat{F}_{\alpha\beta}^+ = \langle T_\tau(\phi_\alpha^+, \phi_\beta^+)\rangle$ is the anomalous Green's function in the superconductor, T_{c0} is the critical temperature in the absence of the proximity effect ($t_1 = t_2 = 0$), and $\omega_n = \pi T_{c0}(2n+1)$ are the Matsubara frequencies.

To calculate $\hat{F}^+$ we introduce the set of imaginary-time Green's functions

$$G_{\alpha,\beta} = -\langle T_\tau(\phi_\alpha, \phi_\beta^+)\rangle, \qquad F_{\alpha,\beta}^+ = \langle T_\tau(\phi_\alpha^+, \phi_\beta^+)\rangle, \tag{8}$$

$$E_{\alpha,\beta}^\psi = -\langle T_\tau(\psi_\alpha, \phi_\beta^+)\rangle, \qquad F_{\alpha,\beta}^{\psi+} = \langle T_\tau(\psi_\alpha^+, \phi_\beta^+)\rangle, \tag{9}$$

$$E_{\alpha,\beta}^\eta = -\langle T_\tau(\eta_\alpha, \phi_\beta^+)\rangle, \qquad F_{\alpha,\beta}^{\eta+} = \langle T_\tau(\eta_\alpha^+, \phi_\beta^+)\rangle. \tag{10}$$

Next, we obtain the system of Gor'kov equations, taking the imaginary-time derivatives of the above Green's functions in the Fourier representation and using the Heisenberg equations for the operators ϕ, ψ, and η:

$$(i\omega_n - \xi)G + \Delta I F^+ - t_1 E^\psi = \hat{1}, \tag{11}$$

$$(i\omega_n + \xi)F^+ - \Delta^* I G + t_1 F^{\psi+} = 0, \tag{12}$$

$$(i\omega_n - \hat{V})E^\psi - t_1 G - t_2 E^\eta = 0, \tag{13}$$

$$(i\omega_n + \hat{V})F^{\psi+} + t_1 F^+ + t_2 F^{\eta+} = 0, \tag{14}$$

$$(i\omega_n - \hat{W})E^\eta - t_2 E^\psi = 0, \tag{15}$$

$$(i\omega_n + \hat{W})F^{\eta+} + t_2 F^{\psi+} = 0. \tag{16}$$

The above system enables an exact analytical solution for $\hat{F}^+$. In the first-order perturbation theory with the gap potential being a small parameter the result is

$$\frac{\hat{F}^+}{\Delta^*} = \left\{(i\omega_n + \xi)\hat{1} - t_1^2\left[(i\omega_n + \hat{V}) - t_2^2(i\omega_n + \hat{W})^{-1}\right]^{-1}\right\}^{-1} \times \hat{I}\left\{(i\omega_n - \xi)\hat{1} - t_1^2\left[(i\omega_n - \hat{V}) - t_2^2(i\omega_n - \hat{W})^{-1}\right]^{-1}\right\}^{-1}, \tag{17}$$

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

The further substitution of (17) into (7) gives the desired critical temperature. Since the transfer integrals are assumed to be small in comparison with T_{c0} before substitution into (7), we take the power expansion of (17) over t_1 and t_2 up to the forth order (see Appendix A) and obtain the explicit analytical result for T_c:

$$T_c(\theta) = T_c(0) + \sum_{\omega_n=-\infty}^{+\infty} \int_{-\infty}^{+\infty} \frac{2T_{c0}^2 t_1^2 t_2^2 h(1-\cos\theta)(\omega_+ + \xi_0) d\xi}{\omega_+^3 \omega_- [(\omega_+ + \xi_0)^2 - h^2]^2}, \tag{18}$$

where $\omega_\pm = i\omega_n \pm \xi$. Integrating over ξ, we find

$$T_c(\theta) = T_c(0) - \sum_{\omega_n>0} \mathrm{Re}\left\{\frac{2\pi T_{c0}^2 t_1^2 t_2^2 h(1-\cos\theta)(2i\omega_n + \xi_0)}{\omega_n^3[(2i\omega_n + \xi_0)^2 - h^2]^2}\right\}. \tag{19}$$

Finally, taking $h = +\infty$, $\xi_0 = +\infty$, and $\xi_0 - h = \varepsilon$, we obtain the critical temperature of the $S/HM_1/HM_2$ spin valve in which the spin-up band in the central half-metal is shifted by the value ε with respect to the energy band in the S layer:

$$T_c(\theta) = T_c(0) + \sum_{\omega_n>0} \frac{\pi T_{c0}^2 t_1^2 t_2^2 \left(4\omega_n^2 - \varepsilon^2\right)(1-\cos\theta)}{4\omega_n^3\left(4\omega_n^2 + \varepsilon^2\right)^2}. \tag{20}$$

For further analysis it is convenient to represent the expression for the critical temperature as

$$T_c(\theta) = T_c(0) + a\frac{t_1^2 t_2^2}{(2\pi T_{c0})^4} T_{c0}(1-\cos\theta). \tag{21}$$

The sign of the parameter a determines whether the standard ($a > 0$) or inverse ($a < 0$) spin-valve effect is realized in the system. Comparing Eq. (21) with Eq. (20), we find

$$a = \sum_{n\geqslant 0} \frac{(2n+1)^2 - (\varepsilon/2\pi T_{c0})^2}{(2n+1)^3[(2n+1)^2 + (\varepsilon/2\pi T_{c0})^2]^2} + O(t^2). \tag{22}$$

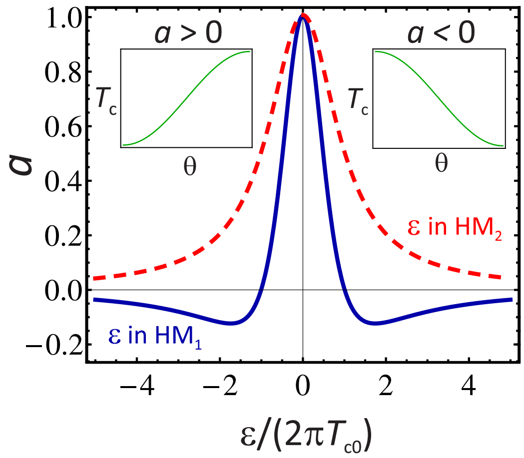

FIG. 2. The critical temperature is represented as $T_c(\theta) = T_c(0) + aT_{c0}[t/(2\pi T_{c0})]^4(1-\cos\theta)$. The dependences of the parameter a on the energy shift ε for the $S/HM_1/HM_2$ spin valve in which the spin-up band is shifted in the HM_1 half-metal (solid blue curve) or in the HM_2 layer (dashed red curve). Insets: the corresponding dependencies of the critical temperature on the angle θ.

If the occupied spin bands in both half-metals coincide with the electron energy band in the superconductor, i.e., $\varepsilon = 0$, then $a > 0$, and $T_c(\pi)$ is higher than $T_c(0)$ (the standard spin-valve effect). However, if $\varepsilon \neq 0$, it is not always the case, and the inverse switching is possible (see Fig. 2, where we have put $t_1 = t_2 \equiv t$). Indeed, the coefficient a becomes negative at $|\varepsilon| = \varepsilon_{cr} \approx 2\pi T_{c0}$ for $|\varepsilon| > \varepsilon_{cr}$, which corresponds to the monotonically decreasing dependence $T_c(\theta)$. Note that for $\varepsilon \gg T_{c0}$ the coefficient a can be estimated as $a \propto -(\pi T_{c0}/\varepsilon)^2$.

Now we investigate if the inverse switching is possible in the case when the spin-up band is shifted in the HM_2 layer instead of the HM_1 one. The corresponding band structure is shown in Fig. 3. For convenience, we assume that the z axis coincides with the spin quantization axis in the HM_1 layer and forms the angle θ with the one in the HM_2 half-metal (see Fig. 3). The Hamiltonian, the system of Gor'kov

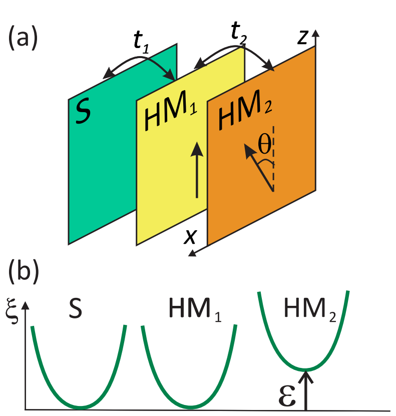

FIG. 3. (a) Sketch and (b) the band structure of the $S/HM_1/HM_2$ spin valve in which the spin-up band in the HM_2 half-metal is shifted by the value ε with respect to the electron energy band in the S layer. The spin quantization axes in half-metals form the angle θ with each other.

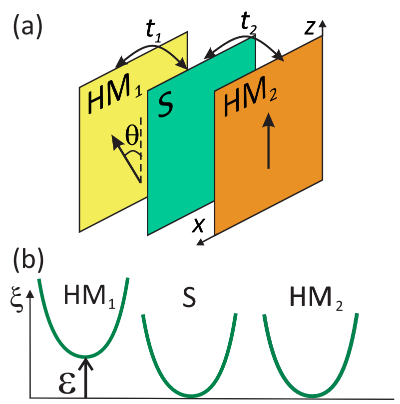

FIG. 4. The $HM_1/S/HM_2$ structure of atomic thickness. (a) Sketch of the spin valve. Here θ is the angle between spin quantization axes in the HM_1 and HM_2 layers. The HM_1 half-metal and the superconductor are coupled by the transfer integral t_1, while the transfer integral t_2 couples the S and HM_2 layers. (b) The band structure of the spin valve.

equations, and its solution for the anomalous Green's function still have the form (1)–(4), (11), and (17), respectively, if one replaces $\hat{V} \to \hat{W}$ and $\hat{W} \to \hat{V}$. Substituting the expansion of the Green's function $\hat{F}^+$ over t_1 and t_2 into (7), we obtain

$$T_c(\theta) = T_c(0) + \sum_{\omega_n=-\infty}^{+\infty} \int_{-\infty}^{+\infty} \frac{T_{c0}^2 t_1^2 t_2^2 h(1-\cos\theta)d\xi}{\omega_+^4 \omega_-[(\omega_+ + \xi_0)^2 - h^2]}. \tag{23}$$

Next, we integrate over ξ and find

$$T_c(\theta) = T_c(0) + \sum_{\omega_n>0} \frac{2\pi T_{c0}^2 t_1^2 t_2^2 h\xi_0(1-\cos\theta)}{\omega_n^3\left[4\omega_n^2 + (h-\xi_0)^2\right]\left[4\omega_n^2 + (h+\xi_0)^2\right]}. \tag{24}$$

Finally, taking $h = +\infty$, $\xi_0 = +\infty$, and $\xi_0 - h = \varepsilon$, we obtain the critical temperature of the $S/HM_1/HM_2$ spin valve:

$$T_c(\theta) = T_c(0) + \sum_{\omega_n>0} \frac{\pi T_{c0}^2 t_1^2 t_2^2 (1-\cos\theta)}{4\omega_n^3\left(4\omega_n^2 + \varepsilon^2\right)}. \tag{25}$$

The corresponding parameter a reads

$$a = \sum_{n\geqslant 0} \frac{1}{(2n+1)^3[(2n+1)^2 + (\varepsilon/2\pi T_{c0})^2]} + O(t^2). \tag{26}$$

From Eq. (25) one sees that $T_c(\pi) > T_c(0)$ for any ε (see Fig. 2). Thus, the shift of the occupied spin band in the side half-metal does not give rise to the inverse spin-valve effect.

III. SPIN-VALVE EFFECT IN HM1/S/HM2 STRUCTURES

In this section we consider spin valves which consist of a superconductor placed between two half-metals (see Fig. 4) and calculate the critical temperature of such a structure. The spin quantization axis in the HM_2 layer is directed along the z axis and forms the angle θ with the one in the HM_1 layer. The spin-up band in the right half-metal coincides with the energy band in the superconductor, while in the left half-metal we assume $\xi_\uparrow = \xi(\mathbf{p}) + \varepsilon$. The Hamiltonian has the form

(1) with H_0, H_s, $\hat{W}$, and $\hat{V}$ satisfying (2), (3), (5), and (6), respectively, and

$$\hat{H}_t = \sum_{\mathbf{p};\alpha=\{1,2\}} [t_1(\phi_\alpha^+\psi_\alpha + \psi_\alpha^+\phi_\alpha) + t_2(\phi_\alpha^+\eta_\alpha + \eta_\alpha^+\phi_\alpha)]. \quad (27)$$

As before, we introduce the minimal set of the Green's functions (8)–(10) required for the calculation of T_c and write down the system of Gor'kov equations (see Appendix B). Their solution for the anomalous Green's function in the linear approximation over the gap potential reads

$$\frac{\hat{F}^+}{\Delta^*} = \left[(i\omega_n + \xi)\hat{1} - t_1^2(i\omega_n + \hat{V})^{-1} - t_2^2(i\omega_n + \hat{W})^{-1}\right]^{-1} \times \hat{I}\left[(i\omega_n - \xi)\hat{1} - t_1^2(i\omega_n - \hat{V})^{-1} - t_2^2(i\omega_n - \hat{W})^{-1}\right]^{-1}. \quad (28)$$

Expanding expression (28) over t_1 and t_2 up to forth order and substituting it into (7), we find

$$T_c(\theta) = T_c(0) + \sum_{\omega_n=-\infty}^{+\infty} \int_{-\infty}^{+\infty} \frac{T_{c0}^2 t_1^2 t_2^2 h(1-\cos\theta)d\xi}{\omega_+^3\omega_-} \times \left\{\frac{2}{\omega_+[(\omega_+ + \xi_0)^2 - h^2]} + \frac{1}{\omega_-[(\omega_- - \xi_0)^2 - h^2]}\right\}. \quad (29)$$

Performing the same analysis as before, we obtain the critical temperature of the $HM_1/S/HM_1$ spin valve of atomic thickness with the spin-up band in HM_1 shifted by the value ε with respect to the electron energy band in the superconductor:

$$T_c(\theta) = T_c(0) + \sum_{\omega_n>0} \frac{\pi T_{c0}^2 t_1^2 t_2^2 \left(68\omega_n^4 - 7\varepsilon^2\omega_n^2 - \varepsilon^4\right)(1-\cos\theta)}{\omega_n^3\left(4\omega_n^2 + \varepsilon^2\right)^3}. \quad (30)$$

In the limit $t_1 \to 0$, $t_2 \to 0$ the corresponding parameter a reads

$$a = \sum_{n\geqslant 0} \frac{17(2n+1)^4 - 7(2n+1)^2(\varepsilon/2\pi T_{c0})^2 - (\varepsilon/2\pi T_{c0})^4}{(2n+1)^3[(2n+1)^2 + (\varepsilon/2\pi T_{c0})^2]^3}. \quad (31)$$

One sees that the behavior $T_c(\theta)$ strongly depends on the value of the energy shift ε (see Fig. 5). Since the parameter a changes sign at $|\varepsilon| = \varepsilon_{cr} \approx 2.8\pi T_{c0}$, the system reveals the standard spin-valve effect for $|\varepsilon| < \varepsilon_{cr}$ and the inverse one in the opposite case.

Note that the sign change in the difference $[T_c(\pi) - T_c(0)]$ appears even if the transfer integrals between the layers are not small. The numerical solution of the self-consistency equation with the anomalous Green's function (28) shows the switching between the standard and inverse spin-valve effects up to $t \lesssim T_{c0}$ (see Appendix C).

IV. CONCLUSION

We developed the theory of the spin-valve effect in the atomically thin $S/HM_1/HM_2$ and $HM_1/S/HM_2$ structures beyond the quasiclassical approximation. We showed that the details of the electron energy band structure in half-metallic layers strongly affect the behavior of the system critical temperature T_c: depending on the position of the only occupied spin band in one of the HM_1 layers, the dependence of T_c on the angle between the spin quantization axes in half-metals can be either monotonically increasing or decreasing, which corresponds to the standard or inverse spin-valve effect, respectively.

The recent experiments on spin valves containing the half-metallic compound $La_{0.7}Ca_{0.3}MnO_3$ demonstrated that this strongly polarized ferromagnet is more stable than CrO_2 [52] and gives rise to the anomalous behavior of T_c [55–58]. We hope that such stability will allow the fabrication complex spin valves with two HM layers and perform experimental verification of our results. Note that our model does not account for the finite thickness of the HM layers. If this thickness is much smaller than the superconducting correlation length ξ_h inside the half-metal, our results should remain qualitatively the same. At the same time, for HM layers with thickness $\sim\xi_h$ the interference effects may have a significant impact on T_c. As a result, we expect that the type of spin-valve effect will be determined by the combination of two factors: the influence of the band structure details and the interference effects.

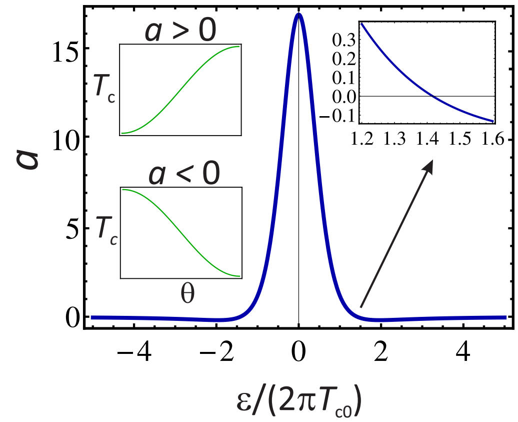

FIG. 5. The critical temperature has the form $T_c(\theta) = T_c(0) + aT_{c0}[t/(2\pi T_{c0})]^4(1-\cos\theta)$. The parameter a vs the energy separation ε for the $HM_1/S/HM_2$ structure. The left insets demonstrate corresponding dependencies of the critical temperature T_c vs the angle θ. The right inset shows in detail the part of the main plot where a changes sign.

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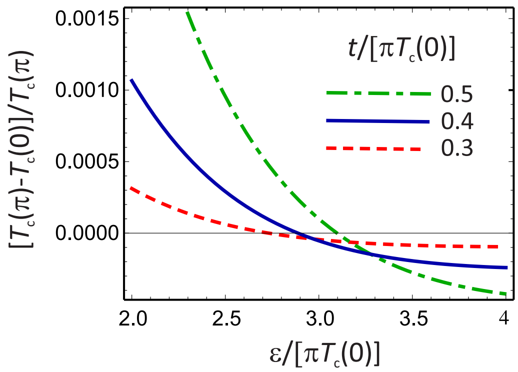

FIG. 6. The dependence of the critical temperature on the energy separation ε of the $HM_1/S/HM_2$ structure calculated numerically for different values of the transfer integral t.

APPENDIX A: ANOMALOUS GREEN'S FUNCTION IN THE S/HM1/HM2 SPIN VALVE OF ATOMIC THICKNESS

Expanding Eq. (17) over t_1 and t_2 up to fourth order, we obtain the following expression:

$$\begin{aligned}\frac{\hat{F}^+}{\Delta^*} \simeq \frac{1}{\omega_+\omega_-}\bigg[\hat{I} &+ t_1^2\left(\frac{1}{\omega_+}\hat{X}_+\hat{I} + \frac{1}{\omega_-}\hat{I}\hat{X}_-\right)\\ &+ t_1^2 t_2^2\left(\frac{1}{\omega_+}\hat{X}_+\hat{Y}_+\hat{X}_+\hat{I} + \frac{1}{\omega_-}\hat{I}\hat{X}_-\hat{Y}_-\hat{X}_-\right)\\ &+ t_1^4\left(\frac{1}{\omega_+^2}\hat{X}_+^2\hat{I} + \frac{1}{\omega_-^2}\hat{I}\hat{X}_-^2\right)\bigg],\end{aligned} \tag{A1}$$

where $\hat{X}_\pm = (i\omega_n\hat{1} \pm \hat{V})^{-1}$, $\hat{Y}_\pm = (i\omega_n\hat{1} \pm \hat{W})^{-1}$.

APPENDIX B: GOR'KOV EQUATIONS FOR THE HM1/S/HM2 STRUCTURE

Using the same procedure as before, we obtain the following system of Gor'kov equations:

$$(i\omega_n - \xi)G + \Delta I F^+ - t_1 E^\psi - t_2 E^\eta = \hat{1},$$

$$(i\omega_n + \xi)F^+ - \Delta^* I G + t_1 F^{\psi+} + t_2 F^{\eta+} = 0,$$

$$(i\omega_n - \hat{V})E^\psi - t_1 G = 0,$$

$$(i\omega_n + \hat{V})F^{\psi+} + t_1 F^+ = 0,$$

$$(i\omega_n - \hat{W})E^\eta - t_2 G = 0,$$

$$(i\omega_n + \hat{W})F^{\eta+} + t_2 F^+ = 0.$$

APPENDIX C: NUMERICAL CALCULATION OF THE CRITICAL TEMPERATURE OF THE S/HM1/HM2 STRUCTURE

Our model enables the exact solution of the critical temperature, which is valid for all $t_1, t_2 \lesssim \Delta$. Solving numerically the self-consistency equation with the exact anomalous Green's function (28), we obtain the sign change of the difference $[T_c(\pi) - T_c(0)]$ at nonzero ϵ even for not very small transfer integrals $t_1, t_2 \lesssim \pi T_{c0}$ (see Fig. 6). This confirms the sign change of the coefficient a, obtained analytically in the limit $t_1, t_2 \to 0$ [see Eq. (31) and Fig. 5].

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