Half-Metallic Superconducting Triplet Spin Valve

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We theoretically study a finite size $S_{F1}N_{F2}$ spin valve, where a normal metal ($N$) insert separates a thin standard ferromagnet ($F_1$) and a thick half-metallic ferromagnet ($F_2$). For sufficiently thin superconductor ($S$) widths close to the coherence length $\xi_0$, we find that changes to the relative magnetization orientations in the ferromagnets can result in substantial variations in the transition temperature $T_c$, consistent with experiment [Singh et al., Phys. Rev. X 5, 021019 (2015)]. Our results demonstrate that, in good agreement with the experiment, the variations are largest in the case where $F_2$ is in a half-metallic phase and thus supports only one spin direction. To pinpoint the origins of this strong spin-valve effect, both the equal-spin $f_1$ and opposite-spin $f_0$ triplet correlations are calculated using a self-consistent microscopic technique. We find that when the magnetization in $F_1$ is tilted slightly out-of-plane, the $f_1$ component can be the dominant triplet component in the superconductor. The coupling between the two ferromagnets is discussed in terms of the underlying spin currents present in the system. We go further and show that the zero energy peaks of the local density of states probed on the $S$ side of the valve can be another signature of the presence of superconducting triplet correlations. Our findings reveal that for sufficiently thin $S$ layers, the zero energy peak at the $S$ side can be larger than its counterpart in the $F_2$ side.

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In the field of superconducting spintronics, there is interest in spin-controlled proximity effects for manipulating the superconductivity in ferromagnet ($F$) and superconductor ($S$) layered systems [1, 2]. When an $S$ layer is in contact with two ferromagnets, creating a superconducting spin valve, the superconducting state can be controlled by changing the relative magnetization directions [3–5]. The basic superconducting spin-valve involves $SFF$ structures [3, 6] where switching between relative parallel and antiparallel magnetizations modifies the oscillatory singlet pairing in the $F$ regions. For strong ferromagnets, these oscillations have limited extent, as they become damped out over very short distances [7]. If however, the mutual magnetizations vary noncollinearly, the broken time reversal and translation symmetries induces a mixture of spin singlet and odd-frequency (or odd-time) spin-triplet correlations with 0 and $\pm 1$ spin projections along the magnetization axis [8, 9]. The triplet pairs with nonzero spin projection can naturally penetrate extensively within the ferromagnet layers [10–16] and result in an enhancement of the DOS at low energies [17, 18]. This long-range triplet component in $S_{F1}F_2$ type spin valves can be manipulated by changing the relative orientations of the magnetizations in $F_1$ and in $F_2$, which creates opportunities for the development of new types of spin-valves and switches for nonvolatile memory applications [19–21]. Because of their simplicity in pinpointing fundamental phenomena and promising prospects in spintronics devices, the $S_{F1}F_2$ spin valve continues to attract broad interest [3, 6, 14, 21–25, 27, 30]. For example, an anomalous Meissner effect has recently been observed [31] that is consistent with the generation of an odd-frequency superconducting state [32].

Recent experiments involving superconducting spin valves have investigated variations in the critical temperature, $T_c$ [33, 34] when varying the relative in-plane magnetization angle. The suppression in $T_c$ for nearly orthogonal magnetizations reflects the increased presence of equal-spin triplet pairs [6]. A spin valve like effect was also experimentally realized [23, 35] in FeV superlattices, where antiferromagnetic coupling between the Fe layers permits gradual rotation of the relative magnetization direction in the $F_1$ and $F_2$ layers. Most experiments involve standard ferromagnets, leading to $\Delta T_c$ sensitivity of several mK. When the outer $F_2$ layer is replaced by a half-metallic ferromagnet, such as CrO$_2$, a very large $\Delta T_c$ has been reported, which is indicative of the presence of odd-frequency triplet superconducting correlations [25].

Besides through studying $T_c$, the existence and type of superconducting correlations in superconducting spin-valves can be identified through signatures of the proximity-induced electronic density of states (DOS) [26]. When triplet correlations are present in an $F$ layer, it has been shown that a zero energy peak (ZEP) in the DOS can arise [27, 28]. The situation where pair correlations from both the spin-0 and spin-1 triplet channels are present can however make its unambiguous detection difficult. Nonetheless, this difficulty can be alleviated if one of the $F$ layers is half-metallic (supporting one spin direction), creating an effective spin-filter that can isolate the spin-1 triplet component due to the large exchange splitting present. Thus it is of interest to investigate $S_{F1}F_2$ structures containing a half-metallic ferromagnet, where the modified triplet proximity effects can result in

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strong spin valves with high sensitivity to magnetization changes and a corresponding $T_c$ suppression. To realistically and accurately model these systems, where $h \approx E_F$, we use a fully microscopic microscopic framework, the Bogoliubov-de Gennes (BdG) equations, to determine the singlet and triplet pair correlations self-consistently. This approach naturally supports the study of a broad range of intermediate ferromagnetic exchange energies, including the half metallic phase, by simply setting the exchange field value close to the Fermi energy. The half metallic regime is also accessible within the quasiclassical approximation [29, 30] by considering the case when the energy splitting of the the spin-up and spin-down bands greatly exceed the Fermi energy, i.e., $h \gg E_F$. Using the BdG formalism, we show how to identify the existence of the equal-spin components by probing the $S$ side of the proposed valve with an STM, revealing signatures in the form of peaks in the density of states (DOS) at zero energy [22, 27].

I. METHODS

A schematic of the spin valve configuration is depicted in Fig. 1. We model the nanostructure as a $SF_1NF_2$ layered system, where $S$ represents the superconducting layer, $N$ denotes the normal metallic intermediate layer, and $F_1$, $F_2$ are the inner (free) and outer (pinned) magnets, respectively. The layers are assumed to be infinite in the $y-z$ plane with a total thickness $d$ in the $x$ direction, which is perpendicular to the interfaces between layers. The ferromagnet $F_2$ has width $d_{F_2}$ and fixed direction of magnetization along $z$, while the free magnetic layer $F_1$ of width $d_{F_1}$ has a variable magnetization direction. The superconducting layer of thickness $d_S$ is in contact with the free layer. The magnetizations in the $F$ layers are modeled by effective Stoner-type exchange fields $\mathbf{h}(x)$ which vanish in the non-ferromagnetic layers.

To accurately describe the physical properties of our systems with sizes in the nanometer scale and over a broad range of exchange fields, where quasiclassical approximations are limited, we numerically solve the microscopic BdG equations within a fully self-consistent framework. The general spin-dependent BdG equations for the quasiparticle energies, $\epsilon_n$, and quasiparticle wavefunctions, $u_{n\sigma}, v_{n\sigma}$, are written:

$$
\begin{pmatrix}
\mathcal{H}_0 - h_z & -h_x & 0 & \Delta(x) \\
-h_x & \mathcal{H}_0 + h_z & -\Delta(x) & 0 \\
0 & -\Delta(x) & -(\mathcal{H}_0 - h_z) & -h_x \\
\Delta(x) & 0 & -h_x & -(\mathcal{H}_0 + h_z)
\end{pmatrix}
\times
\begin{pmatrix}
\begin{bmatrix}
u_{n\uparrow} \\
v_{n\downarrow}
\end{bmatrix}
\end{pmatrix}

= \epsilon_n
\begin{pmatrix}
\begin{bmatrix}
u_{n\uparrow} \\
v_{n\downarrow}
\end{bmatrix}
\end{pmatrix}
,$$

(1)

where $h_i$ ($i = x, z$) are components of the exchange field. In Eqs. (1), the single-particle Hamiltonian $\mathcal{H}_0 = -1/(2m)d^2/dx^2 - E_F + U(x)$ contains the Fermi energy, $E_F$, and an effective interfacial scattering potential described by delta functions of strength $H_j$ ($j$ denotes the different interfaces), namely: $U(x) = H_1\delta(x-d_S) + H_2\delta(x-d_S - d_{F_1}) + H_3\delta(x-d_S - d_{F_2} - d_N)$, where $H_j = k_F^2\lambda_{Bj}/m$ is written in terms of the dimensionless scattering strength $\lambda_{Bj}$. We assume $h_{x,i} = h_i \cos \theta_i$ and $h_{z,i} = h_i \sin \theta_i$ in $F_i$, where $h_i$ is the magnitude of exchange field, and $i$ denotes the region. To minimize the free energy of the system at temperature $T$, the singlet pair potential $\Delta(x)$ is calculated self-consistently [36]:

$$
\Delta(x) = \frac{g(x)}{2} \sum_n [u_{n\uparrow}(x)v_{n\downarrow}(x) + u_{n\downarrow}(x)v_{n\uparrow}(x)] \tanh \left( \frac{\epsilon_n}{2T} \right),
$$

(2)

where the sum is over all eigenstates with $\epsilon_n$ that lie within a characteristic Debye energy $\omega_D$, and $g(x)$ is the superconducting coupling strength, taken to be constant in the $S$ region and zero elsewhere. The pair potential gives direct information regarding superconducting correlations within the $S$ region only, since it vanishes in the remaining spin valve regions where $g(x) = 0$. Greater insight into the singlet superconducting correlations throughout the structure, and the extraction of the proximity effects is most easily obtained by considering the pair amplitude, $f_3$, defined as $f_3 \equiv \Delta(x)/g(x)$.

To analyze the correlation between the behavior of the superconducting transition temperatures and the existence of odd triplet superconducting correlations in our system, we compute the induced triplet pairing amplitudes which we denote as $f_0$ (with $m = 0$ spin projection) and $f_1$ (with $m = \pm 1$ spin projection) according to the following equations [16]:

$$
f_0(x,t) = \frac{1}{2} \sum_n [u_{n\uparrow}(x)v_{n\downarrow}(x) - u_{n\downarrow}(x)v_{n\uparrow}(x)] \zeta_n(t),
$$

(3a)

$$
f_1(x,t) = \frac{-1}{2} \sum_n [u_{n\uparrow}(x)v_{n\downarrow}(x) + u_{n\downarrow}(x)v_{n\uparrow}(x)] \zeta_n(t),
$$

(3b)
where \( \zeta_n(t) \equiv \cos(\varepsilon_n t) - i \sin(\varepsilon_n t) \tanh(\varepsilon_n/(2T)) \), and \( t \) is the time difference in the Heisenberg picture. These triplet pair amplitudes are odd in \( t \) and vanish at \( t = 0 \), in accordance with the Pauli exclusion principle. The quantization axis in Eqs. (3a) and (3b) is along the \( z \) direction. When studying the triplet correlations in \( F_1 \), we align the quantization axis with the local exchange field direction, so that after rotating, the triplet amplitudes \( f_0 \) and \( f_1 \) become linear combinations of the \( f_0 \) and \( f_1 \) in the original unprimed system [27]: \( f'_0(x,t) = f_0(x,t) \cos \theta - f_1(x,t) \sin \theta \), and \( f'_1(x,t) = f_0(x,t) \sin \theta + f_1(x,t) \cos \theta \). Thus, when the exchange fields in \( F_1 \) and \( F_2 \) are orthogonal (\( \theta = \pi/2 \)), the roles of the equal-spin and opposite-spin triplet correlations are reversed. The singlet pair amplitude however is naturally invariant under these rotations.

The study of single-particle excitations in these systems can reveal important signatures in the proximity induced singlet and triplet pair correlations. A useful experimental tool that probes these single-particle states is tunneling spectroscopy, where information measured by a scanning tunneling microscope (STM) can reveal the local DOS, \( N(x, \varepsilon) \), as a function of position \( x \) and energy \( \varepsilon \). We write \( N(x, \varepsilon) \) as a sum of each spin component (\( \sigma = \uparrow, \downarrow \)) to the DOS: \( N(x, \varepsilon) = N^\uparrow(x, \varepsilon) + N^\downarrow(x, \varepsilon) \), where,

\[
N^\sigma(x, \varepsilon) = \sum_n [u^2_{n\sigma}(x) \delta(\varepsilon - \varepsilon_n) + v^2_{n\sigma}(x) \delta(\varepsilon + \varepsilon_n)].
\]

II. RESULTS

We now proceed to present the self-consistent numerical results for the transition temperature, triplet amplitudes, and local DOS for the spin-valve structure depicted in Fig. 1. We normalize the temperature in the calculations by \( T_0 \), the transition temperature of a pure bulk S sample. When in the low-\( T \) limit, we take \( T = 0.05 T_0 \). All length scales are normalized by the Fermi wavevector \( k_F \), so that the coordinate \( x \) is written \( X = k_F x \), and the \( F_1 \) and \( F_2 \) widths are written \( D_{F_1} = k_F d_{F_1} \), for \( i = 1, 2 \). The thick half-metallic ferromagnet \( F_2 \) has width \( D_{F_2} = 400 \), and \( F_1 \) is a standard ferromagnet with \( b_1 = 0.1E_F \). We set \( d_{F_1} = \xi_F \), where \( \xi_F = v_F/(2h_1) \) is the length scale describing the propagation of spin-0 pairs. In dimensionless units we thus have, \( D_{F_1} = (h_1/E_F)^{-1} = 10 \), which optimizes spin mixing of superconducting correlations in the system. The \( S \) width is normalized similarly by \( D_S = k_F d_S \), and its scaled coherence length is taken to be \( k_F \xi_0 = 100 \). Natural units, e.g., \( \hbar = k_B = 1 \), are used throughout.

A. Critical Temperature and Triplet Correlations

We first study the critical temperature of the spin valve system. The linearized self-consistency expression near \( T_c \) takes the form, \( \Delta_i = \sum \mathcal{G}_{ij} \Delta_j \), where \( \Delta_i \) are the expansion coefficients for \( \Delta(x) \) in the chosen basis. The \( \mathcal{G}_{ij} \) are the corresponding matrix elements, which involve sums of the normal state energies and wavefunctions. To determine \( T_c \), we compute the eigenvalues \( \lambda_i \) of the corresponding eigensystem \( \Delta = \lambda \mathcal{G} \Delta \). When \( \lambda > 1 \) at a given temperature, the system is in the superconducting state. Many of the computational details can be found...
in Ref. 33, and are omitted here.

It was experimentally observed [25] that a SF1F2 spin valve is most effective at converting singlet Cooper pairs to spin polarized triplet pairs when F2 is in a half-metallic phase. To examine this theoretically, we investigate the critical temperature and corresponding triplet pair generation as a function of $h_2/E_F$ and $\theta$ ($h_1/E_F = 0.1$ remains fixed). The width of the superconducting layer is maintained at $D_S = 130$, and the nonmagnetic insert has a set width corresponding to $D_N = 5$. The exchange field $b_2$ varies from $0.1E_F$ to $E_F$ where $b_2 = E_F$ corresponds to the situation where only one spin species exists in this region (i.e. the half-metallic phase). As seen in Fig. 2, $T_c$ is nearly constant over the full range of $\theta$ when both ferromagnets are of the same type, i.e., when $h_2/E_F = 0.1$. Upon increasing $h_2$ towards the half-metallic limit, it is apparent that the spin valve effect becomes dramatically enhanced, whereby rapid changes in $T_c$ occur when varying $\theta$. This result therefore clearly supports the assertion that the use of a half-metal generates the most optimal spin-valve effectiveness [25]. Large variations in $T_c$ have also been found using a diffusive quasiclassical approach involving SF1F2 heterostructures lacking the normal layer insert [3, 30]. When comparing $T_c$ in the two collinear magnetic orientations, the self-consistently calculated critical temperatures in Fig. 2 reveal that the parallel state ($\theta = 0^\circ$) has a smaller $T_c$ compared to the antiparallel state ($\theta = 180^\circ$) for moderate exchange field strengths. For these cases, the two magnets can counter one another, leading to a reduction of their effective pair-breaking effects. This creates a more favorable situation for the superconducting state, causing $T_c$ to be larger. The situation reverses for stronger magnets with $h \gtrsim 0.8$, and the maximum $T_c$ now arises for parallel relative orientations of the magnetizations. In between the parallel and antiparallel states, $T_c$ undergoes a minimum that occurs not at the orthogonal orientation ($\theta = 90^\circ$), but slightly away from it. This behavior has been observed in ballistic [5] and diffusive [3] systems where the minimum in $T_c$ arises from the leakage of Cooper pairs that are coupled to the outer $F$ layer via the generation of the triplet component $f_1$ that is largest near $\theta = 90^\circ$.

To demonstrate the correlation between the strong $T_c$ variations and the generation of triplet and singlet pairs, Fig. 3 shows the magnitudes of the equal-spin triplet amplitudes ($f_1$), opposite-spin triplet amplitudes ($f_0$), and the singlet pair amplitudes ($f_3$), each averaged over the S region. For the relative correlations, a representative value for the normalized relative time $\tau$ is set at $\tau \equiv \omega t = 4$. When the ferromagnet ($F_2$) possesses a large exchange field, and the relative magnetization angle between $F_1$ and $F_2$ approaches an orthogonal state, superconductivity becomes severely weakened. Indeed, as Fig. 2 demonstrated, the singlet pair correlations can become completely destroyed at low temperatures ($T \simeq 0.05$), and orientations in the vicinity of $\theta \simeq 90^\circ$, whereby the system has transitioned to a normal resistive state. This is consistent with Fig. 3(c), where the $f_3$ amplitudes vanish in the neighborhood of $\theta \approx 90^\circ$ and $h_2/E_F = 1$. As Fig. 3(a) and (b) illustrates, the triplet amplitudes also vanish due to the absence of singlet correlations at those orientations. For weaker magnets however, the superconducting state never transitions to a normal resistive state over the entire range of $\theta$, and the well known situation arises whereby the equal-spin triplet pairs are largest for orthogonal magnetization configurations, i.e., when the misalignment angle is greatest ($\theta \approx 90^\circ$). In all cases however, the $f_1$ components must always vanish at $\theta = 0$ and $\theta = 180^\circ$, where the relative collinear magnetization alignments are either in the parallel or antiparallel state respectively. It is clear from Figs. 3(a) and 3(b) that the average behavior of $|f_0|$ and $|f_1|$ exhibits their most extreme values when $T_c$ undergoes its steepest variations around $\theta \approx 20^\circ$ [see Fig. 2]. In particular, at the half-metallic phase, $f_1$ is greatly enhanced while $f_0$ is dramatically suppressed. Therefore, the considerable variations in $T_c$ is correlated with the fact that 100% spin-polarized compounds such as CrO$_2$ result in the optimal generation of spin triplet correlations [25]. The suppression of $f_0$ at $\theta \approx 20^\circ$ is fairly robust to changes in the size of the S region. As the bottom panels in Figs. 3 illustrate, increasing $D_S$ by several coherence lengths causes very little change in the location of the first minimum in $f_0$ at $\theta \approx 20^\circ$. The angle $\theta$ that corresponds to a peak in $f_1$ however, noticeably shifts to larger $\theta$, so that at $\theta \approx 20^\circ$, $f_1$ no longer at its peak value. Therefore, the thinnest S layer width considered here, $D_S = 130$, leads to the most favorable conditions for the generation of $f_1$ triplet pairs in the superconductor and limited coexistence with the $f_0$ triplet correlations.

Next, Fig. 4 shows $T_c$ as a function of the out-of-plane misalignment angle $\theta$ for differing (a) superconductor widths $D_S$, (b) normal layer widths $D_N$, and (c) spin-independent interface scattering strengths $H_B$. If the relative magnetizations were to rotate in-plane, the $T_c$ behavior discussed here would be identical, thus providing additional experimental options for observing the predicted effects. In (a), the sensitivity of $T_c$ to the S layer width is shown. The importance of having thin S layers with $d_S \sim \xi_0$ (100 in our units) is clearly seen. In essence, extremely narrow S boundaries restrict Cooper pair formation, causing the ordered superconducting state to effectively become more “fragile”, consistent with other F/S systems containing thin S layers [5]. Indeed, for the thinnest case, $D_S = 100$, superconductivity completely vanishes for most magnetization configurations, except when $\theta$ is near the parallel or antiparallel orientations. At the thickest $D_S$ shown ($D_S = 200$), the sensitivity to $\theta$ has dramatically diminished, as pair-breaking effects from the adjacent ferromagnet now have a limited overall effect in the larger superconductor. For all S widths considered, the minimum in $T_c$ occurs when $\theta$ lies slightly off the orthogonal configuration ($\theta = 90^\circ$), consistent with some quasiclassical systems [3]. Next, in Fig. 4(b) the S layer thickness is set to $D_S = 130$, while several nonmagnetic N metal spacer widths are
FIG. 4. (Color online). Critical temperature $T_c$ as a function of the relative exchange field orientation angle $\theta$. In (a) the normal metal insert has a width of $D_N = 5$, and the $S$ width varies as shown in the legend, from $D_S = 100$ to $D_S = 200$. In (b) the $S$ width is fixed at $D_S = 130$, while the $N$ spacer is varied. In (c) the effects of interfacial scattering are examined, with $D_S = 130, D_N = 5$. The legend depicts the various scattering strengths $H_B$ considered.

The presence of the $N$ layer clearly plays a crucial role in the thermodynamics of the spin valve. Indeed, an optimum $D_N \approx 5$ exists which yields the greatest $\Delta T_c(\theta)$: Increasing or decreasing $D_N$ around this value can significantly reduce the size of the spin valve effect. Physically, this behavior is related to the spin-triplet conversion that takes place in the ferromagnets and corresponding enhancement of the equal-spin triplet correlations in the $N$ layer. This will be discussed in greater detail below. For $D_N$ much larger than the optimal width, a severe reduction in magnetic interlayer coupling occurs and $T_c$ exhibits little variation with $\theta$.

Finally, in Fig. 4(c), we incorporate spin-independent scattering at each of the spin valve interfaces. A wide range of scattering strengths are considered. We assume $H_j \equiv H (j = 1, 2, 3)$, so that interface scattering can be written solely in terms of the dimensionless parameter $H_B = H/v_F$. Overall, the general features and trends for $T_c$ seen previously are retained. With moderate amounts of interface scattering, $H_B = 0.1$, we find $\Delta T_c \approx T_c(\theta = 0^\circ) - T_c(\theta = 90^\circ) \approx 0.3T_D$. It is immediately evident that samples must have interfaces as transparent as possible [25, 27]: the variations in $T_c$ with $\theta$ become severely reduced with increasing $H_B$, as the phase coherence of the superconducting correlations becomes destroyed. In all cases, we observe some degree of asymmetry in $T_c$ as a function of $\theta$, similar to what has been reported in both diffusive [3] and clean [5] spin valves lacking half-metallic elements. If it is assumed that the band splitting in $F_2$ is sufficiently large so that only one spin species can exist, a quasiclassical approach has shown that $T_c$ becomes symmetric with respect to $\theta$ in the diffusive regime [30].

To correlate the large spin-valve effect observed in Fig. 4 with the odd-time triplet correlations, we employ the expressions in Eqs. (3a) and (3b), which describe the spatial and temporal behavior of the triplet amplitudes. We normalize the triplet correlations, computed in the low $T$ limit, to the value of the singlet pair amplitude in the bulk $S$. The normalized averages of $|f_0|$ and $|f_1|$ are plotted as functions of $\theta$ in Fig. 5, at a dimensionless characteristic time of $\tau = 4$. For comparison purposes, the singlet pair correlations, $f_3$, are also shown (third column). In each panel, spatial averages over different segments of the spin valve are displayed as separate curves (see caption). Each row of figures corresponds to different $D_N$: $D_S = 130, 150, 300$ (from top to bottom). One of the most striking observations is the effect of the normal metal spacer, which contains a substantial portion of the equal-spin triplet pairs. We will see below that the $f_1$ triplet correlations within the nor-
FIG. 6. (Color online). Normalized triplet \(f_0, f_1\) and singlet \(f_3\) amplitudes versus the dimensionless coordinate \(X\). The relative magnetization orientation is set to \(\theta = 20^\circ\). The dashed vertical lines identify the locations of the interfaces for the \(SFI_NF_2\) structure. Each segment corresponds to the following ranges: \(X < 130\) \((S\) region\), \(130 \leq X \leq 140\) \((F_1\) region\), \(140 < X \leq 145\) \((N\) region\), and \(X \geq 145\) \((F_2\) region\). The singlet component has been reduced by a factor of 10 for comparison purposes.

For thinner superconductors, where a self-consistent singlet component \(f_3(x)\) can substantially decline, or vanish altogether, in contrast to simple step function. Indeed, the observed disappearance of the singlet and triplet pair correlations for thin superconductors at \(\theta \approx 90^\circ\) (see top panels), can only occur if the pair potential is calculated self-consistently [Eq. (2)], thus ensuring that the free energy of the system is lowest [36]. As will be seen below, this important step permits the proper description of the proximity effects leading to nontrivial spatial behavior of \(\Delta(x)\) in and around the interfaces for both the superconductor and ferromagnets [44]. In common non self-consistent approaches, where \(\Delta(x)\) is treated phenomenologically as a prescribed constant in the \(S\) region, this vital behavior is lost.

Next, in Fig. 6 we present the spatial behavior of the real parts of the triplet and singlet pair correlations throughout each segment of the spin valve. We choose \(\theta = 20^\circ\) in order to optimize the \(f_1\) triplet component in \(S\). The other parameters used correspond to \(D_S = 130\), \(D_N = 5\), and \(T = 0.05\). Proximity effects are seen to result in a reduction of the singlet \(f_3\) correlations in the \(S\) region near the interface at \(X = 130\). As usual, this decay occurs over the coherence length \(\xi_0\). The singlet amplitude then declines within the \(F_1\) region before undergoing oscillations and quickly dampening out in the half-metal. Thus, as expected, the singlet Cooper pairs cannot be sustained in the half-metallic segment where only one spin species exists. Within the half-metal, the triplet component, \(f_0\) (also comprised of opposite-spin pairs), undergoes damped oscillations similar to the \(f_3\) correlations. It is notable that the triplet \(f_0\) component is severely limited in the \(S\) region, in stark contrast to the singlet correlations. Therefore, the \(f_0\) correlations in this situation are confined mainly to the \(F_1\) and \(N\) regions. The equal-spin \(f_1\) triplet component on the other hand, is seen to pervade every segment of the spin valve: The \(f_1\) correlations are enhanced in the \(N\) region, similar in magnitude to \(f_0\), but then exhibit a slow decay in both the \(S\) and half-metallic regions.

To further clarify the role of the triplet correlations in the spin valve, we now discuss the explicit relative time evolution of the triplet states in Fig. 7. Snapshots of the real parts of the triplet amplitudes are shown in equal increments of the relative time parameter \(\tau\). The angle \(\theta\) is fixed at \(\theta = 20^\circ\), again corresponding to when the triplet correlations with \(m = \pm 1\) projection of the \(z\)-component of the total spin in the superconductor is largest (see Fig. 5). The spatial range shown permits visualization of both triplet components throughout much of the system. Starting at the earliest time \(\tau = 0.8\), we find that \(f_1\) mainly populates the nonmagnetic \(N\) region, and then as \(\tau\) increases, propagates into the \(F_1\) and \(F_2\) regions before extending into the superconductor (left of the dashed vertical line). Meanwhile, \(f_0\) is essentially confined to the \(F_1\) and \(N\) regions, with limited presence in the \(S\) and \(F_2\) layers. Since the characteristic length \(\xi_F\) over which the \(f_0\) correlations modulate in \(F_2\) is inversely proportional to
h_2, f_0 declines sharply in the half-metallic region. Also, in agreement with Fig. 5, for θ = 20° and D_S = 130, there is also a limited presence of f_0 in the superconductor. The superconductor therefore has |f_1| >> |f_0|, which by using the appropriate experimental probe, can reveal signatures detailing the presence of equal-spin pairs f_1 [22].

B. Density of States

To explore these proximity induced signatures further, we investigate the experimentally relevant local DOS. An important spectroscopic tool for exploring proximity effects on an atomic scale with sub-meV energy resolution is the scanning tunneling microscope (STM). We are interested in determining the local DOS in the outer S segment of the SF_1 NF_2 spin valve. By positioning a non-magnetic STM tip at the edge of the S region, the tunneling current (I) and voltage (V) characteristics can be measured [22]. This technique yields a direct probe of the available electronic states with energy eV near the tip. The corresponding differential conductance dI(V)/dV over the energy range of interest is then proportional to the local DOS. The vast majority of past works only considered the DOS in the ferromagnet side where the f_1 correlations were expected to dominate [22, 24, 27]. However unavoidable experimental issues related to noise and thermal broadening can yield inconclusive data. As we have shown above, with the proper alignment of relative magnetizations, one can generate a finite f_1 in S accompanied by relatively limited f_0, thus presenting an opportunity to detect the important triplet pairs with spin s = ±1. By avoiding comparable admixtures of the two triplet components, experimental signatures of the equal-spin triplet correlations should be discernible. To investigate this further, the six panels in Fig. 8 show the normalized DOS evaluated near the edge of the superconductor for a wide variety of orientation angles θ. All plots are normalized to the corresponding value in a bulk sample of S material in its normal state. As shown, each panel ranges from a mutually parallel (θ = 0°) to a nearly orthogonal magnetization state (θ = 80°). In each case considered, we again have D_N = 5 and D_S = 130. Examining the top row of panels, traces are seen of the well-known BCS peaks that have now been shifted to subgap energies due to proximity and size effects. There also exists bound states at low energies that arise from quasiparticle interference effects. By sweeping the angle θ from the relative parallel case (θ = 0°) to slightly out of plane (θ = 20°), the zero energy quasiparticle states become significantly more pronounced. This follows from the fact that strong magnets tend to shift the relative magnetizations leading to maximal f_1 generation away...
FIG. 9. (Color online). Top panels: The normalized spatially and energy resolved DOS at three different orientations of the relative magnetization angle: (a) $\theta = 10^\circ$, (b) $\theta = 20^\circ$, and (c) $\theta = 30^\circ$. Panels (a)-(c) pertain to a single system with a narrow $S$ layer of width $D_S = 130$. The spatial region extending from $X = 0$ to 130 therefore corresponds to the superconducting region, and $X > 130$ pertains to the remaining layers of the spin valve. Bottom panels: the DOS is shown for three different $S$ layer thicknesses: (d) $D_S = 150$, (e) $D_S = 200$, and (f) $D_S = 300$, where $\theta$ is now fixed at $20^\circ$. The dashed vertical lines identify the interface between $S$ and $F_1$.

A complimentary global view of the above phenomena is presented in Fig. 9, where both the spatially and energy resolved DOS is shown at various $\theta$ (top panels) and $D_S$ (bottom panels). The top panels (a)-(c) depict the DOS for the same parameters and normalizations used in Fig. 8, and at three orientations: $\theta = 0^\circ$, $10^\circ$, $20^\circ$. It is evident that increasing the misalignment angle $\theta$, causes the ZEP in the $S$ region to become enhanced, reaching its maximum at $\theta \approx 20^\circ$. At this angle the ZEP extends through much of the system, including to a small extent, the $F_2$ side. However, within $S$, the ZEP is clearly more dominate [22]. For the bottom panels, (d)-(f), the relative magnetization orientation is fixed at $\theta = 20^\circ$, and three larger $S$ layers are shown: $D_S = 150$, $D_S = 200$, and $D_S = 300$. Increasing the $S$ layer widths illustrates the ZEP evolution towards a familiar gapped DOS of a BCS form. As seen, the ZEP is maximal in the superconducting region near the $S/F_1$ interface. By increasing $D_S$, the ZEP in the $S$ side becomes diminished until for sufficiently large $D_S$, that is, $D_S \approx 200$, the well-known singlet superconducting gap begins to emerge throughout much of the superconductor. At an even larger $D_S$ ($D_S = 300$), the ZEP has clearly weakened even further. Finally, for the experiment reported in Ref. 25, a peak in the resistive transitions at external fields of $B > 0.25T$ was observed immediately before the critical temperature whereby the system has transitioned to the superconducting phase. This peak in the transition curves was believed to be caused by the influence of the external field, effectively creating a $SF_1F_2F_2'$ type of configuration. We investigated such a configuration for various strengths and orientations of the $F'$ ferromagnet, and no evidence was found that was suggestive of anomalous behavior near $T_c$ for $F'$ with weak exchange fields. Note that the system under consideration is translationally invariant in the $yz$ plane (see Fig. 1). Therefore, the spin valve structure may experience a Fulde Ferrell-Larkin-Ovchinnikov phase during its phase transition from the superconducting to normal phase, although in a narrow region of parameter space [54, 55].

C. Spin Currents

To reveal further details of the exchange interaction which controls the behavior and type of triplet correlations present in the system, we next examine the characteristics of the spin currents that exist within the spin
When the magnetizations in \( F_1 \) and \( F_2 \) are noncollinear, the exchange interaction in the ferromagnets creates a spin current \( \mathbf{S} \) that flows in parts of the system, even in the absence of a charge current. If the spin current varies spatially, the corresponding nonconserved spin currents in \( F_1 \) and \( F_2 \) generate a mutual torque that tends to rotate the magnetizations of the two ferromagnets. This process is embodied in the spin-torque continuity equation [50, 51] which describes the time evolution of the spin density \( \eta \):

\[
\frac{\partial}{\partial t} \langle \eta_i(x) \rangle + \frac{\partial}{\partial x} S_i(x) = \tau_i(x), \quad i = x, y, z, \tag{5}
\]

where \( \tau(x) \) is the spin transfer torque (STT): 
\[
\tau(x) = -(2/\mu_B)\mathbf{m}(x) \times \mathbf{h}(x), \quad \mathbf{m}(x) \text{ is the magnetization, and } \mu_B \text{ is the Bohr magneton (see Appendix A).}
\]

The spin current tensor here has been reduced to vector form due to the quasi-one-dimensional nature of the geometry. We calculate \( S(x) \) by performing the appropriate sums of quasiparticle amplitudes and energies [see Eq. (A10)]. In the steady state, the continuity equation, Eq. (5), determines the torque by simply evaluating the derivative of the spin current as a function of position: 
\[
\tau_i(x) = \frac{\partial S_i(x)}{\partial x}.
\]

The net torque acting within the boundaries of e.g., the \( F_1 \) layer, is therefore the change in spin current across the two interfaces bounding that region:

\[
S_y(d_S + d_{F_1}) - S_y(d_S) = \int_{F_1} dx \tau_y, \tag{6}
\]

In equilibrium, the net \( \tau_y \) in \( F_2 \) is opposite to its counterpart in \( F_1 \). Since no spin current flows in the superconductor, we have \( S_y(d_S) = 0 \), and the net torque in \( F_1 \) is equivalent to the spin current flowing into \( N \).

In our setup, the exchange field in \( F_1 \) is directed in the \( x - z \) plane, and therefore the spin current and torque are directed orthogonal to this plane (along the interfaces in the \( y \) direction). Likewise, if the magnetizations were varied in the \( y - z \) plane, the spin currents would be directed along \( x \). Figure 10 thus illustrates the normalized spin current \( S_y \) as a function of the dimensionless position \( \theta \). The normalization factor \( S_0 \) is written in terms of \( n_c v_F \), where \( n_c = k_F^2/(3\pi^2) \), and \( v_F = k_F/m \). Several equally spaced magnetization orientations \( \theta \) are considered, ranging from parallel \( (\theta = 0^\circ) \), to orthogonal \( (\theta = 90^\circ) \). Within the two \( F \) regions, \( S_y \) tends to undergo damped oscillations, while in \( N \) there is no exchange interaction \( (\mathbf{h} = 0) \), and consequently the spin current is constant for a given \( \theta \). The main plot shows that when \( \theta = 0^\circ \), \( S_y \) vanishes throughout the entire system, as expected for parallel magnetizations. By varying \( \theta \), spin currents are induced due to the misaligned magnetic moments in the \( F \) layers. If the exchange field is rotated slightly out of plane, such that \( \theta < 30^\circ \), it generates on average, negative spin currents in the \( N \) and \( F_1 \) regions. As shown, these spin currents reverse their polarization direction for larger \( \theta \). This behavior is consistent with the inset, which shows how tuning \( \theta \) affects \( S_y \) (or equivalently, the net torque) in \( N \). Thus, by manipulating \( \theta \), the strength and direction of the spin current in the normal metal can be controlled, or even eliminated completely at \( \theta \approx 34^\circ \). By varying \( \theta \) about this angle, the overall torque, which tends to align the magnets in a particular direction, can then reverse in a given magnet.

For \( \theta \approx 15^\circ \) and \( \theta \approx 160^\circ \), the inset also clearly shows an enhancement of the magnitude of the spin currents, which coincides approximately to the orientations leading to an increase in the spin-polarized triplet pairs observed in Fig. 5.

In conclusion, motivated by recent experiments [22, 25], a hybrid \( SF_1N\) \( SF_2 \) spin valve containing a half-metallic ferromagnet has been theoretically investigated, revealing a sizable spin-valve effect for thin superconductors with widths close to \( \xi_0 \). Through self-consistent numerical calculations, the contributions from both the equal-spin \( (f_1) \) and opposite-spin \( (f_0) \) triplet correlations have been identified as the relative magnetization angle \( \theta \) varies. We found that when the magnetization in \( F_1 \) is directed slightly out-of-plane, the magnitude of \( f_1 \) in \( S \) is maximized, while for \( f_0 \) it is very small. By investigating the DOS in the superconductor over a broad range of \( \theta \), we were able to identify the emergence of zero energy peaks (ZEPs) in the DOS that coincide with peaks in the averaged \( f_1 \). Our results show, to a large extent, good agreement with experimental observations as well as the physical origins of these effects. We have thus established a clear, experimentally identifiable role that the triplet correlations play in this new class of half-metallic spin-valve structures. For future work, it would be interesting to study the transport properties of these types of spin valves by investigating the self-consistent charge and spin currents as they pertain to dissipationless spintronics applications.
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Appendix A: Spin Currents

In order to calculate the spin currents flowing within the spin valve, it is convenient to employ the Heisenberg picture to determine the time evolution of the spin density, \( \eta(r,t) \),

\[
\frac{\partial}{\partial t}(\eta(r,t)) = i[\mathcal{H}_{\text{eff}}, \eta(r,t)], \quad (A1)
\]

where \( \eta(r) \) is the spin density operator defined as,

\[
\eta(r) = \psi^+(r)\sigma\psi(r). \quad (A2)
\]

We define the effective BCS Hamiltonian \([36]\), \( \mathcal{H}_{\text{eff}} \), via

\[
\mathcal{H}_{\text{eff}} = \int d^3r \left\{ \psi^+(r)[\mathcal{H}_0(r) - \textbf{h}(r) \cdot \textbf{\sigma}]\psi(r) + \Delta(r)\psi^+_\uparrow(r)\psi_\downarrow(r) + \Delta^*(r)\psi_\downarrow(r)\psi^+_\uparrow(r) \right\}, \quad (A3)
\]

where \( \psi^+_\sigma(r), \psi_\sigma(r) \) denotes the fermionic field operators with spin projections \( \sigma = \uparrow, \downarrow \) along a given quantization axis, and \( \textbf{\sigma} \) is the usual vector of Pauli matrices. Inserting the Hamiltonian, Eq. (A3), into (A1) yields the following continuity equation:

\[
\frac{\partial}{\partial t}(\eta(r,t)) + \frac{\partial \textbf{S}}{\partial x} = \textbf{\tau}, \quad (A4)
\]

where \( \textbf{S} \) is the spin current which in our geometry is a vector (in general it is a tensor). The spin-transfer torque, \( \textbf{\tau} \), is given by:

\[
\textbf{\tau} = -i\langle \psi^+(r)[\textbf{h} \cdot \textbf{\sigma}, \textbf{\sigma}]\psi(r) \rangle - 2\langle \psi^+(r)[\textbf{h} \times \textbf{h}]\psi(r) \rangle. \quad (A5)
\]

Recalling the expression for the local magnetization, \( m(r) \),

\[
m(r) = -\mu_B \langle \eta(r) \rangle, \quad (A6)
\]

this permits the torque in Eq. (A5) to be written as,

\[
\textbf{\tau} = 2\langle \psi^+(r)\textbf{\sigma}\psi(r) \rangle \times \textbf{h} = -\frac{2}{\mu_B} \textbf{m} \times \textbf{h}. \quad (A7)
\]

In the steady state, and when a torque is present, the spin current therefore must have at least one spatially varying component. After taking the commutator in Eq. (A1), the explicit expression for the spin-current is found to be,

\[
\textbf{S} = -\frac{i}{2m}\langle \psi^+(r)\textbf{\sigma}\frac{\partial \psi(r)}{\partial x} - \frac{\partial \psi^+(r)}{\partial x}\textbf{\sigma}\psi(r) \rangle, \quad (A8)
\]

where for our quasi-one-dimensional systems, the vector \( \textbf{S} \) represents the spin current flowing along the \( x \) direction with spin components \( (S_x, S_y, S_z) \). To write the spin current in terms of the calculated quasiparticle amplitudes and energies, the field operators are directly expanded by means of a Bogoliubov transformation \([36]\):

\[
\psi^+_\uparrow(r) = \sum_n (u_{n\uparrow}(r)\gamma_n - v^*_{n\uparrow}(r)\gamma^*_n), \quad (A9a)
\]

\[
\psi_\downarrow(r) = \sum_n (u_{n\downarrow}(r)\gamma_n + v^*_{n\downarrow}(r)\gamma^*_n), \quad (A9b)
\]

where \( u_{n\sigma} \) and \( v_{n\sigma} \) are the quasiparticle and quasihole amplitudes, and \( \gamma_n \) and \( \gamma^*_n \) are the Bogoliubov quasiparticle annihilation and creation operators, respectively. By directly considering the commutation relations for the quantum mechanical operators, the following expectation values must be satisfied throughout our calculations: \( \langle \gamma^*_n \gamma_m \rangle = \delta_{nm} f_n \), \( \langle \gamma^*_\downarrow \gamma^*_\uparrow \rangle = 0 \), \( \langle \gamma^*_n \gamma_m \rangle = 0 \). Here \( f_n \) is the Fermi function which depends on the temperature \( T \) and quasiparticle energy \( \varepsilon_n = fu_n = (\exp[\varepsilon_n/(2T)] + 1)^{-1} \). We can now expand each spin component of the spin current in terms of the quasiparticle amplitudes to obtain \([50, 51]\):

\[
S_x = -\frac{i}{2m} \sum_n \left\{ f_n [u^*_n \frac{\partial u^*_n}{\partial x} + u^*_n \frac{\partial u^*_n}{\partial x} - u_n \frac{\partial u^*_n}{\partial x} - u^*_n \frac{\partial u^*_n}{\partial x}] - (1 - f_n) [v^*_n \frac{\partial v^*_n}{\partial x} + v^*_n \frac{\partial v^*_n}{\partial x} - v_n \frac{\partial v^*_n}{\partial x} - v^*_n \frac{\partial v^*_n}{\partial x}] \right\}, \quad (A10)
\]

\[
S_y = -\frac{1}{2m} \sum_n \left\{ f_n [u^*_n \frac{\partial u^*_n}{\partial x} - u^*_n \frac{\partial u^*_n}{\partial x} - u_n \frac{\partial u^*_n}{\partial x} + u^*_n \frac{\partial u^*_n}{\partial x}] - (1 - f_n) [v^*_n \frac{\partial v^*_n}{\partial x} - v^*_n \frac{\partial v^*_n}{\partial x} + v_n \frac{\partial v^*_n}{\partial x} - v^*_n \frac{\partial v^*_n}{\partial x}] \right\}, \quad (A11)
\]

\[
S_z = -\frac{i}{2m} \sum_n \left\{ f_n [u^*_n \frac{\partial u^*_n}{\partial x} - u^*_n \frac{\partial u^*_n}{\partial x} - u_n \frac{\partial u^*_n}{\partial x} + u^*_n \frac{\partial u^*_n}{\partial x}] - (1 - f_n) [-v^*_n \frac{\partial v^*_n}{\partial x} + v^*_n \frac{\partial v^*_n}{\partial x} + v_n \frac{\partial v^*_n}{\partial x} - v^*_n \frac{\partial v^*_n}{\partial x}] \right\}. \quad (A12)
\]
In the case of $F$ layers with uniform magnetization, there is no net spin current. The introduction of an inhomogeneous magnetization texture however results in a net spin current imbalance that is finite even in the absence of a charge current.

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