$0 - \pi$ Transitions in Josephson Junctions with Antiferromagnetic Interlayers

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We show that the dc Josephson current through superconductor-antiferromagnet-superconductor (S-AF-S) junctions manifests a remarkable atomic-scale dependence on the interlayer thickness. At low temperatures the junction is either a 0 or π junction depending on whether the AF interlayer consists of an even or odd number of atomic layers. This is associated with different symmetries of the AF interlayers in the two cases. In the junction with odd AF interlayers an additional $\pi - 0$ transition can take place as a function of temperature. This originates from the interplay of spin-split Andreev bound states. Experimental implications of these theoretical findings are discussed.

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The developing field of superconducting spintronics subsumes many fascinating physical phenomena with potential applications that may complement nonsuperconducting spintronic devices [1]. In addition there is an increasing interest in the novel properties of interfaces and junctions of superconductors and magnetic materials [2,3]. An important example is the $0 - \pi$ transition in superconductor-ferromagnet-superconductor (S-F-S) junctions where, depending on the temperature and the width of the ferromagnetic interlayer, the ground state of the junction is characterized by an intrinsic phase difference of π between the two superconductors [3–5]. This may be important for superconducting digital circuits, and has been proposed as a possible basis for quantum qubits [6–10]. The interplay of magnetic and superconducting order leads to interesting mesoscopic physical phenomena also at interfaces between antiferromagnets and superconductors. Recent theoretical studies have shown that a characteristic spin-dependent quasiparticle reflection at the AF surface, the so-called Q reflection, combined with Andreev reflection on the superconducting side, leads to novel low-energy bound states near such interfaces [11]. These Andreev bound states have important consequences for the associated proximity effect and can, for example, be detected in tunneling spectroscopy as subgap peaks in the resulting local density of states [12].

In this Letter we investigate effects of the Q reflection on the Josephson current in S-AF-S tunnel junctions in s-wave superconductors. An enhancement of the low-temperature critical current in such junctions was found in the limit of a sufficiently small ratio m/t, where t and m denote the hopping matrix element and the antiferromagnetic order parameter, respectively [11]. As shown below, the parameter m/t becomes sufficiently small in tunnel junctions only under the condition $(m/t) \ll \sqrt{D}$, where D is the transparency coefficient. We will find that in the opposite case $(m/t) \gtrsim \sqrt{D}$, which is also realistic for fabrication, the Josephson current in S-AF-S junctions exhibits new interesting properties. At low-temperature T, the current-phase relation reveals either a 0- or a π-junction state depending on whether the AF interlayer consists of an even or odd number of atomic layers, respectively. This atomic-scale thickness dependence differs from that of S-F-S junctions where the period of the alternation between 0 and π states strongly depends on the exchange field which controls the proximity-induced damped spatial oscillations of the pairing amplitude in the ferromagnetic metal. In contrast, for the S-AF-S junctions the $0 - \pi$ behavior is a true even/odd effect related to the difference in symmetries of the odd and even AF interfaces and the corresponding interface $\mathcal{S}$ matrices, as well as the spectra of the Andreev bound states. For odd (110) AF interlayers, the supercurrent displays a prominent anomaly with increasing T *revealing another* $\pi - 0$ *transition*. We will show that this remarkable result is a consequence of the interplay of spin-split Andreev bound states contributing with opposite sign to the total supercurrent. Lastly, we discuss possible experimental consequences of the effects in question. Our theoretical analysis includes both the self-consistent numerical solutions of the Bogoliubov-de Gennes (BdG) equations and a quasiclassical analytical approach to the superconducting leads, allowing us to describe the AF interface fully microscopically with atomic-scale accuracy, and interpret the results physically.

Model.—The Hamiltonian is defined on a 2D square lattice with superconducting Δ_i and magnetic m_i order parameters, and lattice constant $a = 1$:

$$\hat{H} = -t \sum_{\langle ij \rangle \sigma} \hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} + \sum_i (\Delta_i \hat{c}^{\dagger}_{i\uparrow} \hat{c}^{\dagger}_{i\downarrow} + \text{H.c.}) - \sum_{i\sigma} \mu \hat{n}_{i\sigma} + \sum_i m_i (\hat{n}_{i\uparrow} - \hat{n}_{i\downarrow}). \qquad (1)$$

Here, $\hat{c}^{\dagger}_{i\sigma}$ creates an electron of spin σ on the site i, μ is the chemical potential, and $\hat{n}_{i\sigma} = \hat{c}^{\dagger}_{i\sigma} \hat{c}_{i\sigma}$ is the particle number operator. The associated BdG equations are

$$\sum_j \begin{pmatrix} \mathcal{K}^+_{ij,\sigma} & \mathcal{D}_{ij,\sigma} \\ \mathcal{D}^*_{ij,\sigma} & -\mathcal{K}^-_{ij,\sigma} \end{pmatrix} \begin{pmatrix} u_{n\sigma}(j) \\ v_{n\bar{\sigma}}(j) \end{pmatrix} = E_{n\sigma} \begin{pmatrix} u_{n\sigma}(i) \\ v_{n\bar{\sigma}}(i) \end{pmatrix}. \quad (2)$$

The diagonal blocks are given by $\mathcal{K}^{\pm}_{ij} = -t\delta_{\langle ij\rangle} - \mu\delta_{ij} \pm \sigma m_i \delta_{ij}$, where $\sigma = +1/-1$ for up/down spin and δ_{ij} and $\delta_{\langle ij\rangle}$ are the Kronecker delta symbols connecting on-site and nearest neighbor sites, respectively. The off-diagonal block $\mathcal{D}_{ij}$ describes s-wave pairing $\mathcal{D}_{ij} = -\Delta_i\delta_{ij}$. The net magnetization $M_i = \frac{1}{2}[\langle \hat{n}_{i\uparrow}\rangle - \langle \hat{n}_{i\downarrow}\rangle]$ and the pairing amplitude $F_i = \langle \hat{c}_{i\downarrow}\hat{c}_{i\uparrow}\rangle$ are related to m_i and Δ_i by $m_i = U_i M_i$ and $\Delta_i = -V_i F_i$. The coupling constants U_i (V_i) are site dependent and nonzero on (off) the L atomic chains constituting the AF interlayer. This stabilizes the staggered AF order on the interlayer and the superconducting order outside this region. We choose the x (y) axis to run perpendicular (parallel) to the interface. The calculations for planar tunnel junctions with crystal periodicity along the interface are reduced to a 1D problem by Fourier transforming along y. This introduces a crystal-vector component k_y as a parameter and the BdG equations have to be diagonalized for each k_y.

The dc Josephson current $j_{rr'}$ between two neighboring sites $r = (x, y)$ and $r' = (x', y')$ is $j_{rr'} = -(iet/\hbar)\sum_\sigma[\langle \hat{c}^\dagger_{r\sigma}\hat{c}_{r'\sigma}\rangle - \langle \hat{c}^\dagger_{r'\sigma}\hat{c}_{r\sigma}\rangle]$. Below we report the results for the current per unit length $j_{xx'} = (1/l_y)\sum_y j_{rr'}$ obtained by summing along the interface of length l_y over all neighboring links between x and x' chains near the interface. For the (110) interface $x' = x + (1/\sqrt{2})$ and we get

$$j_{xx'} = -\frac{2iet}{\hbar l_y}\sum_{k_y n\sigma}\cos\left(\frac{k_y}{\sqrt{2}}\right)[u^*_{n\sigma}(x)u_{n\sigma}(x')f(E_{n\sigma}) + v_{n\bar{\sigma}}(x)v^*_{n\bar{\sigma}}(x')f(-E_{n\sigma}) - (x \leftrightarrow x')], \quad (3)$$

where $-\pi/\sqrt{2} < k_y \leq \pi/\sqrt{2}$ and $f(E)$ is the Fermi function. For the (100) junction $x' = x + 1$ and the current takes the form (3), but without the $\cos(k_y/\sqrt{2})$ factor and with $-\pi < k_y \leq \pi$. Since the vector potential generated by the current is not taken into account, we discuss only planar junctions in the tunneling limit when the current j is well below the thermodynamic critical pair-breaking current. Below, we fix the phase of the superconducting order parameter at each end of the system, obtain the self-consistent solutions, and calculate the current based on Eq. (3). As is well known, the current is only conserved when the superconducting order parameter is calculated fully self-consistently [13]. For more details on the numerical and analytical approaches used in this Letter, we refer the reader to Ref. [12].

Results.—We have studied the dc Josephson current in both (100) and (110) S-AF-S junctions. Below, however, we focus on the (110) interfaces where the effects in question are more pronounced. Spins along (across) a (110) AF interlayer are identically aligned (alternate). Figures 1(a) and 1(b) show two representative $T = 0$ current-phase relations for the S-AF-S tunnel junctions with different thicknesses L of the sandwiched (110) AF layer. The curves display striking 0- or π-junction sinusoidal behavior depending on whether the AF interface contains an even [Fig. 1(a)] or odd [Fig. 1(b)] number of chains, respectively. Figure 1(e) shows the critical current as a function of thickness L. The temperature dependence of the critical current $j_c(T)$ is shown in Figs. 1(c) and 1(d) for varying magnetic strength U. Clearly, the magnetism leads to remarkable anomalous T dependence of the critical current. For small values of U, where the influence of the Q reflection is more pronounced since the Andreev bound states have lower energy, $j_c(T)$ deviates from the standard behavior by varying monotonically for the even junctions and nonmonotonically for odd L. In particular, we find that in addition to the low T alternating $0 - \pi$ transitions as a function of L, the odd junctions can exhibit another $\pi - 0$ transition as a function of T. This $\pi - 0$ transition is clearly shown in Fig. 1(f), where we plot the

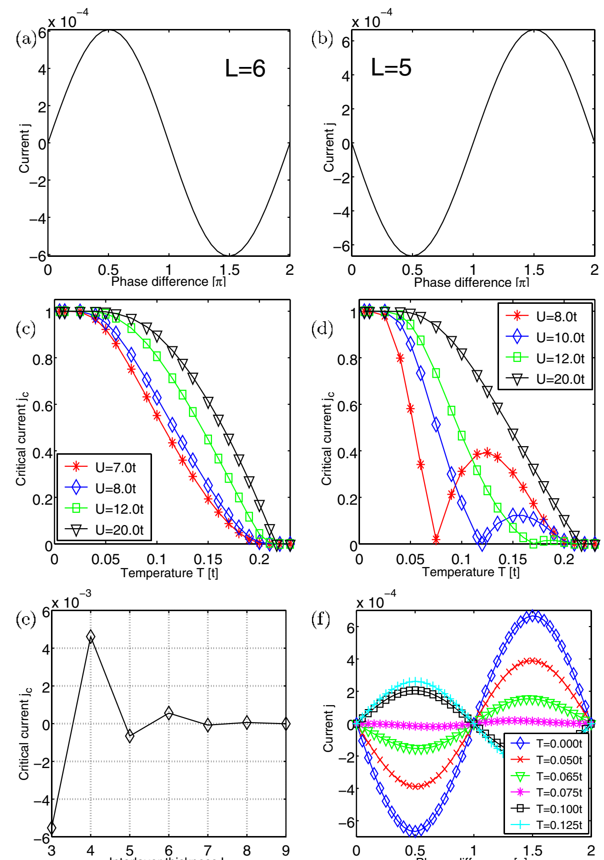

FIG. 1 (color online). Current-phase relation at $T = 0$, $U = 8.0t$ (a), (b) and temperature dependence of the critical current $j_c = |j(\frac{\pi}{2})|$ (c), (d) for S-AF-S (110) junctions with $L = 6$ (a), (c) and $L = 5$ (b), (d). In (c), (d) the graphs have been normalized to their values at $T = 0$. (e) Oscillations of the critical current as a function of the AF thickness L ($U = 8.0t$). (f) Current-phase relation at various temperatures along the $U = 8.0t$ curve in (d). Parameters used in all figures: $V = 2.0t$, $\mu = 0$. Currents are in units of $et/\hbar l_y$.

current-phase relation at various T along the $U = 8.0t$ curve in Fig. 1(d). Note that in Figs. 1(c) and 1(d) the conventional behavior near T_c, $j_c \sim [1 - T/T_c]$, is recovered only in the limit of large U. The anomalous temperature dependence near T_c appears to be associated with the magnetism leaking into the superconducting leads by the proximity effect [12].

In junctions between identical superconductors with a thin interlayer $L \ll \xi_s \sim \hbar v_F/|\Delta|$, the whole Josephson current is carried through the interface by the phase-dependent subgap Andreev bound states. The bound states at the two separate S-AF interfaces [11,12] mix in the junction geometry resulting in qualitatively different bound state bands for the odd or even interlayers. This is seen in Fig. 2 where we show the spin-down eigenspectrum for an even [Fig. 2(a)] and odd [Fig. 2(b)] (110) S-AF-S junction as a function of k_y. In the case of odd L only the total spectrum, including both spin-down and spin-up states, is symmetric with respect to the Fermi surface. For larger values of U, the transparency of the junction decreases, the specular reflection becomes more pronounced, and the bound states move towards the gap edge and become more extended.

We have carried out analytical calculations of the subgap spectrum under the conditions $\Delta \ll m, t, L \ll \xi_s$, whereas our numerical self-consistent studies are applicable in a wider regime. The normal-state spin-dependent reflection and transmission amplitudes are the same on both sides of a (110) odd AF interface: $r_\sigma = \sqrt{R_{\rm odd}}\exp(i\sigma\Theta/2)$, $d_\sigma = i\sigma\sqrt{D_{\rm odd}}\exp(i\sigma\Theta/2)$. Here the transparency coefficient is spin-independent $D_{\rm odd}(k_y) = \cosh^{-2}[2(L+\frac{1}{2})\beta]$, $\sinh\beta = m/[4t\cos(k_y/\sqrt{2})]$, and $R_{\rm odd}(k_y) = 1 - D_{\rm odd}(k_y)$. The difference $\Theta = \Theta_\uparrow - \Theta_\downarrow$ between phases of spin-up and spin-down reflection amplitudes takes the form $\sin\Theta(k_y) = [m/2t\cos(k_y/\sqrt{2})]\{1 + [m/4t\cos(k_y/\sqrt{2})]^2\}^{-1}$. If $m < 4t\cos(k_y/\sqrt{2})$, Θ satisfies the relation $\pi/2 < \Theta < \pi$, whereas for $m > 4t\cos(k_y/\sqrt{2})$ one gets $0 < \Theta < \pi/2$. The narrow regions of k_y near $k_y = \pm\pi/\sqrt{2}$ turn out not to be important for the effects in question and in the estimations one can put $\cos(k_y/\sqrt{2}) \sim 1$.

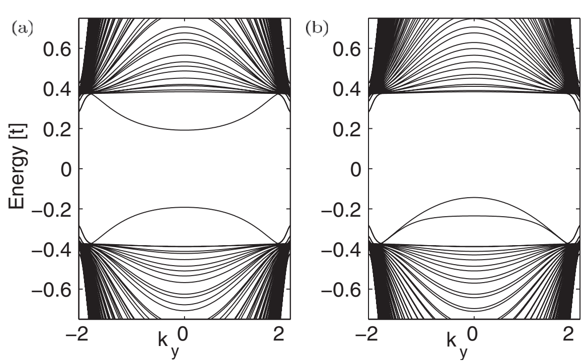

FIG. 2. Spin-down eigenbands for the S-AF-S junctions with $U = 8.0t$ and $\mu = T = \varphi = 0.0$ and $L = 6$ (a) and $L = 5$ (b). As seen, the even or odd number of magnetic layers lead to qualitatively different bound state bands inside the gap.

The key properties of the odd S-AF-S junctions are associated with the fact that they contain *symmetric* magnetic interlayers with respect to the two superconductors. In the (110) odd interlayer both outermost chains belong to the majority spin polarization, defined as "spin-up," and the Andreev states are spin split. The physical origin of the $\pi - 0$ transition at finite T is just the interplay of spin-split Andreev bound states. The general structure of the $\mathcal{S}$ matrix, containing the present reflection and transmission amplitudes, is similar to that found in Ref. [14] for *symmetric* ferromagnetic interfaces. An important distinction to the AF case, however, is the very different expression for the parameter Θ. The presence of the low-energy Q reflection results in quite large values $\Theta > \pi/2$, which ensure the $\pi - 0$ transition with varying temperature in a wide range of the AF order parameter $m < 4t$. Applying the quasiclassical equations to the superconducting leads and taking into account the AF interface properties within the $\mathcal{S}$ matrix approach, we obtain the following spectrum for the Andreev bound states: $E^\pm_\sigma(k_y) = \sigma|\Delta|{\rm sgn}[\sin(\frac{\Theta}{2} \pm \delta)] \times \cos(\frac{\Theta}{2} \pm \delta)$. Here, $\sin\delta = \sqrt{D_{\rm odd}}\cos(\chi/2)$ and χ is the phase difference between the left and right superconducting leads. As seen from the energy spectrum $E^\pm_\sigma(k_y)$, the parameter $m/4t$ becomes negligible in tunnel junctions under quite strict conditions $m/4t \ll \sqrt{D_{\rm odd}}$. This implies $\Theta \approx \pi$ when four dispersive bound states $E^\pm_\sigma(k_y)$ reduce to two doubly degenerate states, leading to the particular results of Ref. [11] for the Josephson current.

Below we consider the different conditions, $\sqrt{D_{\rm odd}} \ll m/4t, 1$ which can be easily satisfied in tunnel junctions. The expression for the Josephson current, which follows from the bound state spectrum in the case $\sqrt{D_{\rm odd}} \ll m/4t, 1$, describes the $\pi - 0$ transition with increasing temperature for $\pi/2 < \Theta < \pi$, and differs only by the additional factor of 1/2 from Eq. (4) of Ref. [14] (with $\alpha = 1$) valid for clean symmetric S-F-S tunnel junctions. At $T = 0$ the current is given by a sum over k_y of the expressions $j^{\rm odd}_{c,k_y}(T=0) = -(1/2)e|\Delta|D_{\rm odd}\cos(\Theta/2)$, whereas near T_c we get $j^{\rm odd}_{c,k_y}(T \approx T_c) = -e|\Delta|^2 D_{\rm odd}\cos\Theta/4T_c$. From this we see that the product $j^{\rm odd}_{c,k_y}(T=0)j^{\rm odd}_{c,k_y}(T \approx T_c)$ is negative for $\pi/2 < \Theta < \pi$ and positive for $\Theta < \pi/2$. Hence, if $\Theta < \pi/2$, there is no $\pi - 0$ transition with increasing T and the π state remains the ground state of the odd (110) S-AF-S junctions for all $T < T_c$.

For the even (110) junctions, the outermost chains of the AF interface have opposite spin polarizations and the Andreev states are spin degenerate. In this geometry the spin-dependent reflection amplitudes on the two sides of the interfaces differ $r_{1,\sigma} = -r^*_{2,\sigma} = \sqrt{R_{\rm ev}}\exp(i\sigma\Theta/2)$. The transmission amplitude is real and spin independent $d = \sqrt{D_{\rm ev}} = 1/\cosh[2(L+1)\beta]$ and the expressions for Θ and β coincide with the odd case. Such structure of the $\mathcal{S}$ matrix is characteristic also for the three-layer ferromagnet-insulator-ferromagnet (FIF) interface with antiparallel orientations of the two ferromagnetic magnetizations [15]. The corresponding spin-degenerate spectrum of the Andreev states in even S-AF-S junctions, $E_{ev}(k_y) = \pm\Delta[D_{ev}(k_y)\cos^2(\chi/2) + R_{ev}(k_y)\cos^2(\Theta/2)]^{1/2}$, has the same form as that found for the FIF three-layer with antiparallel magnetizations [see Eq. (4) in Ref. [15]], but with a significantly different expression for Θ. The Josephson current at zero temperature is a sum over k_y of the expressions $j^{ev}_{c,k_y}(T=0) = e|\Delta|D_{ev}/2\cos(\Theta/2)$, whereas near T_c we obtain $j^{ev}_{c,k_y}(T\approx T_c) = e|\Delta|^2 D_{ev}/4T_c$. There is no $0-\pi$ transition with varying temperature, in agreement with our numerical results and with the S-FIF-S junctions with antiparallel magnetizations.

The different symmetries of even versus odd AF interlayers are also responsible for the low T $0-\pi$ transitions as a function of L. Indeed, the π state is the ground state of clean S-F-S junctions with $\alpha = 1$, $\Theta > \pi/2$ [14], whereas the 0 state is the ground state of the S-FIF-S junctions with antiparallel magnetizations [15]. The direct analogy between the odd (even) AF interfaces and the F interfaces at $\alpha = 1$ (the FIF interfaces with antiparallel magnetizations) results in the correct sequence of the transitions at $T = 0$. The even/odd $0-\pi$ transitions can also be related, within the perturbative approach, to effects of localized spin states in interfaces and the anticommutation of fermions [16–21].

The critical current j_c in odd (110) S-AF-S junctions at $T = 0$ is reduced by the factor $\cos(\Theta/2)$ compared to the standard junctions with the transparency D_{odd}. For $m/t \ll 1$ we have $\cos(\Theta/2) \ll 1$ and the relative suppression is significant. The presumed condition $\sqrt{D_{odd}} \ll m/4t$ gives the smallest value $\cos(\Theta/2) \sim \sqrt{D_{odd}}$ and a reduced current $j^{odd}_c \propto D^{3/2}_{odd}$. Contrary to the odd case, the critical current j^{ev}_c in even junctions at $T = 0$ is enhanced by $1/\cos(\Theta/2)$ compared to standard junctions with the transparency D_{ev}. The maximal relative enhancement is realized for $\cos(\Theta/2) \sim \sqrt{D_{ev}}$, where the applicabilities of the present results border those of Ref. [11]. Then $j^{ev}_c \sim e|\Delta|\sqrt{D_{ev}}$, in qualitative agreement with the net critical current at $T = 0$ found in Ref. [11].

Fabrications of ultrathin AF interfaces [possible candidates are chromium-based materials [22]] with atomic-scale control of the thickness over a macroscopic area, similar to the case of ultrathin films [23,24], would allow observations of the even/odd effect for S-AF-S junctions. Alternatively one should average the Josephson current over interface imperfections. For example, assume that the procedure can be reduced to an averaging over thickness variations within a few layers. If $L \gg 1$, we get $D_{odd}(L) \approx D_{ev}(L \pm 1)$. For $m \ll t$ the critical currents are related as $j^{ev}_c \sim (t/m)^2|j^{odd}_c| \gg |j^{odd}_c|$ at $T = 0$, whereas near $T = T_c$ they are of the same order and sign. Since the current j^{ev}_c strongly dominates $|j^{odd}_c|$ at low T, the result of the averaging is that the ground state is the 0 state with the anomalous critical current $j^{ev}_c(T)$ and there is no $0-\pi$ transition, if $m \ll t$. For $m \sim t$ even and odd currents are of the same order and therefore similar samples can have differing signs of j_c. If $\Theta < \pi/2$, j^{ev}_c and j^{odd}_c have opposite signs and we expect a pronounced suppression of the net critical current at all T. For $\Theta > \pi/2$, the odd and even currents have opposite signs only at low T where a similar cancellation can take place. Therefore, we predict a nonmonotonic temperature dependence of the net critical current in this case.

Conclusions.—We have found a low-temperature even/odd sequence of the 0 and π states of S-AF-S junctions and an additional novel $\pi - 0$ transition with increasing temperature in odd junctions. The even/odd effect is caused by the different symmetries of the even versus odd AF interfaces and the corresponding $\mathcal{S}$ matrices, and is revealed in qualitatively different temperature dependencies of the critical currents for even and odd barrier thicknesses. The $\pi - 0$ transition with varying temperature is induced in the odd junctions by the interplay of the spin-split Andreev bound states.

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