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Magnetic intragap states and mixed parity pairing at the edge of spin triplet superconductors

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We show that a spontaneous magnetic moment may appear at the edge of a spin-triplet superconductor if the system allows for pairing in a subdominant channel. To unveil the microscopic mechanism behind such effect we combine numerical solution of the Bogoliubov-De Gennes equations for a tight-binding model with nearest-neighbor attraction, and the symmetry based Ginzburg-Landau approach. We find that a potential barrier modulating the electronic density near the edge of the system leads to a non-unitary superconducting state close to the boundary where spin-singlet pairing coexists with the dominant triplet superconducting order. We demonstrate that the spin polarization at the edge appears due to the inhomogeneity of the non-unitary state and originates in the lifting of the spin-degeneracy of the Andreev bound-states.

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Introduction. Recognition that the surface states in correlated materials reflect the nature of the interactions and orders in the bulk has led to a significant research effort aimed at the understanding, and potential control, of these electronic states [1–3]. Gapless modes at the boundary of materials whose bulk is gapped are especially interesting since the surface states are robust, and may be topologically protected, i.e. their existence relies on the global symmetries of the bulk state and does not depend on the details of the surface scattering and other sample-dependent parameters [2]. The bulk gap may be due to the band structure, or, in a metal, may arise from electron-electron interaction, as in superconductors [4]. Simple band insulators or conventional superconductors do not support robust low-energy states at the boundary. It is the study of their counterparts, where the bulk is topologically non-trivial, and hence the bulk-boundary correspondence theorem dictates the existence of the surface states, that has been a focus of much recent attention [1, 2, 4].

A prime candidate for the topological superconductivity is Sr_2RuO_4 , where the emergent consensus indicates triplet chiral pairing, with time-reversal symmetry broken by the orbital degrees of freedom [5]. In this material signatures of the predicted topologically protected edge states were recently found in tunnelling spectroscopy [6]. The quasiparticles reflecting off the sample boundary experience the sign change of the superconducting order parameter along their trajectory, which gives rise to so-called Andreev bound states (ABS) near the surface, which contribute to Josephson currents [7]. Emergence of ABS has been investigated in high- T_c cuprates and other unconventional superconductors [4, 8, 9].

In this Letter we investigate the nature of the Andreev bound states at the surface of spin triplet superconductors. We perform a microscopic self-consistent calculation, and include a realistic surface barrier of finite width

and height, and the possibility of pairing in one or more subdominant channels [8]. We find that a) a subdominant *in-phase s-wave* superconducting order exists near the edge of the sample; b) the in-phase *s-wave* component gives a non-unitary superconducting state at the boundary; c) as a result, the ABS are spin-polarized, leading to a finite surface magnetization; d) spin current flows along the interface in this regime; e) surface charge currents exhibit anomalous dependence on the magnetization. We analyze the conditions for the existence of the magnetic surface states, and investigate their spectrum numerically. These results are supported by symmetry analysis of the Ginzburg-Landau expansion of the free energy. Our work strongly suggests that triplet superconductors can be used in spin-active heterostructures.

Model and formalism. We consider a two-dimensional superconductor in a parallel slab geometry in vacuum. If x and y are the directions perpendicular and parallel to the interfaces, respectively, the system is uniform along the y axis, so that the translational symmetry is broken only in the x direction. The Hamiltonian is then defined on a square lattice of size $L \times L$ (the lattice constant is unity), with periodic boundary conditions along y ,

$$H = -t \sum_{\langle \mathbf{i}, \mathbf{j} \rangle, \sigma} (c_{\mathbf{i}\sigma}^\dagger c_{\mathbf{j}\sigma} + \text{h.c.}) - \mu \sum_{\mathbf{i}, \sigma} n_{\mathbf{i}\sigma} - \sum_{\langle \mathbf{i}, \mathbf{j} \rangle} V (n_{\mathbf{i}\uparrow} n_{\mathbf{j}\downarrow} + n_{\mathbf{i}\downarrow} n_{\mathbf{j}\uparrow}) + \sum_{\mathbf{i}} U(i_x) n_{\mathbf{i}\sigma}. \quad (1)$$

Here the lattice sites are labelled by $\mathbf{i} \equiv (i_x, i_y)$, with i_x and i_y integers between 0 and L , $\langle \mathbf{i}, \mathbf{j} \rangle$ denote nearest-neighbor sites, and μ is the chemical potential. The nearest-neighbor attractive interaction $-V$ ($V > 0$) is effective in both singlet and triplet pairing channels. All the energies are in units of the hopping parameter t . The slab edges are located at $i_x = 0$ and $i_x = L$, and we introduce a site-dependent potential $U(i_x)$ to

model the interface barrier. To investigate the model of Eq. (1) we decouple the interaction term in the Hartree-Fock approximation by introducing the pairing amplitude on a bond, $\Delta_{ij} = \langle c_{i\uparrow}c_{j\downarrow} \rangle$, so that $Vn_{i\uparrow}n_{j\downarrow} \simeq V(\Delta_{ij}c_{j\downarrow}^\dagger c_{i\uparrow}^\dagger + \Delta_{ij}^*c_{i\uparrow}^\dagger c_{j\downarrow} - |\Delta_{ij}|^2)$. These pairing amplitudes yield the spin singlet (S) and triplet (T) components, $\Delta^{S,T} = (\Delta_{ij} \pm \Delta_{ji})/2$, that define the superconducting order parameters (OPs) with s - or p -wave symmetry, i.e. $\Delta_s(\mathbf{i}) = (\Delta_{i,i+\hat{x}}^S + \Delta_{i,i-\hat{x}}^S + \Delta_{i,i+\hat{y}}^S + \Delta_{i,i-\hat{y}}^S)/4$ and $\Delta_{p_x(y)}(\mathbf{i}) = (\Delta_{i,i+\hat{x}(\hat{y})}^T - \Delta_{i,i-\hat{x}(\hat{y})}^T)/2$, which are then determined self-consistently [10]. Singlet d -wave superconductivity is possible but does not appear in the parameter range where we work [10]. In the bulk ($U = 0$) the most favorable pairing state for this model depends on the electron density, n , and the chiral $p_x + ip_y$ order is stabilized in the region between half-filling, $\mu \simeq 0$, and high (low) density ($|\mu| \simeq 2.5$) [11]. Hence, we choose $|\mu| \simeq 1.8$, in this window of stability, so that for $U = 0$ the filling is $n \simeq 0.4$. All the numerical results below have been obtained for a pairing interaction $V = 2.5$, a rectangular potential barrier of height U near the left edge of the system, $0 \leq i_x \leq 8$, and a system size $L = 80$; greater values of L leave the results qualitatively unchanged. We also determine the local spin and charge currents, $J_s(i_x) = J_\uparrow(i_x) - J_\downarrow(i_x)$, and, $J_c(i_x) = J_\uparrow(i_x) + J_\downarrow(i_x)$, with $J_\sigma(i_x) = \frac{2t}{L_y} \sum_{k_y} \sin(k_y) \langle c_{k_y\sigma}^\dagger c_{k_y\sigma} \rangle$ [12]. We find qualitative differences between our results for the extended barrier, and those obtained assuming a sharp step-like potential at the surface [13]. One crucial distinction is that a finite-width barrier changes the electron density near the boundary, and, if it is strong enough to drive the density into the regime where superconducting components competing with the dominant triplet order are stabilized, leads to the coexistence of two distinct pairing states near the interface. This coexistence is at the root of the phenomena we describe.

Numerical results. Figs.1,2 show representative results for the electron density, spin polarization, spin and charge currents, as well as the evolution of the superconducting order parameters for different strength of the surface potential. For $U = 0$, Fig.1(a), we find the expected result: the interface is pairbreaking for the p_x component of the OP, while the p_y component remains essentially constant. Finite U depletes the electron density near the edge, Fig.2(a), and, as U exceeds a critical magnitude, here found to be $U_c \simeq 0.19$, the surface electron density reaches the value where a subdominant s -wave component of the order parameter first appears, Fig.1(b)-(d). Consequently, there is a substantial region of coexistence of the superconducting OPs with different parity. Note that mixed parity is allowed here since the presence of the barrier breaks the inversion symmetry. Remarkably, the emergence of the mixed-parity phase is accompanied by the appearance of a finite spin polarization in that same region, Fig.2(b), as well as that of

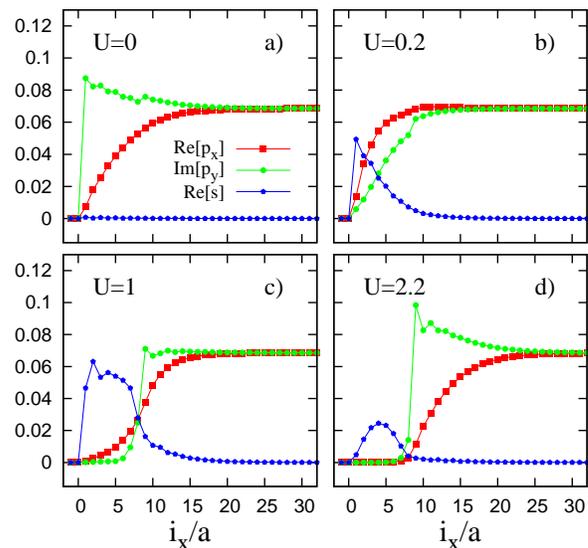


FIG. 1: (color online) Evolution of the order parameters for different heights of the potential barrier U extending from $i_x = 0$ to $i_x = 8$. Label s -wave refers to nearest-neighbor pairing; Note that the s -wave amplitude is purely real.

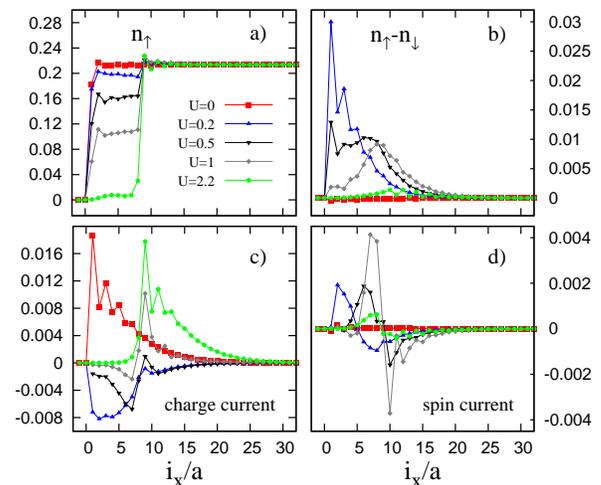


FIG. 2: (color online) Evolution of the majority spin electron density: (a), spin-polarization (b), as well as of the spin (c) and charge currents (d) for several values of the potential U . Note the sign change of the charge current in the regime where the magnetization appears. Also, the spin polarization and the spin current are peaked in the range where the superconducting orders of different symmetry coexist, cf. Fig. 1.

a spin current, Fig.2(d). At the same time the surface charge current, initially present simply due to the chiral nature of the bulk superconducting state [5], changes sign, Fig.2(c). As the barrier height increases, fewer carriers remain in the boundary layer, and the magnetization and other signatures of the unconventional surface states gradually disappear. Note that the charge cur-

rents at the interface give rise to a magnetic field, and, therefore, to a spin polarization [14, 19]. However, as discussed in the supplementary material [21], the origin and the spatial profile of this field are very different from those of the spin polarization shown in Fig.2(b).

The analysis of the energy spectrum $E_n(k_y)$ (due to translational invariance along the interface k_y is a good quantum number) obtained from the numerical solution of the Bogoliubov-De Gennes equations confirms that the local magnetization is due to the gapless modes propagating in one direction along the boundary. This is evident from Fig. 3, where the two originally spin-degenerate chiral edge states (Fig. 3(a)) associated with the left boundary split once the barrier potential exceeds $U_c \simeq 0.19$ (Fig. 3(b)-(d)). This splitting appears together with the spin polarization at that edge (of course, the counterpropagating mode at the right edge is not affected). It is clear, for example, from Fig. 3(b), that splitting leads to the unequal number of occupied ($E_n(k_y) < 0$) states for the two spin-split modes. In addition, new intragap states appear close the bottom and the top of the gap edge. They evolve from an asymmetric band (peak at $k_y > 0$) for $U = 0.2$ and 1.0 (Fig. 3(b)-(c)), when singlet-triplet coexistence is significant, to a symmetric “bump” around $k_y = 0$ for $U = 2.2$ (Fig. 3(d)). This feature contributes significantly to the spin current and is in large part responsible for the change in sign of the charge current. Note that the branches crossing the gap are piecewise-linear, so that $J_\sigma \propto \sum_{\mathbf{k}} dE_\sigma/dk \Theta(-E_{\sigma,\mathbf{k}})$ nearly compensates between the spin-split central branches. As the barrier height U increases the splitting between the edge modes at the edge diminishes, and magnetization is reduced as the boundary region becomes depleted.

Our result shows that a spin accumulation may occur in a triplet superconductor *without the proximity coupling to an exotic system*. This situation is quite different from the case discussed in Refs.15–17, where spin polarization appears at the sharp interface between semi-infinite triplet and a singlet superconductors with no coexistence region, when analyzed using the BTK scattering formulation [13]. In Refs. 15–17 such magnetization appears only for a non-trivial phase difference between the two superconductors, exactly the opposite to what we find in our geometry.

The essential ingredient of our finding is the coexistence of the singlet and triplet OPs in the same material over a finite range near the interface, obtained from a fully self-consistent solution of the Bogoliubov-de Gennes equations in the presence of a realistic boundary potential. In our case the magnetization exists near the surface over the same length scale as the density gradient: this is because for our parameter values the superconducting coherence length, ξ_0 , is comparable to that width. If screening of the surface potential occurs on a shorter scale, the surface barrier nucleates the subdominant s -

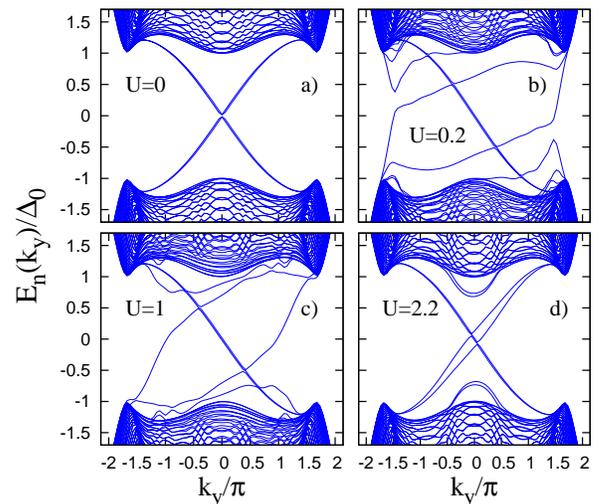


FIG. 3: (color online) Energy spectrum of the solutions of the Bogoliubov-de Gennes equations scaled to the superconducting gap Δ_0 of the homogeneous spin triplet superconductor. a) pure chiral phase. Two dispersing branches crossing $E = 0$ correspond to the modes along the left and the right edges of the sample. b)-d): mixed-parity phases. The right edge mode remains unchanged while the modes along the left edge become spin-split. Extra midgap states which are spin-polarized appear at the bottom (occupied) and the top edge (unoccupied) of the gap reflecting the occurrence of a mixed-parity coexisting region. The latter and the spin-split chiral states both contribute to the overall spin accumulation.

wave component, and the coexistence range is set by the coherence length.

Symmetry analysis. To elucidate the origin of the spin polarization we analyse the problem from the symmetry perspective. The main insight from the numerical results is that the singlet and the triplet OPs coexist near the edge due to the finite range of the boundary potential, and the absence of the inversion symmetry. We first note that in this situation the OP is non-unitary. In the 2x2 spin space the order parameter is [18] $\Delta_{\mathbf{k}} = i[(\mathbf{d}_{\mathbf{k}} \cdot \boldsymbol{\sigma}) + \psi_{\mathbf{k}}]\sigma_y$, where σ_i are Pauli matrices, and $\mathbf{d}_{\mathbf{k}}$ and $\psi_{\mathbf{k}}$ are the three triplet and the singlet pairing amplitudes respectively. The gauge-invariant product is given by $\Delta \Delta^\dagger = |\mathbf{d}_{\mathbf{k}}|^2 \sigma_0 + |\psi_{\mathbf{k}}|^2 \sigma_0 + \mathbf{q}_{\mathbf{k}} \cdot \boldsymbol{\sigma}$ with $\mathbf{q}_{\mathbf{k}} = \psi_{\mathbf{k}} \mathbf{d}_{\mathbf{k}}^* + \psi_{\mathbf{k}}^* \mathbf{d}_{\mathbf{k}} + i[\mathbf{d}_{\mathbf{k}} \times \mathbf{d}_{\mathbf{k}}^*]$. In our case the bulk triplet superconductor is unitary, $\mathbf{d} \parallel \hat{\mathbf{z}}$ and therefore $\mathbf{d}_{\mathbf{k}} \times \mathbf{d}_{\mathbf{k}}^* = 0$. However, in the coexistence region, $\mathbf{q}_{\mathbf{k}} = 2\text{Re}[\psi_{\mathbf{k}} \mathbf{d}_{\mathbf{k}}^*] \neq 0$ since, as Fig. 1 shows, the self-consistent solution yields the *in-phase* singlet and triplet p_x components.

The net spin polarization of the Cooper pairs, $s_i = (1/2) \sum_{\mathbf{k}} (\mathbf{q}_{\mathbf{k}} \cdot \boldsymbol{\sigma}) \sigma_i$, does not appear for *uniform* mixed parity system (with unitary triplet component) since the singlet and triplet order parameters have opposite parity. Hence their product is odd in momentum and its average over \mathbf{k} vanishes. The same argument does not hold in a

system without translational invariance such as the one considered here, and the \mathbf{q} -vector that is non-uniform in space yields spin-splitting of the edge states. To analyse this situation we consider a Ginzburg-Landau (GL) magnetic free energy density f_m in the region of coexistence. We choose the direction of the magnetization \mathbf{m} parallel to $\mathbf{d}(\mathbf{r}) = \hat{\mathbf{z}}(\eta_x(\mathbf{r}) + i\eta_y(\mathbf{r}))$, along the $\hat{\mathbf{z}}$ -axis, as required by the spin rotation invariance, and assume that the pairing amplitudes depend only on the coordinate x normal to the boundary. The GL expansion includes terms linear in m and the gradient of the p_x -component of the triplet pairing,

$$f_m = m^2 + (\partial_x m)^2 + \alpha m \left\{ \beta \partial_x [\eta_x \psi^* + \eta_x^* \psi] + [\psi^* (\partial_x \eta_x) + \psi (\partial_x \eta_x^*)] - [\eta_x^* (\partial_x \psi) + \eta_x (\partial_x \psi^*)] \right\}. \quad (2)$$

Such linear coupling means that in the region of the coexistence a finite magnetization always appears unless the singlet and the triplet p_x components are out of phase (and the product $\eta_x \psi$ is purely imaginary). This emphatically brings forth the distinction between our results and those for the S-I-S junction [15–17], where the spin accumulation only occurs if the two pairing components are out of phase, the exact opposite of the result we find. We note that this term (and its analog derived in Ref. [20]) has a structure which is different from the well-known contributions that relate the inhomogeneity in $\eta(\mathbf{r}) \times \eta^*(\mathbf{r})$ [19] to spontaneous charge-currents at the edge and a magnetic field [21].

Only the p_x -component of the triplet appears in the GL expansion above; in principle the term $\partial_y \eta_y$ is also allowed by symmetry [20], but vanishes under the assumption of the translational invariance along the interface. It follows that the time-reversal symmetry breaking by the bulk chiral triplet state is not at the origin of the magnetization of the Andreev bound states: the same result would be achieved for purely real p_x bulk triplet superconductivity, while for the imaginary p_x bulk pairing with real subdominant s -wave pairing near the interface no magnetization appears. The results in the supplementary material [21] show precisely this behavior. Note that the terms written in Eq. (2) do not contribute to the currents along the interface as the only gradient is along the x direction. To obtain such currents, higher order terms involving the η_y component of the order parameter are needed. For non-chiral single-component p_x triplet order parameter no substantial spin and charge currents exist, even though the magnetization still appears. Such currents are allowed by symmetry, but their magnitude is strongly suppressed, likely by a power of T_c/t .

Discussion. We showed that Andreev bound states near a boundary of a triplet superconductor can be spin-polarized and yield nontrivial spin and charge currents near the interface. The origin of the spin polarization is in the emergence of the coexistence regime of the triplet

and the subdominant singlet pairing components near the boundary above a critical surface barrier. Our numerical results demonstrate that the two are phase-locked, and both the numerical fully self-consistent solution of the Bogoliubov-de Gennes equations and the Ginzburg-Landau analysis indicate that magnetization inevitably appears when the two order parameters lead to a non-unitary configuration and are spatially varying. We find that the symmetry-breaking at the surface is unrelated to the chiral nature of the bulk superconducting state, and therefore may be expected in a much wider class of triplet superconductors. It would also be very interesting to check whether similar effects occur at the interfaces involving non-centrosymmetric superconductors, where the singlet and the triplet components are intrinsically mixed in the bulk yielding measurable spin effects at the interface [22–25], as well as in the proximity structures with topological materials. We leave this for future investigations.

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Supplementary material for “Magnetic intragap states and mixed parity pairing at the edge of spin triplet superconductors”

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In this supplementary material to the main text we show that the behavior of the magnetic field induced by the edge currents in a chiral spin-triplet superconductor is very distinct from that of the spin polarization, emphasizing the different origin of the two. Furthermore, to elucidate this difference on the basis of the Ginzburg-Landau approach, we numerically demonstrate that in a triplet superconductor with a single component order parameter that does not break time-reversal symmetry, the non-vanishing magnetization at the edge of the system occurs because of the non-unitary character of the mixed parity order parameter near the boundary, while the edge currents are absent.

MAGNETIC FIELD INDUCED BY EDGE CURRENTS

A chiral spin-triplet superconductor can sustain spontaneous currents at the edge due to the time-reversal symmetry breaking in the orbital channel. These currents, in turn, lead to the appearance of a magnetic field near the boundary. One may ask whether this field causes the spin polarization that we found in the manuscript. The answer is negative, and below we show that the spatial profile and the properties of the induced field are very different from those of the spin-polarized states. Moreover, the spin polarization persists even when there are no edge currents, in agreement with our analysis.

We first compute the field due to the edge current. In principle, this field is screened in the bulk on the scale of the London penetration depth. However, in the immediate vicinity of the interface the screening has little effect, and the field distribution can be obtained directly from the spatial dependence of the currents. For the two-dimensional slab configuration analyzed in the paper, according to the Maxwell’s law $\nabla \times \mathbf{B} = \mu_0 \mathbf{J}_c$, the magnetic field is perpendicular to the plane (z -direction). At a distance i_x from the edge it has an amplitude $B_{\text{orb}}^z(i_x) = -\mu_0 \sum_{j_x=1}^{i_x} J_c(j_x)$ with μ_0 being the magnetic permeability constant [2].

In Fig.1 we show the behavior of B_{orb} as a function of the potential at the edge. For $U = 0$ there is an induced magnetic field but no net spin magnetization, while above the threshold both exist (see Fig. 2(b) in the main text). As expected, due to the different mechanisms generating the spin polarization and the orbital magnetic field, the spatial profile of B_{orb} is very different from that of the magnetization. The spin-polarization is always of the same sign as a function of the potential U (see Fig. 2 in the main text), and is peaked in the regime of the coexistence of the order parameters of different parity. On the other hand, the orbital magnetic field changes sign twice: around $U = 0.2$, and then again $U \geq 1$, when the spin-polarization vanishes. The two are clearly of

very different origin.

We note that the magnitudes of the field generated by both mechanisms are comparable. To check this we convert the spin-polarization into a magnetic field intensity [2]. The spin-polarization yields a local magnetic field given by $B_{\text{pol}}^z(i_x) = -\frac{\mu_0 \mu_B}{a^2 c} (n_{\uparrow}(i_x) - n_{\downarrow}(i_x))$, where $\mu_B = \frac{\hbar e}{2m}$ is the Bohr magneton and c the lattice constant along the z direction [2]. The ratio between the prefactors of B_{orb} and B_{pol} is $r = (\mu_0 \frac{e t}{\hbar a}) / (\frac{\mu_0 \mu_B}{a^2 c}) \sim t m (\frac{c}{a})$. Since the hopping amplitude is related to the inverse of the effective mass m^* , for a generic filling the ratio $r \sim O(1)$, thus implying that the two magnetic fields are of the same order of magnitude. Hence, the field generated by the spin polarization near the boundary will not have the same profile as that due to the edge-currents.

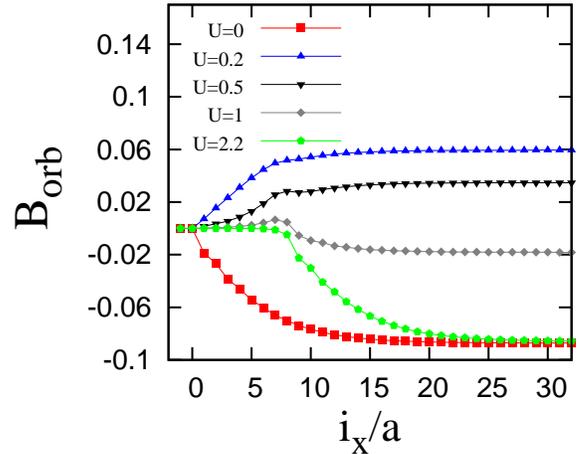


FIG. 1: (color online) Evolution of the magnetic field induced by the edge currents for a chiral spin-triplet superconductor for several values of the potential U . The scale of B_{orb} is in unit of $\frac{e t}{\hbar a} \mu_0$. We neglect here the Meissner currents that affect the field distribution on the scale of the London penetration depth, which is much greater than several lattice spacings.

SPIN-POLARIZED EDGE STATES FOR SINGLE COMPONENT SPIN-TRIPLET SUPERCONDUCTORS

According to the symmetry constraints, only the p_x -component of the spin-triplet order parameter appears in the Ginzburg-Landau expansion (Eq. 2 of the main text). In principle, the term $\partial_y \eta_y$ is also allowed [1], but does not contribute if the translational invariance along the interface holds. Then, the time-reversal symmetry breaking by the bulk chiral triplet state is not a necessary condition for the occurrence of the magnetization of the Andreev bound states. Indeed, the same result is obtained for purely real p_x bulk triplet superconductivity, while for the imaginary p_x bulk pairing with real subdominant s -wave pairing near the interface no magnetization appears.

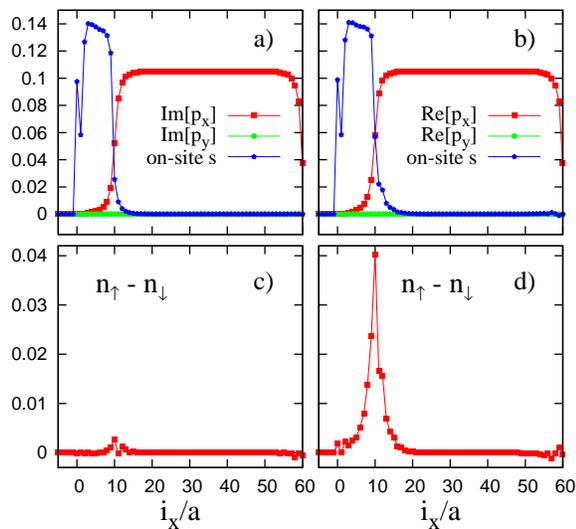


FIG. 2: (color online) Spatial evolution of singlet and triplet order parameters and of the magnetization in the case of unitary, a) and c), and non-unitary states, b) and d), respectively, as realized in a thin vertical slab of the system around the point ($i_x = 10$). A real spin singlet on-site pairing amplitude and a purely real or a purely imaginary triplet pairing amplitude are assumed in input ($i_x < 10$ and $i_x > 10$, respectively).

To explore this connection, we consider a situation when in proximity of the left edge ($0 < i_x < \bar{i}_x$, with $\bar{i}_x = 10$) a purely local s -wave potential is the only source of pairing, with V still effective in the remaining part of the system, and use as input a real s -wave order parameter for $0 < i_x \leq \bar{i}_x$ and a purely imaginary p_x -wave one for $i_x > \bar{i}_x$. Working at the same electron density as before (with $U = 0$), and without the self-consistent iterative procedure (which would unavoidably lead to a mixing of real and imaginary components), we see from the panels a) and c) of Fig. 2 that, in spite of the parity mixing occurring around $i_x = \bar{i}_x$, no appreciable spin polarization is observed. On the other hand, when in the same configuration one uses for $i_x > \bar{i}_x$ a purely real p_x input order parameter to generate a non-unitary mixed phase around $i_x = \bar{i}_x$, a significant magnetization clearly develops in the mixing region. This is exhibited in the panels b) and d) of Fig. 2, and supports our conclusion based on symmetry arguments.

In this case of a single component spin-triplet superconductor there are no edge currents and thus the spin-polarization due to the non-unitary character of the order parameter is the unique source of magnetization at the boundary.

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