Self-organized topological superconductivity in a Yu-Shiba-Rusinov chain

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We study a chain of magnetic moments exchange coupled to a conventional three-dimensional superconductor. In the normal state the chain orders into a collinear configuration, while in the superconducting phase we find that ferromagnetism is unstable to the formation of a magnetic spiral state. Beyond weak exchange coupling the spiral wave vector greatly exceeds the inverse superconducting coherence length as a result of the strong spin-spin interaction mediated through the subgap band of Yu-Shiba-Rusinov states. Moreover, the simple spin-spin exchange description breaks down as the subgap band crosses the Fermi energy, wherein the spiral phase becomes stabilized by the spontaneous opening of a p-wave superconducting gap within the band. This leads to the possibility of electron-driven topological superconductivity with Majorana boundary modes using magnetic atoms on superconducting surfaces.

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The prospect of performing topological quantum computation [1] has stimulated intense investigations into condensed-matter systems harboring Majorana bound states [2–13]. One potential platform involves magnetic atoms arranged in a regular lattice on an s-wave superconducting substrate [14]. This system has received renewed interest due to recent scanning tunneling microscopy (STM) data possibly supporting the existence of Majorana bound states in a self-assembled one-dimensional (1D) array of atomically spaced Fe atoms on the surface of superconducting Pb [15–17].

We focus on the case of an STM-assembled magnetic atom chain whose spacing is several substrate lattice sites [18], where the overlap of atomic wave functions is negligible. In that case, each atom acts as an isolated magnetic moment giving rise to localized, subgap Yu-Shiba-Rusinov (YSR) states [19–24] within the superconductor. Overlap between YSR states leads to the formation of an effectively spinless subgap band that can undergo a topological superconducting transition controlled by the magnetic ordering of the magnetic atoms (spin chain) [25,26] (see Fig. 1). On the other hand, the ordering of the spin chain is dictated by the indirect exchange mediated by electrons in the superconductor, allowing the possibility of an electron-driven “self-organized” topological superconducting phase.

Although many important aspects of spin chains on superconductors have been theoretically studied by several authors [25–36] (see also Refs. [37–40]), a generic conceptual account of the collective ordering mechanism of the magnetic and electronic degrees of freedom in a bulk (D > 1) superconductor remains elusive (the 1D case is special due to 2kF nesting and was studied in Refs. [28–30]; see also Ref. [37]).

In this Rapid Communication, we establish the existence of spiral magnetic order and self-organized topological superconductivity in the case of a magnetic adatom chain on a three-dimensional (3D) substrate using an exactly solvable minimal model. We provide the conceptual framework to describe the ordering mechanism in a general setting, which we find to be entirely distinct from the 2kF mechanism that can occur for a 1D substrate [28–30,37]. In particular, we show that ferromagnetism of the spin chain is unstable to the formation of a spiral state due to the presence of singlet superconductivity in the host. The corresponding spiral wave vector exhibits a nonmonotonic dependence on the spin-lattice exchange coupling to the superconductor. The wave vector grows rapidly as the exchange increases from zero due to a strong indirect spin interaction mediated by YSR states, and decreases after the YSR band crosses the Fermi energy due to the double-exchange mechanism. In the latter regime the YSR chain exhibits self-sustained p-wave superconductivity with the possibility of Majorana boundary modes, depending on the lattice spacing. Our main results are summarized in Fig. 2, with details related to various technical calculations delegated to the Supplemental Material [41].

A system of magnetic atoms exchange coupled to a 3D superconductor may be described by the following Bogoliubov–de Gennes Hamiltonian,

$$H = \frac{1}{2} \sum_k \frac{1}{2} \left[ \Psi_k^\dagger \left( \hat{\xi}_k \tau_z + \Delta \tau_x \right) \Psi_k + \frac{1}{2} J \int \frac{d^2 r}{\gamma} \Psi_{r}^\dagger \mathbf{S} \cdot \sigma \Psi_r \right],$$

where \( \hat{\xi}(k) = \frac{k^2 - \xi^2}{2m} \) (\( k, \mathbf{r} \), and \( m \) are the electron momentum, position, and mass, respectively, while \( k_F \) is the Fermi momentum), and \( \Psi = (\psi_\uparrow, \psi_\downarrow, \psi_\downarrow^*, \psi_\uparrow^*)^T \) is the 4-component electron wave function.

FIG. 1. Magnetic atoms on the surface of a superconductor induce local spin-polarized, subgap YSR states (black curves). YSR wave-function overlap (shaded red) leads to hopping and p-wave pairing due to hybridization with singlet Cooper pairs in the host. This hybridization can drive the spin chain into a spiral state that, in turn, induces spontaneous topological superconductivity within the YSR chain.
Nambu spinor written in terms of electron annihilation (creation) operators $\psi_\sigma$ ($\psi_\sigma^\dagger$) with spin projection $\sigma$. Here, $\sigma_i$ and $\tau_i$ are, respectively, Pauli matrices acting in the spin and particle-hole spaces while $S_j = \sum_j \delta(r - r_j)S_j$ is the sum of spins $j$ at sites $r_j$ with lattice spacing $a$ and $J$ is the exchange interaction constant.

We provide the exact phase diagram of Eq. (1) within the classical spin approximation [20] assuming a planar spiral ansatz, $S_j \cdot S_j = S^2 \cos Qa(i - j)$, where the spiral wave vector $Q$ is treated as a variational parameter determined by minimizing the total electronic energy of the system, $\mathcal{Q}_{\text{min}} = q$. The main results of this procedure are shown in Fig. 2, with technical details provided in the Supplemental Material [41]. Below, we focus on extracting only the most important and physically relevant ordering mechanisms, which we verify against the exact results.

**Magnetic atom order.** The spin-chain magnetic order is easiest to determine in the limit of small exchange coupling, where one may integrate out electrons to second order in $\hbar I_1$ since $\mathcal{Q}_{\text{min}} = q$. The main results of this procedure are shown in Fig. 2, with technical details provided in the Supplemental Material [41]. Below, we focus on extracting only the most important and physically relevant ordering mechanisms, which we verify against the exact results.

The electron-induced spin-spin exchange coupling in Eq. (2) is $(\hbar I_1 = 1$) [42–45]

$$I(r) \propto J^2 e^{-2r/\xi} \left[ \frac{v_F}{2\pi r} \cos(2k_F r) + \frac{\Delta}{r^2} \sin^2(k_F r) \right],$$

where $v_F$ is the Fermi velocity and $\xi = v_F/\Delta$ is the coherence length of the superconductor. We note that solving for the superconducting order parameter self-consistently is not important in the dilute atom regime ($k_F a \gg a^{-1}, \xi^{-1}$) since the YSR energy and electron propagator between spins are hardly modified [46]. We do not consider the dense atom limit $k_F a < 1$, where a collective depletion of $\Delta(r)$ near the chain should be taken into account.

The first term in square brackets in Eq. (3) is the familiar Rudermann-Kittel-Kasuya-Yosida (RKKY) interaction [47–49], while the second, strictly antiferromagnetic, term arises from the anomalous component of the electronic spin susceptibility and disfavors the pair-breaking effect of a polarized exchange field. The spin-chain ground-state energy is given by the minimum Fourier component of the exchange interaction, $E_0 = I_q$.

In the normal state ($\Delta = 0$), one finds from Eq. (3) a ferromagnet ($q = 0$) in the range $n + 1/4 < k_F a/\pi < n + 3/4$, with integer $n$ and an antiferromagnet ($q = \pi/\alpha$) otherwise. We emphasize that the $q = 2k_F$ spiral phase that may arise when the electron gas is also one dimensional [28–30,37] does not occur here; the spin chain is always in a collinear state. However, superconducting correlations in a 3D electron gas generally make ferromagnetism unstable towards spiral formation due to the long-range superconducting correction in Eq. (3) (in a 1D electron gas the $q = 2k_F$ order is hardly modified by superconductivity [28–30]). Indeed, for $\Delta \neq 0$ the minimum Fourier component $I_q \sim q^2 - |q|/\xi$ is shifted to the wave vector $q \sim \xi^{-1}$. This magnetic instability is similar to the Anderson-Suhl transition in 2D and 3D spin lattices [43,50] and results from the compromise between the shorter-range ferromagnetic RKKY interaction and the longer-range antiferromagnetic interaction.

The spiral formation is stable and strongly reinforced by the inclusion of higher-order terms beyond the Born approximation in Eq. (3). The crucial effect responsible for this behavior is the formation and overlap of the subgap YSR bound states induced by the magnetic atoms. Formally, these subgap states are encoded in the single magnetic atom $T$.
matrices,
\[ T_j(\omega) = JS_j \cdot \sigma \left( 1 + \frac{\pi J v_F \omega \tau_0 + \Delta \tau_1}{2} \sqrt{\Delta^2 - \omega^2} S_j \cdot \sigma \right)^{-1}, \]  
(4)
where \( v_F \) is the normal state density of states at the Fermi energy. The presence of the bound state is signified by the subgap pole of \( \det T_j(\omega) \) on the real energy axis \( \omega = \pm \varepsilon \),
\[ \varepsilon = \Delta \frac{1 - (\pi J S v_F/2)^2}{1 + (\pi J S v_F/2)^2}. \]  
(5)
To see this we follow Ref. \[45\] and consider two YSR states, in particular, one may replace the bare magnetic atom potential with its \( T \) matrix, Eq. (4). Computing the exchange coupling to second order in \([\varepsilon, \Delta] = \text{const.} \) and \( \text{perturbative result} \) \[3\], we find for small \( \varepsilon \) an enhanced antiferromagnetic component \( \sim 1/|\varepsilon| \) due to the exchange coupling mediated via the YSR states \[45\]. This effect strongly increases the spiral wave vector of the spin chain. Indeed, in the range \( n + 1/4 \leq k_F a/\pi \leq n + 3/4 \) for integer \( n \), one finds \( I_q \sim q^2 - |q|\varepsilon^{-1}\Delta/|\varepsilon| \), with \( \Delta \) the ground-state wave vector \( q \sim \varepsilon^{-1}\Delta/|\varepsilon| \) rapidly growing as \( \varepsilon \) approaches zero. This behavior is consistent with the exact numerical result, shown in Fig. 2(b), as long as \( |\varepsilon|/\Delta \) is not too small. The apparent divergence of Eq. (5) as \( |\varepsilon| \rightarrow 0 \) signifies its inapplicability for small enough \( \varepsilon \), since the effective exchange energy cannot physically exceed the splitting between YSR energies caused by their finite overlap.

This suggests that below a characteristic value of \( \varepsilon \), a crossover (for two spins) to a new regime occurs. To see this we follow Ref. \[45\] and consider two YSR states hybridizing with a Cooper pair from the superconducting condensate. This process can be described by the matrix element \( U(r) = \Delta e^{-|r|/\xi} \cos(k_F r)/(k_F r) \) representing the overlap between YSR states (see Fig. 1). The energy difference between the ground state and the excited state with the YSR states occupied/unoccupied is \( 2|\varepsilon| \). As long as \( U < 2|\varepsilon| \), the change of the ground-state energy can be computed perturbatively, \( U^2/2|\varepsilon| \), leading to the second term in the brackets of Eq. (5). Thus, for the spin chain, Eq. (5) is valid down to the scale \( |\varepsilon| \sim U(a) \sim \Delta/k_F a \) (assuming \( \xi \gg a \)), at which point \( q \sim k_F a/\xi \). When the Fermi energy crosses the YSR band \( |\varepsilon| \lesssim U(a) \approx \Delta/k_F a \), the perturbation theory in \( U/|\varepsilon| \) fails since Cooper pairs in the bulk strongly hybridize with the YSR states. This signals a fundamental change of the ground state, and corresponds to a \( p \)-wave superconducting phase transition in the YSR chain which harbors Majorana boundary states (provided spiral order remains stable).

We now wish to show that in the regime of strong hybridization [where the effective spin model Eqs. (2) and (6) is inapplicable] ferromagnetism remains unstable to spiral formation (i.e., the topological superconductivity is stable). The complication is that a new competing tendency arises once the Fermi energy lies in the YSR band: The gain of kinetic energy associated with electrons hopping along the YSR chain is maximized for a ferromagnetic arrangement of the spin chain since this maximizes the YSR bandwidth, analogous to the double-exchange mechanism. However, the presence of a spiral leads to a superconducting gap in the YSR band, leading to a concomitant gain of the corresponding condensation energy, depicted in Fig. 3. At small \( q \), it is easy to see that the energy gain from the opening of the superconducting gap \( \Delta E_{\text{gap}} \propto -q^2(\delta q \Delta k)^2 \ln \left( \frac{|q|}{q_a} \right) \) is always larger than the loss of kinetic (or RKKY) energy \( \Delta E_{\text{kin}} \propto q^2 \), where the coefficient of the logarithm is proportional to the square of the YSR gap at the YSR Fermi points \( \pm k_s \) (see Fig. 3) expanded for small \( q \), \( \Delta k \approx q \delta q \Delta k \) (\( \Delta k = 0 \) for \( q = 0 \) since Cooper pairs cannot hybridize with a ferromagnetic chain). Qualitatively, we thus find that ferromagnetism is generically unstable to the formation of spiral phase with wave vector \( q \propto e^{-1/\lambda} \), where the parameter \( \lambda \propto (\delta q \Delta k)^2 \) entering the exponent depends on \( k, \Omega = \Omega(a) \), and is provided below Eq. (8). The case \( q = 0 \) can only occur if the gap at the YSR Fermi points, and thus \( \lambda \), vanishes for \( k_s = 0, \pi/a \).

We study this possibility and the quantitative variation of \( q \) on \( \varepsilon \) by evaluating the YSR contribution to the total energy numerically [the above gap RKKY contribution, the first term in the brackets of Eq. (5), only weakly depends on \( |\varepsilon| \ll \Delta \) here],
\[ E_{\text{YSR}} = -\frac{1}{2} \sum_k E_k, \quad E_k = \sqrt{(h_k - \varepsilon)^2 + \Delta_k^2}. \]  
(7)
Here, the hopping \( h_k = h_{-k} \) and \( p \)-wave pairing \( \Delta_k = -\Delta_{-k} \) energies are the same as those derived in Ref. \[25\], up to the energy shift \( \varepsilon \) which enters Eq. (7) only as an effective chemical potential for the YSR band. The precise forms of \( h_k, \Delta_k \) are provided in the Supplemental Material \[41\], but are not essential in the following; their salient features are sketched in Fig. 3. In particular, one sees that \( \Delta_k \) indeed may have extra nodes away from \( k = 0, \pi/a \) due to the long-range nature of the pairing (i.e., higher odd harmonics beyond sin \( ka \) are relevant).
Generally, we find that when $\Delta_k = h_k = 0$ have simultaneous zeros, double exchange wins and the system exhibits a gapless electronic spectrum and ferromagnetism in the spin chain. Remarkably, the exact location of these gapless critical lines in the phase diagram of Fig. 2(a) can be extracted:

$$\varepsilon_c = \frac{\Delta}{k_F a} \left[ \pi/2 - (k_F a \bmod \pi) \right].$$  

(8)

In the spiral regions of Fig. 2, the magnetic order in the close vicinity of Eq. (8) is exponentially suppressed $\sim e^{-\varepsilon_c/k_F a}$, where $\lambda \sim \left( \frac{\varepsilon_c}{\Delta k_F a} \right)^2$. Away from this line $q$ grows to the scale $q \sim k_F a/\xi$ at $\varepsilon \sim \Delta/k_F a$, beyond which it crosses over to the $T$-matrix dependence $q \sim \Delta/|\varepsilon|$, as shown in Fig. 2(b) for the case $k_F a = 15.5\pi$ ($\varepsilon_c = 0$). This leads to the nonmonotonic behavior of $q$ on the YSR energy $\varepsilon$, with a peak around $\varepsilon \sim \Delta/k_F a$ of order $q_{\text{max}} \sim k_F a/\xi$. The magnetic order determined from minimizing the electronic energy of Eq. (1), shown in Fig. 2(b), indeed exhibits this crossover behavior and is well described by the $T$-matrix approximation when $|\varepsilon| > \Delta/k_F a$ and the YSR approximation when $|\varepsilon| < \Delta/k_F a$.

We now briefly discuss the topological properties of the model in Eq. (1), delegating a more detailed account to the Supplemental Material. As discussed in Refs. [32,33,51–54], the topological class of the YSR chain in the planar spiral configuration is BDI due to hidden time-reversal and chiral symmetries. Different topological phases are therefore distinguished by a $Z$ topological invariant (winding number), which can only change when the gap in the YSR spectrum closes. This occurs when the YSR band crosses the Fermi energy or when the system is tuned across the gapless ferromagnetic line, Eq. (8), leading to the topologically nontrivial and distinct $\text{TS}^\pm$ phases with winding numbers $\pm 1$ (for a fixed rotation axis of the spiral), shown in Fig. 2(a). As a result, the boundary between $\text{TS}^+$ and $\text{TS}^-$ systems will host a pair of zero-energy Majorana bound states protected by chiral symmetry, whereas the boundary of either system with vacuum will only host a single Majorana bound state. The presence of two Majorana bound states also occurs for a single system in either of the $\text{TS}^\pm$ phases if there is a $q \rightarrow -q$ domain wall [53–55].

Experimental outlook. The YSR topological gap $\Delta_t$ obtains a broad maximum as a function of magnetic atom spacing (i.e., from one period $n$ of the topologically nontrivial part of the phase diagram to the next, $k_F a \rightarrow k_F a + \pi$). This is because if the magnetic atoms are spaced too closely ($a \rightarrow 0$), $\Delta_t \propto q_{\text{max}} \Delta/k_F a \propto \Delta a/\xi$ becomes small, while if the atoms are too dilute ($a \rightarrow \infty$), the overall energy scale $\Delta/k_F a$ is diminished. The maximum thus occurs for an optimal spacing $a_{\text{opt}}$ determined by $q_{\text{max}} \sim 1$, giving $k_F a_{\text{opt}} \sim \sqrt{\Delta k_F a/\xi}$. At this spacing, for $k_F a = 2000$, we find $\Delta_t \sim 200\,\text{mK}$, assuming $\Delta = 10\,\text{K}$ (by comparison for Fe on Pb experiments show $\Delta \lesssim 1\,\text{K}$ [15,16]).

The influences of anisotropy and temperature on the topological phase are expected to be unimportant as long as the associated energy scale remains below $\Delta_t$. The magnetic order can also be destroyed by thermal fluctuations, but such effects will be quenched either by finite chain size or anisotropy [28–30,33]. For the case of single-ion anisotropy, described by the Hamiltonian $H_D = -D S_j^z$, we find that when $D < 0$ (easy plane) the spiral is merely fixed to lie in the $xy$ plane (i.e., the spiral axis lies along $z$), while for $D > 0$ the spiral axis lies in the $xy$ plane and is orthogonal to the $\xi$ axis. For sufficiently strong anisotropy $D \gtrsim \Delta_t \sim 20\,\text{mK}$ we expect the ground state to become a topologically trivial, collinear magnetic phase. This restricts the self-organized topological phase to easy-plane systems or those with sufficiently weak easy-axis anisotropy.

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See Supplemental Material at http://link.aps.org supplemental/10.1103/PhysRevB.93.140503 for the derivation of the exact ground-state energy as a function of the spiral wave vector. We also provide the formula determining the exact subgap YSR spectrum and topological phase boundaries.


