Self-Organized Topological State with Majorana Fermions

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Most physical systems known to date tend to resist entering the topological phase and must be fine-tuned to reach that phase. Here, we introduce a system in which a key dynamical parameter adjusts itself in response to the changing external conditions so that the ground state naturally favors the topological phase. The system consists of a quantum wire formed of individual magnetic atoms placed on the surface of an ordinary s-wave superconductor. It realizes the Kitaev paradigm of topological superconductivity when the wave vector characterizing the emergent spin helix dynamically self-tunes to support the topological phase. We call this phenomenon a self-organized topological state.

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Topological phases, quite generally, are difficult to come by. They either occur under rather extreme conditions (e.g., the quantum Hall liquids [1], which require high sample purity, strong magnetic fields, and low temperatures) or demand fine-tuning of system parameters, as in the majority of known topological insulators [2–4]. Many perfectly sensible topological phases, such as the Weyl semimetals [5] and topological superconductors [4,6], remain experimentally undiscovered.

The paucity of easily accessible, stable topological materials has been in large part responsible for the relatively slow progress towards the adoption of topological phases in mainstream technological applications. A question that naturally arises is the following: Is there a fundamental principle behind this "topological resistance"? Although unable to give a general answer to this question, we provide in this Letter a specific counterexample to this conjectured phenomenon of topological resistance. We consider a simple model system, which, as we demonstrate, *wants* to be topological in a precisely defined sense. The key to this "topofilia" is the existence in the system of a dynamical parameter that adjusts itself in response to changing external conditions so that the system self-tunes into the topological phase. The specific model system we consider is depicted in Fig. 1(a) and consists of a chain of magnetic atoms, such as Co, Mn, or Fe, deposited on the atomically flat surface of an ordinary s-wave superconductor, as described in a recent experimental study [7]. We note that scanning tunneling microscopy (STM) techniques now enable fairly routine assembly of such and even much more complicated nanostructures [8,9].

It has been pointed out previously [10–12] that if the magnetic moments in the chain exhibit a spiral order then the electrons in the chain can form a one-dimensional (1D) topological superconductor (TSC) with Majorana zero modes localized at its ends [13]. For a given chemical potential μ, however, the spiral must have the correct pitch in order to support the topological phase. This connection is illustrated in Figs. 1(b) and 1(c) and will be discussed in more detail below. Exactly how the pitch of the spiral depends on the system parameters and its thermodynamic stability are two key issues that have not been previously discussed. In this Letter, we show that, remarkably, under generic conditions the pitch of the spiral that minimizes the free energy of the system coincides with the one required to establish the topological phase.

The physics behind the self-organization phenomenon outlined above is easy to understand and is similar to that leading to the spiral ordering of nuclear spins proposed to occur in 1D conducting wires [14,15] and two-dimensional electron gases [16]. Some experimental evidence for such an ordering has been reported [17,18]. If we

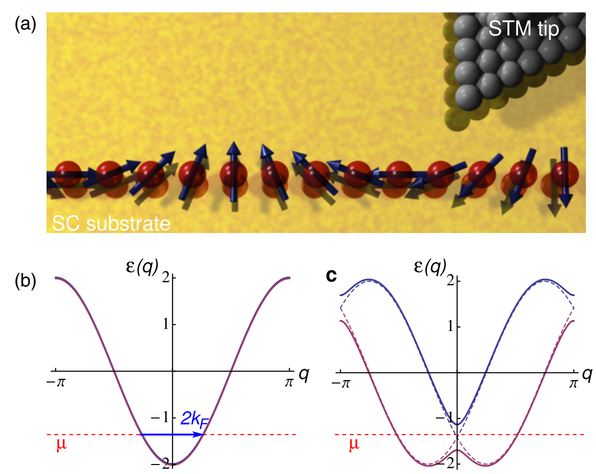

FIG. 1 (color online). Chain of magnetic atoms on a superconducting substrate. (a) Schematic depiction of the system with the red spheres representing the adatoms and blue arrows showing their magnetic moments arranged in a spiral. (b) Two spin-degenerate branches of the normal-state spectrum of the system in the absence of magnetic moments modeled by the nearest-neighbor tight-binding model Eq. (1). (c) With the magnetic moments the two branches shift in momentum by $\pm G$ and the gap JS opens at $q = 0, \pi$. Dashed lines show the shifted spectral branches indicated in panel (b) with no gap for comparison.

for a moment neglect the superconducting order and assume a weak coupling of the adatoms to the substrate then the electrons in the chain can be thought of as forming a 1D metal. The natural wave vector for the spiral ordering in such a 1D metal is $G = 2k_F$ where k_F denotes its Fermi momentum. This is because the static spin susceptibility $\chi_0(q)$ of a 1D metal has a divergence at $q = 2k_F$. Electron scattering off such a magnetic spiral results in the opening of a gap in the electron excitation spectrum but only for one of the two spin-degenerate bands [14,15]. In the end, we are left with a single, nondegenerate Fermi crossing at $\pm 2k_F$, illustrated in Fig. 1(c). According to the Kitaev criterion [13], this is exactly the condition necessary for a 1D TSC to emerge. In the following, we will show that this reasoning remains valid when we include superconductivity from the outset and when we describe the chain by a tight-binding model appropriate for a discrete atomic chain.

We begin by studying the simplest model of tight-binding electrons coupled to magnetic moments $\boldsymbol{S}_i$ described by the Hamiltonian

$$\mathcal{H}_0 = -\sum_{ij\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} - \mu \sum_{i\sigma} c^\dagger_{i\sigma} c_{i\sigma} + J \sum_i \boldsymbol{S}_i \cdot (c^\dagger_{i\sigma} \boldsymbol{\sigma}_{\sigma\sigma'} c_{i\sigma'}). \tag{1}$$

Here, $c^\dagger_{j\sigma}$ creates an electron with spin σ on site j, J stands for the exchange coupling constant, and $\boldsymbol{\sigma} = (\sigma^x, \sigma^y, \sigma^z)$ is the vector of Pauli spin matrices. We assume that the substrate degrees of freedom have been integrated out, leading to a superconducting order Δ in the chain described by

$$\mathcal{H} = \mathcal{H}_0 + \sum_j (\Delta c^\dagger_{j\uparrow} c^\dagger_{j\downarrow} + \text{H.c.}). \tag{2}$$

We consider a coplanar helical arrangement of atomic spins as indicated in Fig. 1(a),

$$\boldsymbol{S}_j = S[\cos(Gx_j), \sin(Gx_j), 0], \tag{3}$$

where G is the corresponding wave vector and the chain is assumed to lie along the x axis. We note that the Hamiltonian in Eq. (2) is invariant under the simultaneous global SU(2) rotation of the electron and atomic spins, so the discussion below in fact applies to any coplanar spiral.

To find the spectrum of excitations, it is useful to perform a spin-dependent gauge transformation [11]

$$c_{j\uparrow} \to c_{j\uparrow} e^{(i/2)Gx_j}, \qquad c_{j\downarrow} \to c_{j\downarrow} e^{-(i/2)Gx_j}, \tag{4}$$

upon which the Hamiltonian becomes translationally invariant and can be written in the momentum space as

$$\mathcal{H} = \sum_q [\xi(q) c^\dagger_{q\sigma} c_{q\sigma} + b(q) c^\dagger_{q\sigma} \sigma^z_{\sigma\sigma'} c_{q\sigma'} + JS c^\dagger_{q\sigma} \sigma^x_{\sigma\sigma'} c_{q\sigma'} + (\Delta c^\dagger_{q\uparrow} c^\dagger_{-q\downarrow} + \text{H.c.})]. \tag{5}$$

In the above, $\xi(q) = \frac{1}{2}[\epsilon_0(q - G/2) + \epsilon_0(q + G/2)] - \mu$, and $b(q) = \frac{1}{2}[\epsilon_0(q - G/2) - \epsilon_0(q + G/2)]$ with $\epsilon_0(q) = -\sum_j t_{0j} e^{iqx_j}$ the normal-state dispersion in the absence of the exchange coupling. We note that the Hamiltonian of Eq. (5) is essentially a lattice version of the model semiconductor wire studied in Refs. [19,20] with $b(q)$ playing the role of the spin-orbit coupling and JS standing for the Zeeman field. Its normal-state spectrum is given by

$$\epsilon(q) = \xi(q) \pm \sqrt{b(q)^2 + J^2 S^2} \tag{6}$$

and is displayed in Fig. 1(c) for the case of nearest-neighbor hopping with $\epsilon_0(q) = -2t \cos q$.

If viewed as a rigid band structure, then according to the Kitaev criterion [13] the chain will support topological superconductivity when there is an odd number of Fermi crossings in the right half of the Brillouin zone. This requires μ such that $|\mu \pm 2t \cos(G/2)| < JS$. However, in the SU(2) symmetric model under consideration, G is a dynamical parameter that will assume a value that minimizes the system free energy. Taking $\boldsymbol{S}_i$ to be classical magnetic moments and working at $T = 0$, we thus proceed to minimize the ground-state energy of the electrons $E_g(G)$ for a given value of μ and Δ. The result of this procedure is shown in Fig. 2(a) and confirms that at minimum $G \approx 2k_F$, as suggested by the general arguments advanced above. More importantly, for almost all relevant values of μ and Δ the self-consistently determined spiral pitch G is precisely the one required for the formation of the topological phase. This fails only close to the half filling ($\mu = 0$) where $G = \pi$ indicates an antiferromagnetic ordering. In this case, the symmetry of the band structure prohibits an odd number of Fermi crossings, so the system must be in the trivial phase. Also, it is clear that no value of G can bring about the TSC phase when μ lies outside of the tight-binding band and the system is an insulator. The resulting topological phase diagram is displayed in Fig. 2(b).

These results indicate that, as we argued on general grounds, the pitch of the magnetic spiral self-tunes into the topological phase for nearly all values of the chemical potential μ for which such a tuning is possible. The emergence of Majorana zero modes at the two ends of such a topological wire [13,19,20] and their significance for the quantum information processing have been amply discussed in the recent literature [21–23].

We now address the adatom coupling to the substrate in greater detail. We consider a more complete Hamiltonian $\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_{SC} + \mathcal{H}_{cd}$, where $\mathcal{H}_0$ is defined in Eq. (1), whereas

$$\mathcal{H}_{SC} = \sum_{\boldsymbol{k}} [\xi_0(\boldsymbol{k}) d^\dagger_{\boldsymbol{k}\sigma} d_{\boldsymbol{k}\sigma} + (\Delta_0 d^\dagger_{\boldsymbol{k}\uparrow} d^\dagger_{-\boldsymbol{k}\downarrow} + \text{H.c.})] \tag{7}$$

describes the SC substrate with electron operators $d^\dagger_{\boldsymbol{k}\sigma}$. The substrate is characterized by a three-dimensional

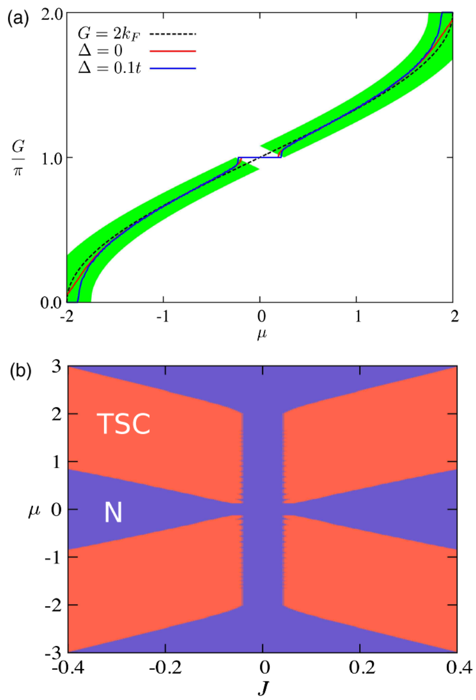

FIG. 2 (color online). The pitch of the spiral and the topological phase diagram. Panel (a) shows the spiral wave vector G that minimizes the system ground-state energy $E_g(G)$ as a function of μ, the latter in units of t. The parameters are $S = 5/2$, $J = 0.1t$, and $\Delta = 0$ (red line), $\Delta = 0.1t$ (blue line). The dashed line represents $G = 2k_F$ whereas the green band shows the region in which G must lie for the system to be topological for a given μ. Panel (b) shows the topological phase diagram in the μ-J plane, both in units of t, for $\Delta = 0.1t$. To distinguish the two phases, we have calculated the Majorana number $\mathcal{M}$ as defined in Ref. [13]. Topological phase (TSC) is indicated when $\mathcal{M} = -1$ whereas $\mathcal{M} = +1$ indicates the topologically trivial phase (N).

normal-state dispersion $\xi_0(\boldsymbol{k}) = k^2/2m - \epsilon_F$ and the bulk gap amplitude Δ_0. The coupling is effected through

$$\mathcal{H}_{cd} = -r\sum_{j\sigma}(d^\dagger_{j\sigma}c_{j\sigma} + \text{H.c.}), \quad (8)$$

where $d_{j\sigma} = (1/\sqrt{N})\sum_{\boldsymbol{k}} e^{-i\boldsymbol{k}\cdot\boldsymbol{R}_j} d_{\boldsymbol{k}\sigma}$, N is the number of adatoms in the chain, and $\boldsymbol{R}_j$ denotes their positions.

We now wish to integrate out the substrate degrees of freedom and ascertain their effect on the magnetic chain. Since the Hamiltonian $\mathcal{H}$ is noninteracting, this procedure can be performed exactly. As outlined in the Appendix of Ref. [21], a simple result obtains in the limit of the substrate a bandwidth much larger than the chain bandwidth $4t$, which we expect to generically be the case. In this limit, the Green's function of the chain reads

$$\mathcal{G}^{-1}_{\text{eff}}(i\omega_n, q) = \mathcal{G}^{-1}_0(i\omega_n, q) - \pi\rho_0 r^2 \frac{i\omega_n - \tau^x\Delta_0}{\sqrt{\omega_n^2 + \Delta_0^2}}, \quad (9)$$

where $\omega_n = (2n+1)\pi T$ is the Matsubara frequency, $\rho_0 = ma^2/2\pi\hbar^2$ is the substrate normal density of states projected onto the chain (with a the adatom spacing), and

$$\mathcal{G}^{-1}_0(i\omega_n, q) = -i\omega_n + \tau^z[\xi(q) + \sigma^z b(q)] + \sigma^x JS \quad (10)$$

the bare chain Green's function. The above Green's functions are 4×4 matrices in the combined spin and particle-hole (Nambu) space, the latter represented by a vector of Pauli matrices $\boldsymbol{\tau}$. In the low-frequency limit $\omega \ll \Delta_0$, relevant to the physics close to the Fermi energy, Eq. (9) implies two effects. First, the bare chain parameters t, μ, and J are reduced by a factor of $\Delta_0/(\Delta_0 + \pi r^2\rho_0)$. Second, a SC gap $\Delta = \pi r^2\rho_0\Delta_0/(\Delta_0 + \pi r^2\rho_0)$ is induced in the chain. In the limit of a weak chain-substrate coupling $r^2 \ll \Delta_0/\rho_0$, the latter is seen to become $\Delta \simeq \pi r^2\rho_0$, independent of the substrate gap Δ_0.

In order to visualize the above effects, we display in Fig. 3 the relevant spectral function, defined as

$$A_{\text{eff}}(\omega, q) = -\frac{1}{2\pi}\text{Im}\,\text{Tr}[(1+\tau^z)\mathcal{G}_{\text{eff}}(\omega + i\delta, q)] \quad (11)$$

where δ represents a positive infinitesimal. The figure clearly shows how the bands self-consistently adjust to the changing chemical potential as well as the expected topological phase transitions taking place between the trivial and the TSC phases.

Our results thus far relied on the mean field theory and ignored interactions beyond those giving rise to superconductivity. There are several effects that can in principle destabilize the topological state found above, but we now argue that the latter remains stable against both interactions and fluctuations. First, one may worry that the adatom magnetic moments would be screened by the Kondo effect at temperatures $T < T_K = \epsilon_F e^{-1/\rho(\epsilon_F)J}$, where $\rho(\epsilon_F)$ is the density of states in the substrate at the Fermi level. For a normal metal, T_K can indeed be sizeable—tens of Kelvins—and the ground state is then nonmagnetic [24]. In the presence of superconductivity, however, $\rho(\epsilon_F) = 0$ and a more elaborate treatment of the Kondo problem in the presence of a gap shows that T_K is much reduced [25], possibly to zero when J is sufficiently small. Thus, generically, we expect the system to avoid the Kondo fixed point and remain magnetic at most experimentally relevant temperatures. Electron-electron interactions in the wire are additionally expected to enhance the magnetic gap [14,16] compared to its noninteracting value JS, which will ultimately further improve the stability of the topological phase.

Second, one must consider thermal and quantum fluctuations that will tend to destroy any ordering present in a 1D wire. Since the SC order in the wire is phase-locked to the substrate we may ignore its fluctuations. However, fluctuations in the magnetic spiral order must be considered. In a realistic system, spin-orbit coupling will induce a Dzyaloshinsky-Moriya interaction of the form

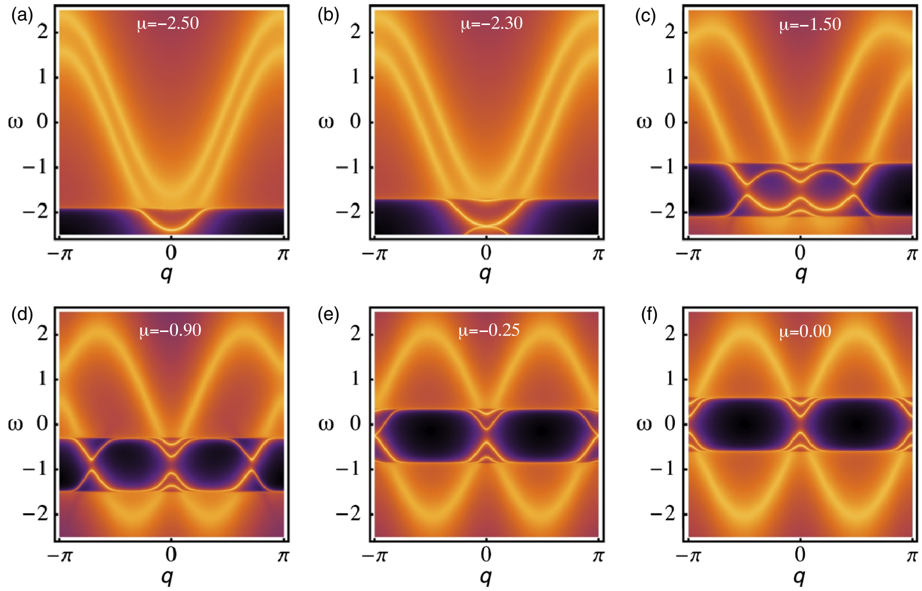

FIG. 3 (color online). Spectral function of the adatom chain. $A_{\mathrm{eff}}(\omega, q)$ defined in Eq. (11) is represented as a density plot for several representative values of the chemical potential μ, with the appropriate self-consistently determined spiral pitch G shown in Fig. 2(a). In panel (a), μ is below the bottom edge of the chain band and the system is in the trivial phase. When μ reaches the band edge, a topological phase transition occurs through a gap closing shown in panel (b). Further increase of μ puts the system into the topological phase illustrated in (c) and (d) until the gap closes again near half filling (e) placing the system back into the trivial phase (f). A similar sequence of phases occurs for positive values of μ for which the spectral function can be obtained by simply flipping the sign of the frequency ω. The dark band around the chemical potential reflects the bulk SC gap. In all panels, frequency ω is in units of t whereas $JS = 0.4t$, $\Delta_0 = 0.6t$, $\rho_0 r^2 = 0.05t$, and $\delta = 0.002t$ is used to give a finite width to the spectral peaks.

$\mathbf{D}_{ij} \cdot (\boldsymbol{S}_i \times \boldsymbol{S}_j)$ in the effective spin Hamiltonian. The latter breaks the SU(2) spin symmetry and pins the spiral order so that the spins rotate in the direction perpendicular to $\mathbf{D}$. The remaining low-energy modes of such a spiral are magnons. The relevant spin-wave analysis and the origin of the DM interaction are outlined in the Supplemental Material [26]. We find a single linearly dispersing gapless magnon $\omega_q = c|q|$ that will reduce the classical ordered moment according to

$$\langle S^x \rangle \simeq S - a \int_{\mathrm{BZ}} \frac{dq}{2\pi} \frac{1}{e^{\beta\hbar\omega_q} - 1}. \tag{12}$$

For an infinite wire, the integral diverges logarithmically at long wavelengths, signaling the expected loss of the magnetic order in the thermodynamic limit. We are, however, interested in a wire of finite length L where the divergence is cut off at $q \sim \pi/L$. A crude estimate of the transition temperature in this case is obtained by assuming $\beta\hbar\omega_q \ll 1$ over the Brillouin zone and setting $\langle S^x \rangle = 0$ in Eq. (12). This gives

$$k_B T^* \approx \frac{\pi S}{\ln N} \frac{\hbar c}{a}, \tag{13}$$

with $N = L/a$ the number of adatoms in the chain. For $N = 100$, $S = 5/2$, and typical model parameters $t = 10$ meV, $J = 5$ meV, and μ appropriate for the topological phase we find T^* of tens of Kelvins (see also the Supplemental Material [26]). Because of the $\ln N$ factor, T^* is only weakly dependent on the chain length.

Our results provide strong support for the notion of a self-organized topological state. Magnetic moments of atoms assembled into a wire geometry on a superconducting surface are indeed found to self-organize into a topological state under a wide range of experimentally relevant conditions. The emergent Majorana fermions can be probed spectroscopically by the same STM employed in building the structures and will show as zero-bias peaks localized near the wire ends. The system can be tuned out of the topological phase by applying magnetic field $\boldsymbol{B}$, which, when strong enough, will destroy the helical order by polarizing the adatom magnetic moments. An attractive feature of this setup is the possibility of assembling more complex structures, such as T junctions and wire networks that will aid future efforts to exchange and braid Majorana fermions with the goal of probing their non-Abelian statistics [27]. We also note that the general self-organization principle described above should apply to other 1D structures, most notably quantum wires with nuclear spins considered in Ref. [14]; however, the energy scales are expected to be much smaller due to the inherent weakness of the nuclear magnetism.

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Note added.—Upon completion of this work we learned about two studies [28,29] reaching similar conclusions regarding topological order in helical spin chains.

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