

Moiré dispersion of edge states in spin chains on superconductors

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Our calculations of ferromagnetic spin chains on *s*-wave superconductors show that the energy oscillations of edge states with the chain's length are due to a moiré pattern emerging from the electronic interactions in the superconductor and the discreteness of the spin-chain lattice. By modifying the spin lattice, the moiré dispersion of edge states can be controlled. In particular, we can engineer nondispersive edge states that remain at fixed energy regardless of the size distribution of the spin chains. This is an important step in the study of edge states of spin chains that can be fabricated with a certain size dispersion.

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Majorana bound states (MBS) have gained increasing interest in recent years due to their non-Abelian statistics and potential application to topological quantum computing [1,2]. The search for MBS in condensed matter systems pays particular attention to one-dimensional (1D) structures that combine superconductivity, spin-orbit coupling (SOC), and magnetic interactions [3–8]. Under the right conditions, these structures are able to mimic a Kitaev chain where MBS arise at the edges of finite systems [3]. Studies have focused on two main approaches: spin chains on superconducting surfaces [8–17], and semiconducting nanowires with Rashba spin-orbit coupling and proximitized superconductivity [18–21]. These edge states are expected to appear at zero energy, however, the spatial overlap between MBS at both edges of finite systems results in non-zero-energy edge states [17,18,22–24].

Due to the finite size of these systems, not only do MBS interact with each other but also with non-zero-energy states [25]. These interactions result in the mixing of MBS. The resulting states appear at finite energies and quasiperiodically evolve with the system's size [16,17,26]. Edge-state energy oscillations have also been found as a function of applied magnetic field [21,27,28]. Despite the mixing of states at the origin of the found oscillations, the new states maintain interesting topological properties [29]. Unfortunately, the oscillations in energy make the control of MBS challenging, and it would be desirable to find them at a fixed energy. Particularly, in the large-scale manufacturing of spin chains, we expect to find a distribution of sizes. Having all topological edge states at a fixed energy regardless of spin-chain size is an important step in their study and reproducibility.

In this Letter, we make a theoretical study of edge states on ferromagnetic (FM) spin chains on a BCS superconductor. Using the model presented in Ref. [26], we observe energy oscillations of the edge states as we vary the number of atoms in the magnetic chain. Similar results have been recently observed in experiments [17]. Here, we show that the oscillations about zero can be found for topological and trivial states of the chain. We trace back the origin of the periodicity to a 1D moiré pattern resulting from the discrete nature of the spin chain reflected in its lattice parameter a_c , and the substrate-mediated interactions governed by the substrate's Fermi wavelength λ_F . As the two structures interact, the resulting edge-state energies rapidly change, producing a rich variety of patterns akin to the many different schemes of energy bands found in 2D moiré systems [30,31]. The dependence of the edge-state energies on a_c and λ_F allows us to control their dispersion. In this way, we can engineer magnetic chains for which the topological edge states remain fixed at a finite energy regardless of the actual size of the spin chain beyond a minimal size.

To simulate the FM spin chain on an *s*-wave superconductor, we solve the Bogoliubov-de Gennes equations [32] for a superconducting surface modeled as a 2D array of points, spaced by the lattice parameter a (see Refs. [26,33]). The superconductor is defined by the order parameter Δ , the Fermi vector of the material k_F , and the metallic electron density N_0 . These parameters fix the BCS correlation length ξ that we use here. The effect of the magnetic impurities is modeled by the local Hamiltonian

$$\hat{H}_{\text{impurity}} = \sum_{j,\sigma}^N [K_j \hat{c}_{j\sigma}^\dagger \hat{c}_{j\sigma} + J_j \vec{S}_j \cdot \hat{\vec{s}}(j)], \quad (1)$$

where J is the magnetic exchange interaction of the impurities with the superconductor, $\vec{S}_j$ is the spin of impurity j that is assumed to be classical, K_j is the corresponding nonmagnetic scattering potential, and $\hat{\vec{s}}(j)$ is the electron spin operator at the tight-binding orbital localized at j corresponding to the creation and annihilation operators $\hat{c}_{j\sigma}^\dagger$ and $\hat{c}_{j\sigma}$. The exchange

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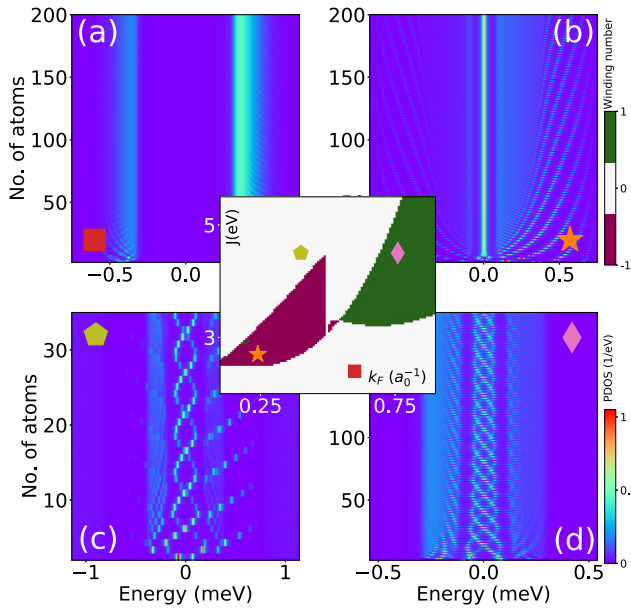


FIG. 1. Topological phase diagram and evolution of edge states with number of atoms. Inset: Winding number calculated for infinite FM chains as a function of the magnetic coupling J and the Fermi vector k_F . The green and magenta areas correspond to the topological phases $w = 1$ and $w = -1$, respectively, and the white area is the trivial region. (a)–(d) Projected density of states (PDOS) as a function of the number of magnetic atoms in the spin chain. The J and k_F parameters are indicated by the position of the corresponding shape. (a) $J = 2.4$ eV, $k_F = 0.6a_0^{-1}$, red square. (b) $J = 2.7$ eV, $k_F = 0.24a_0^{-1}$, orange star. (c) $J = 4.5$ eV, $k_F = 0.4a_0^{-1}$, yellow pentagon. (d) $J = 4.5$ eV, $k_F = 0.75a_0^{-1}$, pink diamond. Other parameters are $\Delta = 0.75$ meV, $N_0 = 0.037/\text{eV}$, $\alpha_R = 3.0$ eV Å, $K = 5.5$ eV, and $a_c = 3.36$ Å. The correlation length is the BCS one, and for (d) it is $\xi = 4852$ Å.

interaction of the magnetic impurities with the Cooper pairs in the superconductor results in the emergence of localized states inside the superconducting gap known as Yu-Shiba-Rusinov (YSR) states [34–36]. By creating a chain of such impurities, the localized states can hybridize creating YSR bands that can go into the topological phase [37–39]. In the case of FM chains, the system can be in the topological phase when the Rashba spin-orbit coupling α_R is different from zero [40].

Figure 1 relates the energy behavior of edge states to the topological phase of the chain. In the inset of Fig. 1, we reproduce the phase space from Ref. [26]. The winding number [40] w of an infinite FM chain is plotted as a function of the magnetic coupling of the impurities J and the Fermi vector k_F . In Ref. [26] we showed that the winding number matches the behavior of the Pfaffian topological invariant and its use can be extended to the case of 2D Rashba coupling. The winding number yields more information than the Pfaffian because it comes in three values for the present system [41,42] with $w = 0$ the topologically trivial phase and $w = \pm 1$ the nontrivial phases. The green and magenta areas on the phase diagram correspond to the topological phases of $w = 1$ and $w = -1$, respectively. On this phase diagram, we select four pairs of parameters and study the evolution of the edge states as we change the length of the chain.

In Figs. 1(a)–1(d) we plot the projected density of states (PDOS) on the edge atom of the chain as a function of energy (x axis) and chain length (y axis). Figure 1(a) corresponds to a nontopological case where the in-gap states are still far from zero energy and delocalized along the chain (see Ref. [43]). As we increase the number of atoms, the edge states remain at a fixed energy. In Fig. 1(b) we plot the in-gap states for a case in the topological region ($w = 1$), where the system has undergone a topological phase transition (TPT) and a MBS appears at the edge of the chain for chains as short as five atoms. In Fig. 1(c) the system has gone through a new TPT, and it is again on the trivial phase. At the lower energies, states oscillate around zero as the number of atoms in the chain increases with a periodicity of ~ 5 atoms. These states are also localized at the edges, as shown in Ref. [43], however, the winding number shows they are topologically trivial. Finally, Fig. 1(d) depicts the evolution of edge states in the $w = -1$ topological phase. Here, the oscillations have a higher periodicity of ~ 60 atoms as well as two different branches that can be separated into even and odd number of atoms. These results show that the presence or absence of oscillating edge states around zero cannot be linked to the topology of the spin-chain phase.

Friedel oscillations arise from the presence of impurities on different substrates with extended electronic states such as on superconductors [36,44,45]. The oscillation follows the relation $\cos(2k_F r + \delta)$, where r is the electronic coordinate, k_F the Fermi wave vector, and δ a phase shift [36]. However, if we try to apply this to understand the periodicity observed in Fig. 1, the resulting oscillations should have a much shorter period than the ones we observe for the chains. Another surprising fact is that small changes of the interimpurity distance a_c or of k_F can lead to very large nonmonotonic variations of the period of the oscillations [43]. To understand these edge-state oscillations with system size, we develop a simple model.

The model considers the periodical effect of spins that are inducing in-gap states in the superconductor. The superconductor is subjected to an effective interaction that follows the behavior obtained in Ref. [37], $E_J = -\Delta \sin(k_F r)/k_F r e^{-r/\xi}$, where r is the spatial coordinate, Δ is the superconducting gap, and ξ the correlation length. On this simplified expression of the interaction exerted on the electronic states by the spins, we add the fact that the spins are regularly spaced, creating a 1D array of periodicity a_c that acts locally on the spin, Eq. (1). To approximately take into account the imposed locality of the spin interaction, we use a mask function that renders the interaction zero at all r values that do not match a spin site. This function $f(r)$ is in principle a comb of delta functions. To simplify, we take its first harmonic, $f(r) \approx \cos(2\pi r/a_c)$. Then the values of the YSR states of the spin chain appear at

$$E_{\text{YSR}}(r) = E_J \times f(r). \quad (2)$$

To understand the oscillations, we just take the oscillatory part of the above function that is

$$\sin(k_F r) \cos\left(\frac{2\pi r}{a_c}\right) = \frac{1}{2} \left[\sin\left(k_F r - \frac{2\pi r}{a_c}\right) + \sin\left(k_F r + \frac{2\pi r}{a_c}\right) \right]. \quad (3)$$

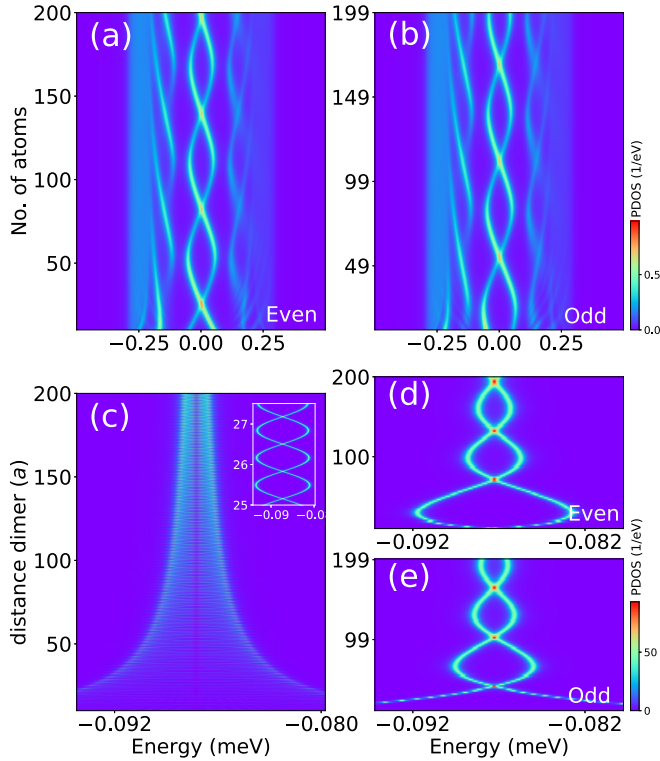


FIG. 2. Projected density of states (PDOS) on the edge atom of a spin chain as a function of the number of atoms in the chain for an (a) even and (b) odd number of atoms, respectively. When (a) and (b) are combined, we recover Fig. 1(d). (c) Dimer PDOS as the distance between the two atoms is varied in a continuous way. Inset: Zoom-in area between distances 25–27.5 a_c . The PDOS from (c) is plotted at selected distances in (d) and (e) corresponding to integer multiples of a_c , even and odd integers, respectively. This clearly shows that the observed oscillations are a consequence of the discrete sampling of the continuous PDOS in (c) and they match the periodicity of the oscillations in (a) and (b), revealing the moiré nature of the latter [the parameters are the same as in Fig. 1(d) and the above (a) and (b)].

This leads to the sum of two oscillations, one at a lower wave number $k_1 = k_F - \frac{2\pi}{a_c}$ and one at a higher wave number, $k_2 = k_F + \frac{2\pi}{a_c}$, explaining the overall behavior of the low-energy in-gap states with increasing size. The higher wave number k_2 is responsible for the even-odd effect, visible in Fig. 1(d). To better illustrate this, Figs. 2(a) and 2(b) depict the split PDOS for even and odd chain lengths, respectively. The split number is too high to be visible in the discrete lattice of the chain and thus results in an alternating signal when we add atoms to the chain, or to a fast atom-to-atom oscillation in the wave function [43]. The lower wave vector k_1 leads to the longer period oscillations.

To reveal the effect of spins on the superconductor, we plot the energy of the induced state as a function of the interspin distance. This is easily done by solving the Bogoliubov–de Gennes equations for a dimer on a jellium-like superconductor [26,33]. If the interspin distance r is continuously varied, we retrieve the behavior of E_J [Fig. 2(c)]. The obtained periodicity is the one given by $2\pi/k_F$, which has nothing to do with the one for the spin chains [Figs. 2(a) and 2(b)].

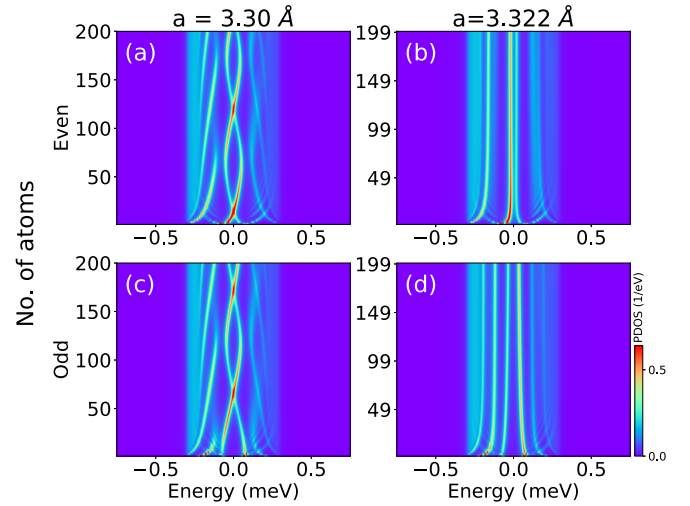


FIG. 3. PDOS on the edge atom of spin chains for *slightly* different interimpurity distances a_c . In the right panels, $a_c = 3.30$ Å, the period of the resulting oscillations is ~ 107 atoms, shown for (a) even and (c) odd numbers of atoms. In (b) and (d), $a_c = 3.322$ Å, we do not observe any evolution of the edge states as we vary the number of atoms. These plots can be compared with Figs. 2(a) and 2(b), $a_c = 3.36$ Å, where we find the period of the oscillations to be 60 atoms. The parameters other than a_c are the same as in Fig. 1(d).

But the periodicity agrees if we apply the mask for an even [Fig. 2(d)] or odd [Fig. 2(e)] number of lattice distances. The new periodicity is a consequence of how the approximately continuous in-gap interactions are sampled by the discrete spin chain.

We conclude that the observed oscillations can be rationalized by the presence of two periodical structures: One is the substrate-mediated oscillation, with a wave vector given by k_F , and the other one is the discrete spatial sampling by the spin chain, controlled by the interimpurity distance a_c giving a wave vector $2\pi/a_c$. The resulting periodic structure is a moiré pattern and the emerging periodicity depends on the two parameters k_F and a_c . As corresponds to moiré patterns, small changes in these two parameters can lead to large differences in the observed periods.

The high dependence of the resulting pattern on k_F and a also allows for tuning the period of the oscillations. We plot two different types of chains in Fig. 3, using *slightly* different lattice parameters. For $a_c = 3.30$ Å, we find again oscillating edge states that can be split into lengths of even and odd numbers of atoms. The period of the oscillations is found to be ~ 105 atoms. For chains with $a_c = 3.322$ Å, we find two sets of in-gap states that can be again divided into even and odd, but the periods of these two oscillations are very large. If we increase roughly by 1% the lattice parameter corresponding to the previous distance between impurities of $a_c = 3.36$ Å [same chains as in Figs. 2(a) and 2(b)] the oscillations are found to have a much smaller period, ~ 60 atoms. As a result of the underlying moiré pattern, small changes in a_c lead to drastically different periods. Very similar results are obtained for small variations in k_F , and the simple arithmetic stemming from Eq. (3) explains the drastic behavior of the oscillations [43].

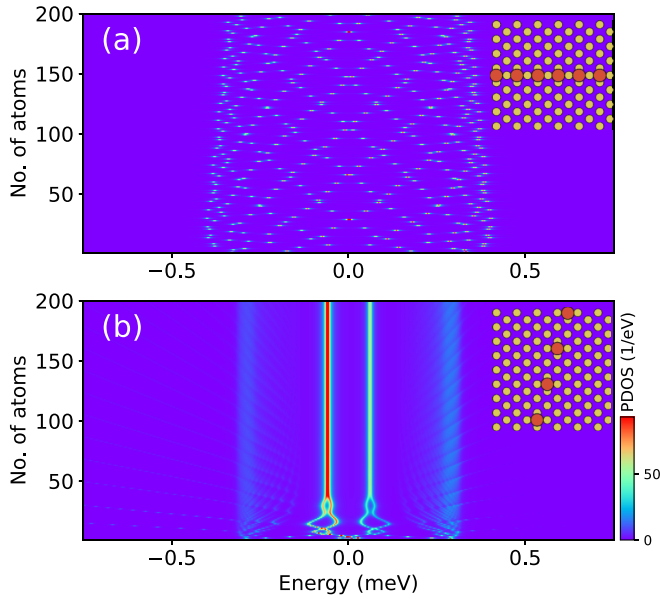


FIG. 4. PDOS obtained on the edge atom of Mn chains of increasing length on Nb (110). (a) The atomic chains are oriented along the $[1\bar{1}0]$ direction, resulting in a distance between impurities of $a_c = 4.67$ Å. (b) The chains are oriented along the $[\frac{1}{2}, \frac{1}{2}, \frac{5}{2}]$ direction, where the distance between impurities is $a_c = 8.56$ Å. The parameters of the calculation are $k_F = 0.1886a_0^{-1}$, such that $2\pi/k_F = 17.6$ Å roughly twice a_c , $J = 0.125$ eV, $\Delta = 1.5$ meV, $N_0 = 1.0$ eV $^{-1}$, $\alpha_R = 1.0$ eV Å, $K = 0.063$ eV, and $a = 3.294$ Å. The BCS correlation length is $\xi = 576$ Å. The insets show schemes of the crystal surface and the chain orientations.

A practical application of our calculations is to reproduce the experimental results by Schneider *et al.* [17]. These authors studied the in-gap states on Mn chains built along the $[1\bar{1}0]$ direction of a superconducting Nb (110) surface. They observed energy oscillations about zero as they increase the number of atoms in the chain with an even-odd behavior similar to the behavior of Figs. 2(a) and 2(b). In Fig. 4(a) we plot the calculated PDOS on the edge atom obtained using parameters extracted from Ref. [17]. Our results are in overall agreement with the experiment, in particular reproducing the even-odd behavior and the finite energy range of the in-gap states. However, if we compute the in-gap electronic structure

when the spin chains are oriented along the $[-\frac{1}{2}, \frac{1}{2}, \frac{5}{2}]$ direction, we obtain the results of Fig. 4(b). As we can observe, in this case the edge states do not evolve for chains longer than ~ 20 atoms, and they remain at a fixed finite energy. This behavior is a consequence of matching the spin-chain lattice parameter a_c to a multiple of $2\pi/k_F$ [43]. However, the matching is not perfect (about 2.05 times) and a simple use of Eq. (3) would give some oscillations that we do not observe in the actual calculation, showing that the effect is indeed more robust when evaluated without the approximations of Eq. (3). Choosing the growth direction of the spin chain on the surface permits us to tailor the dispersion of edge states with spin-chain length without the need for a mathematical match between the different periodical scales of the problem.

In summary, solving Bogoliubov–de Gennes equations for a local model of classical magnetic impurities on an s -wave superconductor predicts oscillations in the energy of edge states as a function of the length of the impurity chain. The origin of the period of the oscillation is a moiré pattern resulting from the discrete sampling produced by the spin chain on the spin-superconductor interaction. The sampling produces a natural wave number of $2\pi/a_c$ where a_c is the interimpurity distance, added on the spin-substrate interaction that itself oscillates with the substrate’s Fermi vector k_F . The origin of the edge-state oscillation is thus independent of its topological character. We have found that by modifying the spin-chain geometry, it is possible to tune the moiré pattern to display edge states at fixed finite energy. We predict that these nondispersive states can be realized on Mn chains on a Nb (110) crystal by assembling a spin chain along the $[-\frac{1}{2}, \frac{1}{2}, \frac{5}{2}]$ direction of the Nb (110) surface. It is then possible to create edge states with an important topological character [17] at fixed finite energies that are independent of the distribution of lengths in the creation of spin chains. The idea of having topological states at finite energy opens the door for a wider range of experiments involving MBS.

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- [43] See Supplemental Material at <http://link.aps.org/supplemental/10.1103/PhysRevResearch.4.L032010> for extra information on the decay length of MBS, profiles of MBS and low-energy modes, and the moiré behavior of wave functions, which includes Ref. [46].
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