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Topological Nodal Point Superconductivity in Checkerboard Magnet-Superconductor Hybrid Systems

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We demonstrate that checkerboard magnet-superconductor hybrid (MSH) systems possess a rich phase diagram exhibiting both strong topological superconducting (STSC) and topological nodal point superconducting (TNPSC) phases. We show that TNPSC phases exist both for ferromagnetic and antiferromagnetic systems, yielding a plethora of qualitatively different edge mode structures. Checkerboard MSH systems also facilitate the emergence of STSC phases which can be induced even in the limit of vanishing magnetization. Our results provide a new path for the quantum engineering of topological superconducting phases using atomic manipulation techniques.

Introduction Magnet-superconductor hybrid (MSH) systems provide a versatile platform for the quantum engineering of topological superconductivity and the ensuing Majorana zero modes. The versatility of MSH systems arises from the fact that their topological phase diagram can be manipulated by changing the MSH system's magnetic structure. While experimentally, only two-dimensional (2D) ferromagnetic (FM) [1–3] and antiferromagnetic (AFM) [4] MSH systems have been realized so far, intriguing topological phase diagrams – involving strong, weak and higher-order topological superconducting phases – have been theoretically proposed to exist in bicollinear AFM [5], skyrmionic [6], 3Q [7], and stacked magnetic structures [8]. Advances in atomic manipulation techniques [9, 10] have raised the intriguing possibility to quantum engineer MSH systems [2, 11] that interpolate between these various magnetic structures, potentially giving rise to intriguing new topological phase diagrams.

In this Letter, we consider one of these possibilities by studying MSH systems with two sublattices of different magnetic adatoms, yielding a checkerboard magnetic structure [see Fig. 1(a)]. We demonstrate that such systems possess a rich topological phase diagram, exhibiting not only strong topological superconducting (STSC) phases [12, 13] characterized by non-zero Chern numbers, but also extended regions of topological nodal point superconductivity (TNPSC) [5, 14–17]. The latter were recently reported to exist in the AFM MSH system Mn/Nb(110) [4], as well as in 4Hb-TaS₂ [18]. We show that TNPSC phases do not only exist in AFM checkerboard systems, but also in FM MSH systems where the AFM chiral symmetry is broken. Moreover, the interplay between the magnetic structures of edges and their real space direction yields a plethora of qualitatively different edge mode structures. We demonstrate that in checkerboard MSH systems STSC phases can be induced even in the limit of vanishing magnetization, in contrast to uniform FM MSH systems [12, 13]. Finally, we show that TNPSC phases can be created using a single species of

magnetic adatoms, simplifying their experimental realization. Our results provide a new path to quantum engineer topological superconducting phases using atomic manipulation techniques.

Theoretical Model To study an MSH systems with a magnetic checkerboard structure [see Fig. 1(a)], we consider a two-dimensional superconducting surface and magnetic layer with the same square lattice structure. The two sublattices of the magnetic layer are occupied by different types of magnetic adatoms, and the entire system is described by the Hamiltonian [12, 13]

$$\begin{aligned} \mathcal{H} = & -t \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle, \sigma} c_{\mathbf{r}, \sigma}^\dagger c_{\mathbf{r}', \sigma} - \mu \sum_{\mathbf{r}, \sigma} c_{\mathbf{r}, \sigma}^\dagger c_{\mathbf{r}, \sigma} \\ & + i\alpha \sum_{\mathbf{r}, \delta, \sigma, \sigma'} c_{\mathbf{r}, \sigma}^\dagger (\delta \times \sigma)_{\sigma, \sigma'}^z c_{\mathbf{r} + \delta, \sigma'} \\ & - \Delta \sum_{\mathbf{r}} \left(c_{\mathbf{r}, \uparrow}^\dagger c_{\mathbf{r}, \downarrow}^\dagger + c_{\mathbf{r}, \downarrow} c_{\mathbf{r}, \uparrow} \right) \\ & - \sum_{\mathbf{r}, \sigma, \sigma'} (J + J_{\mathbf{Q}} e^{i\mathbf{Q} \cdot \mathbf{r}}) c_{\mathbf{r}, \sigma}^\dagger \mathbf{S}_{\mathbf{r}} \cdot \sigma_{\sigma, \sigma'} c_{\mathbf{r}, \sigma'} . \end{aligned} \quad (1)$$

Here, the operator $c_{\mathbf{r}, \alpha}^\dagger$ creates an electron of spin α at site $\mathbf{r}$, $-t$ is the nearest-neighbor hopping amplitude, μ is the chemical potential, α is the Rashba spin-orbit coupling between nearest-neighbor sites $\mathbf{r}$ and $\mathbf{r} + \delta$, and Δ is the s -wave superconducting order parameter. The last term in Eq.(1) describes the coupling between the adatom's spin $\mathbf{S}_{\mathbf{r}}$ of magnitude S at site $\mathbf{r}$ and the conduction electrons, with exchange couplings $J \pm J_{\mathbf{Q}}$ in the two sublattices, and $\mathbf{Q} = (\pi, \pi)$ [for details, see Supplemental Material (SM) [19] Sec.I]. Due to the hard superconducting gap, which suppresses Kondo screening, we can consider the spins of the magnetic adatoms to be classical in nature [20, 21]. Below, we consider a somewhat large superconducting order parameter of $\Delta = 0.3t$ in order to ensure a localization length of the edge modes, $\xi_l \sim v_F/\Delta$, which is much smaller than the system size that we can consider numerically. However, the qualitative nature of our results remains unchanged by the particular value of Δ , see SM [19] Sec. II.

To characterize the strong topological phases, we compute its topological invariant, the Chern number, via [22]

$$C = \frac{1}{2\pi i} \int_{\text{BZ}} d^2k \text{Tr}(P_{\mathbf{k}}[\partial_{k_x} P_{\mathbf{k}}, \partial_{k_y} P_{\mathbf{k}}])$$

$$P_{\mathbf{k}} = \sum_{E_n(\mathbf{k}) < 0} |\Psi_n(\mathbf{k})\rangle \langle \Psi_n(\mathbf{k})| \quad (2)$$

where $E_n(\mathbf{k})$ and $|\Psi_n(\mathbf{k})\rangle$ are the eigenenergies and the eigenvectors of the Hamiltonian in Eq.(1), with n being a band index, and the trace is taken over Nambu, spin and sublattice space. Since STSC phases occur only for $J \neq 0$, they belong to the topological class D [16, 23, 24]. Finally, for antiferromagnetic TNPS phases ($J = 0$) the chiral symmetry of the system allows us to compute a topological charge and characteristic angle associated with nodal points (see SM [19] Sec. III). We note that trivial nodal point superconductivity was previously discussed in the context of antiferromagnetic semimetals [25].

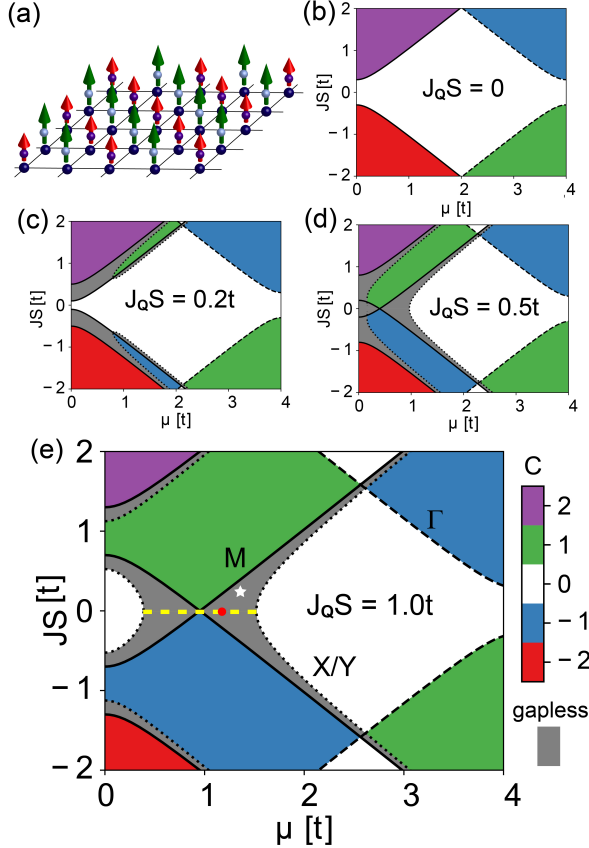


FIG. 1. (a) Schematic structure of the checkerboard magnetic structure with exchange couplings $J \pm \Delta J$ in the two sublattices. (b)-(e) Topological phase diagrams of the MSH system in the (μ, JS) -plane for different values of $J_Q S$ with $(\alpha, \Delta) = (0.2, 0.3)t$.

Results We begin by considering the topological phase diagram of the Hamiltonian in Eq.(1), which is presented

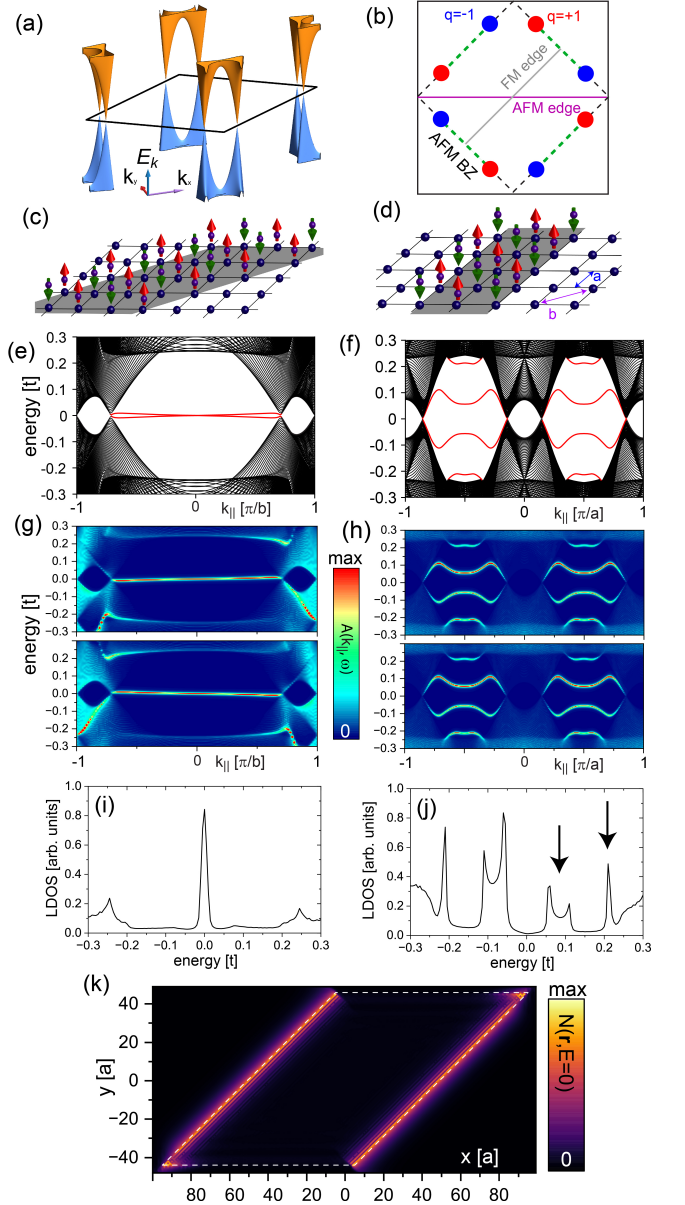


FIG. 2. (a) Energy dispersion of the bulk system in the magnetic BZ. (b) Nodal points and edge modes (dashed green lines) projected onto momenta parallel to the FM and AFM edges. Schematic representation of (c) diagonal (FM) and (d) vertical (AFM) edges. Electronic structure of a ribbon with (e) FM and (f) AFM edges. (g), (h) Spectral functions at the ribbon's left (upper panel) and right (lower panel) edges corresponding to (e) and (f). (i), (j) LDOS at the edges corresponding to (e) and (f). (k) Zero-energy LDOS of a magnetic island (dashed white line) with FM and AFM edges. $(\mu, \alpha, \Delta, JS, J_Q S) = (1.2, 0.2, 0.3, 0, 1.0)t$.

in Figs. 1(b)-(e) for different values of $J_Q S$ (the qualitative form of these phase diagrams is independent of the particular values of α and Δ , see SM [19] Sec. II). For simplicity, we confine our discussion to the $JS \geq 0$ part of the phase diagrams. In addition to the strong topo-

logical $C = 2, -1$ phases which are already present for $J_{\mathbf{Q}}S = 0$, two new features appear in the phase diagram with increasing $J_{\mathbf{Q}}S$. First, a $C = 1$ phase emerges due to the backfolding of the Brillouin zone (BZ), and the splitting of the bands at the X/Y -points. Secondly, an extended region of the phase diagram (shown in grey), lying between the gap closing lines of the M - (solid black line) and X/Y -points (dotted black line), becomes gapless (an analytic expression for the phase transition lines is given in SM [19] Sec. IV). As one moves in the gapless region between these two gap closing lines, the nodal points move along the magnetic BZ boundary from the M to the X/Y -points. For $J_{\mathbf{Q}}S \geq \sqrt{2\alpha^2 + \Delta_0^2}$, the strong topological $C = \pm 1$ phases touch at a single antiferromagnetic ($JS = 0$) point in the phase diagram with chemical potential $\mu_c = \sqrt{(J_{\mathbf{Q}}S)^2 - \Delta^2}$. At this point, any non-zero magnetization, which can be induced by arbitrarily small magnetic fields, pushes the system into a STSC phase, in contrast to uniform FM MSH systems, where $JS > \Delta$ is required [12, 13] for the emergence of strong topological phases.

To exemplify the electronic structure of an antiferromagnetic MSH system ($JS = 0$) in the gapless region around μ_c [yellow line in Fig. 1(e)], we consider a system with $\mu = 1.2t$ [red dot in Fig. 1(e)]. In Fig. 2(a) we present the resulting electronic structure exhibiting eight nodal points located along the boundary of the magnetic BZ. Due to the chiral symmetry of the system along the $JS = 0$ line, we find that these nodal points possess a non-zero topological charge $q = \pm 1$ [see Fig. 2(b)], the corresponding characteristic angles are shown in SM [19] Sec. III. The presence of nodal points with opposite topological charges allows for the emergence of edge modes connecting such nodal points [schematically shown as dashed green lines in Fig. 2(b)] in MSH systems exhibiting edges [5, 14–17]. When considering MSH systems in a ribbon geometry possessing diagonal ferromagnetic (FM) or vertical/horizontal antiferromagnetic (AFM) edges [see Figs. 2(c) and (d)], we find that their electronic structures indeed exhibit such in-gap edge modes as shown by red lines in Figs. 2(e) and (f), respectively. However, in contrast to an MSH system with AFM edges, the edge modes along FM edges disperse only weakly around zero-energy. To understand this qualitative difference, we note that the projection of the bulk band structure onto momenta parallel to either an FM or AFM edge leads to two overlapping (in momentum space) edge modes (see Fig. 2(b), and SM[19] Sec. V). These two edge modes can in general hybridize, and thus split in energy. The spectral functions at the FM and AFM edges, shown in the upper and lower panels of Figs. 2(g) and (h), respectively, for the two edges of each ribbon, provide insight into the different nature of the resulting edge modes. In contrast to the AFM edge, the edge mode along the FM edge is chiral in nature [13] (due to the broken time-reversal symmetry along

the edge) with opposite Fermi velocities on the two FM edges, as shown in Fig. 2(g). Thus, the two modes along the FM edges are spatially separated, and thus do not hybridize. In contrast, the spectral functions at the AFM

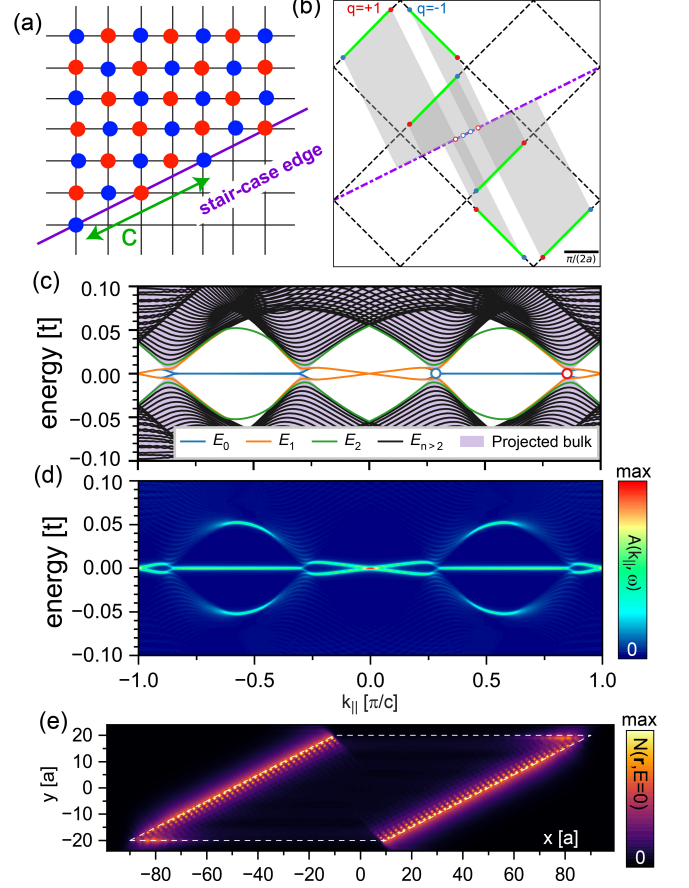


FIG. 3. (a) Schematic picture of a stair-case edge. (b) Projection of edge modes (green lines) connecting nodal points of opposite topological charge onto the momentum axis parallel to the stair-case edge (dashed-dotted purple line). Only projected nodes [open blue and red circles] for $-\pi/c \leq k_{||} \leq \pi/c$ are shown. Dark gray areas represent two overlapping projections. (c) Electronic structure of the ribbon, with projected nodal points shown in (b). (d) Edge spectral function. (e) Zero-energy LDOS for a magnetic island with horizontal and stair-case edges. Parameters are $(\mu, \alpha, \Delta, JS, J_{\mathbf{Q}}S) = (1.2, 0.2, 0.3, 0, 1.0)t$.

edges [see Fig. 2(h)] show that both modes exist at the same edge and thus strongly hybridize, leading to the much larger energy splitting. This qualitative difference leads to distinct signatures in the local density of states (LDOS) of FM and AFM edges: while the LDOS at an FM edge exhibits a large zero-energy peak [see Fig. 2(i)], the LDOS at the AFM edge exhibits only a low-energy V-like shaped LDOS [see Fig. 2(j)], with the signatures of the edge modes seen only at higher energies [see black arrows]. As a result, a spatial plot of the zero-energy LDOS of a finite magnetic island [see Fig. 2(k)] reveals

large spectral weight along the FM edges, and vanishing spectral weight along the AFM edges.

To obtain flat, non-dispersive edge modes, it is necessary to consider edges in real space such that the projected edge modes do not completely overlap in momentum space, as is the case for the FM and AFM edges (see SM [19] Sec. V). For example, by considering a stair-case like edge in real space [see Fig. 3(a)], we find that the resulting projection of the nodal points onto momenta parallel to the stair case edge [Fig. 3(b)] yields momentum regions with even and odd numbers of projected modes. In those regions where three projected modes overlap, one edge mode is non-dispersive and located at zero energy [see black arrows in Fig. 3(c)], while the other two projected modes hybridize and thus shift to higher energies. This is also confirmed by a plot of the edge spectral function shown in Fig. 3(d). As a result, a magnetic island that possesses both vertical and stair-case edges [see Fig. 3(e)] again shows a large zero-energy LDOS along the stair-case edges, and vanishing spectral weight along the vertical edges.

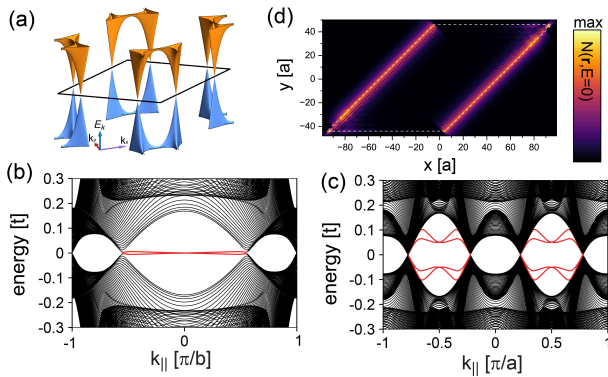


FIG. 4. (a) Energy dispersion of the bulk system in the magnetic BZ. Electronic structure of a ribbon with (b) FM and (c) AFM edges, as a function of momentum parallel to the edge. (d) Zero-energy LDOS of a magnetic island (dashed white line) with FM and AFM edges. $(\mu, \alpha, \Delta, JS, J_Q S) = (1.4, 0.2, 0.3, 0.25, 1.0)t$.

The question immediately arises whether the nature of the edge modes persists in those gapless regions of the phase diagram where the chiral symmetry of the AFM is broken due to a non-zero JS . To answer this question, we consider a system in the gapless region above the antiferromagnetic line, as indicated by a white star in Fig. 1(e). The electronic bulk structure of this system again reveals 8 nodal points along the magnetic BZ boundary, as shown in Fig. 4(a). The electronic dispersions for ribbons with FM and AFM edges [Figs. 4(b) and (c), respectively] reveal the same qualitative nature of the respective edge modes as in the $JS = 0$ case discussed in Fig. 2. However, since the chiral symmetry of the AFM edge is broken due to the non-zero JS , the double-degeneracy of the AFM edge modes is lifted, leading to

a further energy splitting among them. The zero-energy LDOS of a magnetic island [see Fig. 4(d)] thus again reveals large spectral weight along the FM edges, and vanishing spectral weight along the AFM edges. Similar results are obtained not only for any point in the gapless regions around μ_c [see Fig. 1(e)], but also in the gapless regions induced by much smaller values of $J_Q S$ [see Figs. 1(c),(d)], we conclude that checkerboard MSH systems are ideally suited to quantum engineer topological nodal point superconductivity as the occurrence of TNPSC phases does not require the fine-tuning of parameters. Of particular interest here are MSH systems with large Rashba spin-orbit coupling since the extent of gapless regions in the phase diagram increases with α (see SM [19] Sec. II). Our findings provide further support for the conclusion of recent scanning tunneling spectroscopy (STS) experiments [4] that the presence or absence of (near) zero-energy edge modes at various edges in the AFM MSH system Mn/Nb(110) are characteristic signatures of the underlying TNPSC phase.

A special case of the magnetic checkerboard structure arises when $J = J_Q$, implying that only a single species of magnetic adatoms is present in one of the two sublattices, as schematically shown in Fig. 5(a). In Fig. 5(b)

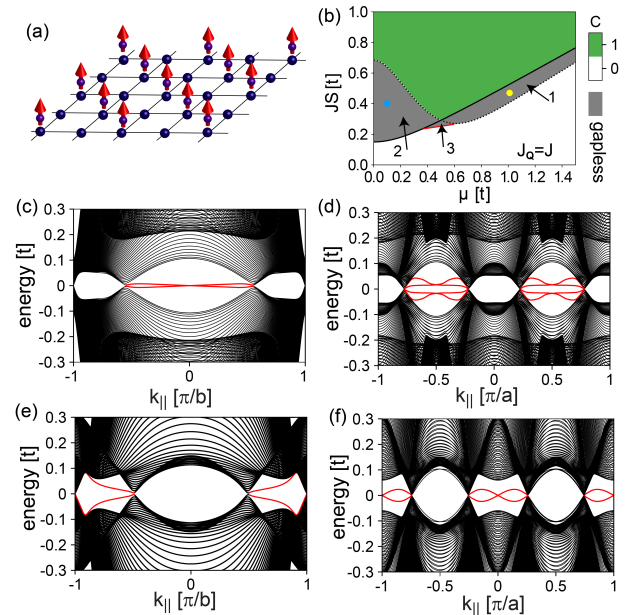


FIG. 5. (a) Schematic structure of the checkerboard magnetic structure for $J = J_Q$. (b) Topological phase diagram for $(\alpha, \Delta) = (0.2, 0.3)t$. Electronic structure of an MSH ribbon with (c),(e) FM and (d),(f) AFM edges for $(\mu, JS) = (1.0, 0.47)t$ [yellow dot in (b)], and $(\mu, JS) = (0.1, 0.4)t$ [blue dot in (b)], respectively.

we present the resulting phase diagram. In addition to the strong topological $C = 1$ phase, we obtain three types of gapless regions. Region 1 is entered from the gapped trivial ($C = 0$) region via a gap closing at the

X/Y -points. As a result, the edge modes connect the nodal points of opposite topological charge that are located on the same edge of the magnetic BZ. In this region, the electronic structure along FM and AFM edges [see Figs. 5(c) and (d)] is similar to that shown in Fig. 2. In contrast, the transition into region 2 from the trivial phase requires a gap closing at the M -points, which yields edge modes connecting the nodal points of opposite topological charge on neighboring edges of the magnetic BZ [see Figs. 5(e) and (f)]. In this case, neither edge shows a (nearly) non-dispersive edge mode, implying the absence of any pronounced zero-energy peak in the LDOS at the edges. Finally, the transition line into region 3 (red line) shows gap closings that vary along the magnetic BZ boundary between the M and X/Y -points. We thus conclude that by using a single species of magnetic adatoms, it is possible to create a TNPSC phase.

Discussion We have shown that checkerboard MSH systems are ideally suited to quantum engineer STSC as well as TNPSC phases, with the latter existing both for AFM ($J = 0$) and FM ($J \neq 0$) structures. The nature of edge modes in the TNPSC phases is determined by the projection of nodal points onto the edge momenta, and the magnetic structure of the edge. This allows for the emergence of edge modes that are dispersive in some momentum ranges, and non-dispersive (flat) in others. Our results further support the conclusions of recent STS experiments in the AFM MSH system Mn/Nb(110) [4] that the underlying TNPSC phase can be identified through the presence or absence of (near) zero-energy edge modes along different edges in the system. The finding that TNPSC can be created in checkerboard MSH systems where the chiral symmetry is broken, such as the ones discussed in Figs. 4 and 5, and that the characteristic dependence of edge modes on the edge structure persists, opens new classes of materials for the exploration of TNPSC. Advances in atomic manipulation techniques all but ensure that such checkerboard MSH systems and the ensuing TNPSC phases can be quantum engineered in the near future.

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