PHYSICAL REVIEW B **88**, 020407(R) (2013)

Proposal for realizing Majorana fermions in chains of magnetic atoms on a superconductor

S. Nadj-Perge, I. K. Drozdov, B. A. Bernevig, and Ali Yazdani*

Department of Physics, Joseph Henry Laboratories, Princeton University, Princeton, New Jersey 08544, USA

(Received 18 January 2013; published 25 July 2013)

We propose an easy-to-build easy-to-detect scheme for realizing Majorana fermions at the ends of a chain of magnetic atoms on the surface of a superconductor. Model calculations show that such chains can be easily tuned between trivial and topological ground states. In the latter, spatially resolved spectroscopy can be used to probe the Majorana fermion end states. Decoupled Majorana bound states can form even in short magnetic chains consisting of only tens of atoms. We propose scanning tunneling microscopy as the ideal technique to fabricate such systems and to probe their topological properties.

DOI: 10.1103/PhysRevB.88.020407 PACS number(s): 71.10.Pm, 03.67.Lx, 74.20.−z

The interest in topological quantum computing and non-Abelian braiding has inspired many recent proposals to create Majorana fermions (MFs) in various experimental systems. Following Kitaev's seminal proposal,[1] many approaches have been considered including those based on topological insulators,[2,3] atoms trapped in optical lattices,[4–6] semiconductors with strong spin-orbit interaction in two dimensions (2D) and one dimension (1D),[7–9] coupled quantum dots,[10,11] and those that combine magnetism of and superconductivity.[12–15] The aim of these approaches is to create a topological superconductor in which MFs emerge as the single excitations at the boundaries. Since MFs are their own antiparticles, they are predicted to appear in tunneling spectroscopy experiments as zero-bias peaks.[16–19] Such peaks have indeed been observed in several experiments and have been interpreted as the signatures of MFs.[20–22] However, these experiments are not spatially resolved to detect the position of the MFs. Additionally, in many instances, the presence of disorder can result in spurious zero-bias anomalies even when the system is not topological.[23,24] It is, therefore, desirable to identify easy-to-fabricate condensed-matter systems in which MFs can be spatially resolved and can be distinguishable from spurious disorder effects.

In this Rapid Communication, we theoretically investigate conditions for which a chain of magnetic atoms on the surface of an s-wave superconductor can host MF modes. We explore the parameter space for which this system is topological and show that even relatively short chains made of only ~ 50 atoms can host robust localized MFs. Our proposed structures can be fabricated using scanning tunneling microscopy (STM), which has previously been used to assemble structures of various shapes with tens of atoms using lateral atomic manipulation techniques.[25–27] Spatially resolved STM spectroscopy of such disorder-free chains can be used to probe the presence of MF end modes.

As shown in Fig. 1, we consider an array of magnetic atoms (such as atoms of $3d$ or $4f$ metals with a net magnetic moment), which are deposited on a single-crystal surface of an s-wave superconductor [such as niobium (Nb) or lead (Pb)] and are arranged into chains using the STM. The interaction of a single magnetic moment with the superconductor gives rise to the so-called Yu-Shiba-Rusinov states[28–31] that have previously been detected from both $3d$ and $4f$ atoms on the surface of Nb and Pb using an STM.[32,33] The results of these previous experiments (with Gd and Mn deposited on Nb) agree well with model calculations in which the magnetic moment is assumed to be static.[32,34,35] In addition, recent spin-polarized STM studies indicate that in magnetic arrays with $\gtrsim 10$ atoms spin dynamics is greatly suppressed.[36] It is, therefore, reasonable to model moments of magnetic atoms as static classical spins. In general, magnetic moments in these chains can form various configurations including a spiral.[37]

To describe this system we use a two-dimensional tight-binding model Hamiltonian of an s-wave superconductor with an array of magnetic atoms,

$$H = \sum_{\langle i,j\rangle\alpha}(t f_{i\alpha}^\dagger f_{j\alpha} + \mathrm{H.c.}) - \mu \sum_{i\alpha} f_{i\alpha}^\dagger f_{i\alpha} + \sum_{n\alpha\beta}(\vec{B}_n \cdot \vec{\sigma})_{\alpha\beta} f_{n\alpha}^\dagger f_{n\beta} + \sum_i (\Delta_i f_{i\uparrow}^\dagger f_{i\downarrow}^\dagger + \mathrm{H.c.}). \quad (1)$$

The operators f and $f^\dagger$ correspond to electron annihilation and creation, respectively, t is the hopping amplitude between adjacent sites $\langle i,j\rangle$ of a *two-dimensional* lattice, μ is the chemical potential, and Δ_i is the local superconducting gap associated with a host superconductor (equal to Δ_0 in the absence of magnetic atoms). The effective magnetic field $\vec{B}_n$ gives rise to a local Zeeman energy on the atoms which are arranged in a *one-dimensional* array of sites $\{n\}$. We consider the case of identical atoms, i.e., $|\vec{B}_n| = B$. Throughout this Rapid Communication, we normalize all simulation parameters to the value of Δ_0.

In order to obtain the two-dimensional gap profile in the vicinity of the atomic chain, we self-consistently solve the resulting Bogoliubov–de Gennes equations (BdG).[38] We assume a constant on-site pairing coupling V for a grid of $N_a \times N_b$ lattice sites in the middle of which N_a local magnetic moments with strength B are embedded (see Ref. 39, Sec. 1 for details). The calculations are performed with open boundary conditions (BCs) in the N_b direction and both open and periodic BCs in the N_a direction to show the presence or absence of MFs at the end of the chain and to compute the Pfaffian (Pf) index.[1] Previous calculations showed that a single magnetic moment gives rise to a state inside the superconducting gap that has an energy close to Δ_0 for low B. As the value of B is increased the energy of this state is continuously tuned to zero.[34,35,40] This zero crossing is a signature of a quantum phase transition at which the impurity site traps a single quasiparticle.[29,41] A similar phase transition

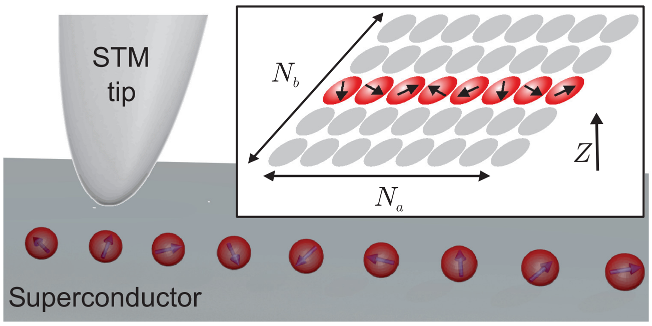

FIG. 1. (Color online) Schematic of the experimental setup. An array of magnetic atoms (red spheres) is assembled using a scanning tunneling microscope on the surface of the s-wave superconductor (gray background). The system is modeled by the two dimensional $N_a \times N_b$ array in which magnetic atoms are embedded (inset). Throughout the paper we consider the case where magnetic moments are in the plane defined by the N_a and Z directions.

occurs in the case of a few magnetic moments.[40,42] The transition obviously coincides with a change in the sign of the Pfaffian (computed in a periodic geometry) for the system, indicating a change in the fermion parity in the ground state. This is the characteristic signature of a topological nontrivial phase with MF end modes.[1]

An example of a transition into a topologically nontrivial phase for our atomic chain is illustrated in Fig. 2, which shows the lowest-energy level and the Pfaffian as a function of B in the case of 96 magnetic moments. The angle between adjacent magnetic moments θ plays a key role in determining whether this system is topological (see below) and has been assumed to be $2\pi/3$ for the results shown in Fig. 2. The most important feature of this calculation is that in the parameter window $2.2 < B/\Delta_0 < 3.45$ in which for periodic BCs in the N_a direction the Pfaffian is negative, and the spatial extent of the lowest excited state [Fig. 2(b)] (for open BCs) shows the presence of MFs at the ends of the chain. This behavior can be contrasted with that of $B/\Delta_0 = 2.1$ [Fig. 2(c)]. In this case Pfaffian is positive and the lowest-energy excitation is distributed approximately evenly along the chain. A calculation of the local density of states (LDOS) as a function of energy shown in Fig. 2(d) clearly demonstrates that the topological case shows a zero-bias peak associated with MFs when tunneling at the end of the chain, whereas, the middle of the system exhibits a minigap. In the nontopological phase sufficiently far away from the transition point, the system shows a clear gap throughout the chain and the absence of zero energy end modes [Fig. 2(e)].

The emerging MF end modes considered here are localized on a very short length scale at the last few sites of the atomic chain. This situation can be contrasted to the proposals involving semiconductor nanowires in proximity with superconductors where the coherence length of the superconductor sets the length scale for MFs.[9] The spatial extent of our MFs is reminiscent of the extent of the Yu-Shiba-Rusinov states created by single atoms, which have been shown both experimentally and theoretically to decay on length scales associated with the Fermi wavelength of a superconductor.[32,35] Note that these states do have long tails associated with the superconducting coherence length, however, this decay is strongly enhanced with an algebraic decay prefactor.[34,35]

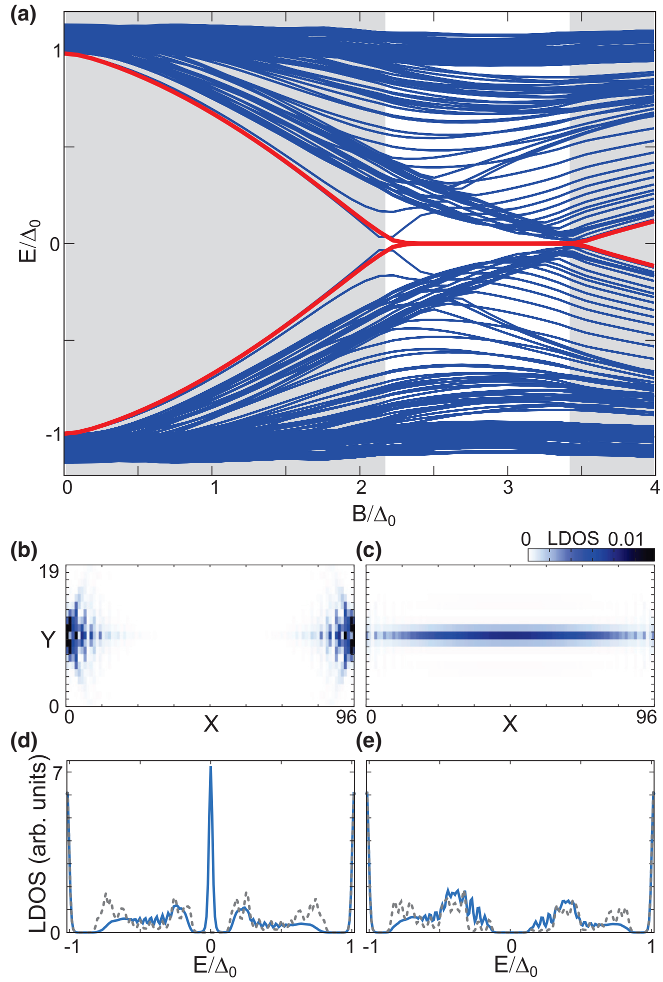

FIG. 2. (Color online) (a) Calculated energy spectrum, marked by blue lines for 96 classical spins placed in the middle of the $N_a \times N_b = 96 \times 19$ grid using periodic BCs. Parameters for the plot are as follows: $\mu/\Delta_0 = 2.12$, $t/\Delta_0 = 2.34$, $V/\Delta_0 = 2.81$, and $T/\Delta_0 = 0.01$. The regions corresponding to the trivial phase (Pf > 0) are shaded gray. The red thick line represents the lowest-energy excitation using open BCs. (b) and (c) The spatial distribution of the local density of states corresponding to the lowest excitation state in the nontrivial ($B/\Delta_0 = 2.87$, Pf < 0) and the trivial ($B/\Delta_0 = 2.23$, Pf > 0) phase. Lattice coordinates X and Y correspond to the N_a direction (along the chain) and N_b direction (orthogonal to the chain), respectively. (d) and (e) Local density of states at the chain ends (blue solid line) and in the middle of the chain (gray dashed line) as a function of energy for nontrivial and trivial phases taking into account the first 96 energy eigenvalues. The intrinsic linewidth of the energy eigenstates is taken to be $\omega/\Delta_0 = 1 \times 10^{-3}$ for this plot.

Although we used a self-consistent BdG calculation for realistic modeling of the experimental situation, a more efficient approach to gain physical insight into this system is to consider an effective 1D model of magnetic atoms on superconducting sites, which is just the $N_b = 1$ limit of our 2D model. Note that in 1D, all information about the superconductor is simply included in the strength of the on-site s-wave gap Δ_0 and the hopping term describes

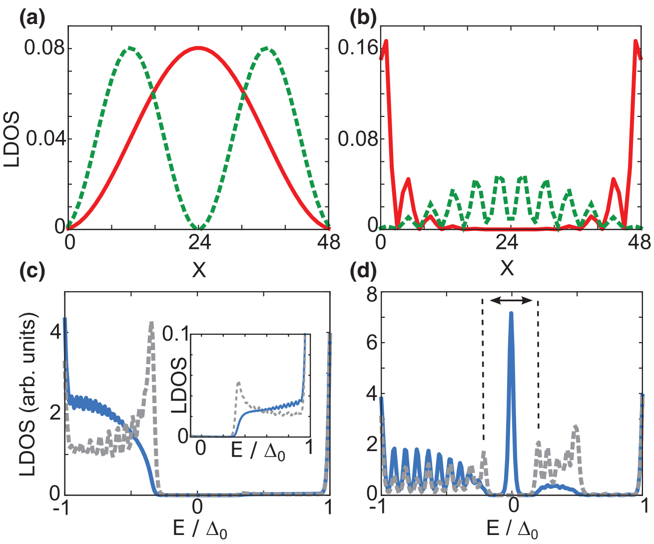

FIG. 3. (Color online) (a) and (b) The spatial profile of the two lowest excitation states of the magnetic chain containing 48 atoms for $\mu/\Delta_0 = 4$, $B/\Delta_0 = 5$, and $\theta = \pi/2$ (marked by red solid and green dashed lines, respectively). Tuning the hopping term t drives quantum phase transition from the (a) trivial ($t/\Delta_0 = 0.4$, Pf > 0) to the (b) topological ($t/\Delta_0 = 1$, Pf < 0) phase. (c) and (d) Local density of states calculated for the same parameters as in (a) and (b) at the chain ends (blue solid line) and in the middle of the chain (gray dashed line). Note that for this choice of parameters spectrum in (c) is asymmetric in energy (see inset). Importantly, in (d) the two MF states around zero energy are separated by the effective minigap Δ_p from the other states in the spectrum (marked by the double arrow line).

coupling between the impurities on superconducting sites only (as opposed to the superconductor bandwidth in the BdG model above, see Ref. 39, Sec. 2). Figure 3 shows that a 1D model qualitatively gives similar results as the 2D model. Importantly, the hopping term, which can be tuned experimentally by placing atoms at different distances, may also drive quantum phase transition from the trivial phase (Pf > 0) to the topological phase (Pf < 0) with MFs at the ends. A one-dimensional version of this Hamiltonian is also considered in Ref. 12 in the context of MFs in disordered magnetic islands on a superconductor.

A key advantage of the 1D model is that it lends itself to an analytical solution, which shows that for a given angle θ between adjacent moments, the Pfaffian for the system is negative when

$$\sqrt{\Delta_0^2 + [|\mu| + 2|t\,\cos(\theta/2)|]^2} > |B|,$$
$$|B| > \sqrt{\Delta_0^2 + [|\mu| - 2|t\,\cos(\theta/2)|]^2} \qquad (2)$$

(see Ref. 39, Sec. 3 for the derivation). The negative value of the Pfaffian is a necessary condition for this system to be in a topological phase; however, it not sufficient, as the bulk of the atomic chain remains must also be gapped. For example, $\theta = 0,\pi$ have the widest range of negative Pfaffian in Eq. (2); unfortunately, this full range is gapless. The minigap for the low-energy excitation is related to the strength of the p-wave pairing that emerges on the chain because of the combination of

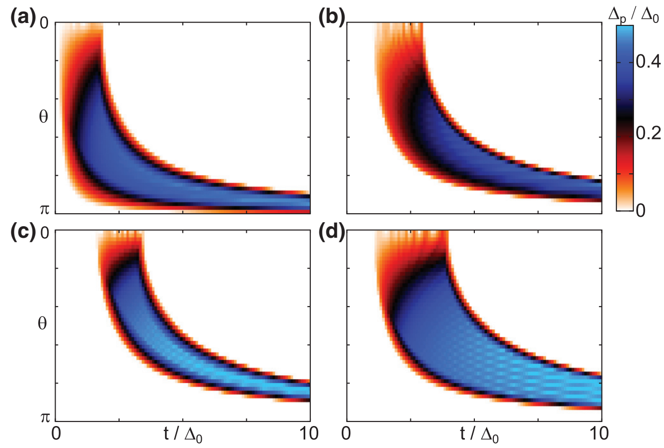

FIG. 4. (Color online) The value of the minigap as a function of tunnel coupling and angle θ calculated for the 1D model: (a) $\mu/\Delta_0 = 2$ and $B/\Delta_0 = 3$; (b) $\mu/\Delta_0 = 2$ and $B/\Delta_0 = 5$; (c) $\mu/\Delta_0 = 5$ and $B/\Delta_0 = 2$; (d) $\mu/\Delta_0 = 5$ and $B/\Delta_0 = 4$.

hopping, pairing, and local Zeeman terms in the Hamiltonian. Calculations of the spectra in both 2D and 1D models described above reveal the energy scale, which separates the zero energy MF states (localized at the two ends) from the next available excitation of the system. In a certain limit, the 1D model can be directly mapped[12] to the original proposal by Kitaev for realization of the MF end mode, which is a superconducting wire with nearest-neighbor pairing,[1] but general eigenvalues can be obtained even without this mapping, see Ref. 39, Sec. 2. The value of this minigap depends on the relative values of μ, t, B, and angle θ (see Fig. 4).

A noncollinear arrangement of magnetic moments in a chain is essential to realize robust MF end modes. When transformed to a basis parallel to the spiraling on-site magnetic field, the hopping becomes spin dependent giving rise to spin-orbit coupling and, hence, to the usual mechanisms for MF end modes. Without detailed modeling of the surface magnetism it is difficult to predict whether specific magnetic atomic chains would have a spiral spin arrangement. We suggest that exploring the full freedom of the linear chain geometry may provide a feasible approach to create favorable conditions for noncollinear magnetic moments of adjacent atoms. For example, double or zigzag chain structures with antiferromagnetic interactions are likely to become frustrated and result in spiral orientation of magnetic moments in the chain.[37] To explore some of these possible geometries [Fig. 5(a)], we map these chains into equivalent linear chains

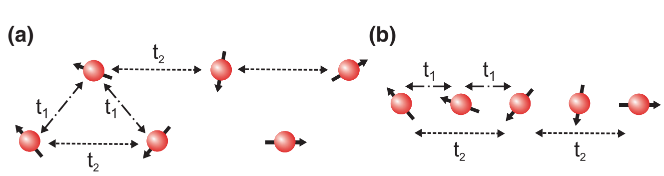

FIG. 5. (Color online) (a) Array of magnetic atoms arranged in two rows (zigzag chain). The coupling among neighboring atoms corresponding to different rows is t_1, and the coupling between atoms within the same row is t_2. (b) Equivalent magnetic moment configuration represented as a single chain with the next-nearest coupling.

with the nearest t_1 and the next nearest t_2 hopping as shown in Fig. 5(b). In the simplest case for which θ is assumed constant, we show that these chains can also support the topological phase when

$$\begin{gathered}\sqrt{\Delta_0^2 + [\mu + 2\cos(\theta/2)t_1 - 2\cos(\theta)t_2]^2} > |B|,\\ |B| > \sqrt{\Delta_0^2 + [\mu - 2\cos(\theta/2)t_1 - 2\cos(\theta)t_2]^2}\end{gathered} \tag{3}$$

(see Ref. 39, Sec. 3a for further details). We note again that these chains may provide easy-to-fabricate structures that would ensure noncollinear spin arrangements required for the realization of MF end modes.

Lastly, we comment on the experimental feasibility of the proposed approach. As shown here the strength of the minigap associated with the p-wave pairing can sometimes exceed 30%–40% of the gap of the host superconductor (Fig. 4). Nevertheless, using an s-wave superconductor with large gap Δ_0 (and measuring at the lowest temperatures) would increase the chance of experimental success. Other factors, such as size of the magnetic moment B or hopping matrix element t are also important and can be optimized experimentally using magnetic atoms with different spin or building chains with different spacing. A systematic experimental approach can start by characterizing the single-impurity states and their modification when impurities are brought close enough to interact.[33] These measurements could be used to map effective 1D model parameters (effective hopping, chemical potential, and exchange coupling) and could allow investigation of the finite-size effects on the excitation spectrum. A different approach would be to start from magnetic chains grown using self-assembled techniques. Note that self-assembled chains consisting of ∼50 atoms with spiral arrangements of magnetic moments are already reported.[37] Such chains would be an ideal starting point to investigate interaction between Majorana fermions. For example, examining coupled chains can provide direct experimental means to demonstrate the Z_2 character of the MF end modes by showing that they appear only in odd numbers of coupled chains. Finally, as structures of different shapes are equally easy to assemble in STM, one can envision a viable route towards braiding experiments in arrays of coupled chains in a similar fashion as proposed for semiconductor nanowire structures.[43–45]

We thank R. Lutchyn and J. Seo for the discussions. This work was supported by NSF-DMR1104612 and NSF-MRSEC programs through the Princeton Center for Complex Materials (Grant No. DMR-0819860), ONR, ARO, and DARPA-SPAWAR Grant No. N6601-11-1-4110. S.N.-P. acknowledges support from the European Community under a Marie-Curie OEF fellowship. B.A.B. acknowledges support from the programs CAREER Grants No. DMR-095242, No. ONR-N00014-11-1-0635, and No. ARMY-245-6778 and the Packard Foundation.

*Corresponding author: yazdani@princeton.edu

[1] A. Y. Kitaev, Phys. Usp. **44**, 131 (2001).
[2] L. Fu and C. L. Kane, Phys. Rev. Lett. **100**, 096407 (2008).
[3] A. R. Akhmerov, J. Nilsson, and C. W. J. Beenakker, Phys. Rev. Lett. **102**, 216404 (2009).
[4] M. Sato, Y. Takahashi, and S. Fujimoto, Phys. Rev. Lett. **103**, 020401 (2009).
[5] S. Diehl, E. Rico, M. A. Baranov, and P. Zoller, Nat. Phys. **7**, 971 (2011).
[6] L. Jiang, T. Kitagawa, J. Alicea, A. R. Akhmerov, D. Pekker, G. Refael, J. I. Cirac, E. Demler, M. D. Lukin, and P. Zoller, Phys. Rev. Lett. **106**, 220402 (2011).
[7] J. D. Sau, R. M. Lutchyn, S. Tewari, and S. Das Sarma, Phys. Rev. Lett. **104**, 040502 (2010).
[8] R. M. Lutchyn, J. D. Sau, and S. Das Sarma, Phys. Rev. Lett. **105**, 077001 (2010).
[9] Y. Oreg, G. Refael, and F. von Oppen, Phys. Rev. Lett. **105**, 177002 (2010).
[10] J. D. Sau and S. Das Sarma, Nat. Commun. **3**, 964 (2012).
[11] I. C. Fulga, A. Haim, A. R. Akhmerov, and Y. Oreg, New J. Phys. **15**, 045020 (2013).
[12] T.-P. Choy, J. M. Edge, A. R. Akhmerov, and C. W. J. Beenakker, Phys. Rev. B **84**, 195442 (2011).
[13] S. Gangadharaiah, B. Braunecker, P. Simon, and D. Loss, Phys. Rev. Lett. **107**, 036801 (2011).
[14] I. Martin and A. F. Morpurgo, Phys. Rev. B **85**, 144505 (2012).
[15] M. Kjaergaard, K. Wölms, and K. Flensberg, Phys. Rev. B **85**, 020503 (2012).
[16] K. T. Law, P. A. Lee, and T. K. Ng, Phys. Rev. Lett. **103**, 237001 (2009).
[17] K. Flensberg, Phys. Rev. B **82**, 180516 (2010).
[18] J. D. Sau, S. Tewari, R. M. Lutchyn, T. D. Stanescu, and S. Das Sarma, Phys. Rev. B **82**, 214509 (2010).
[19] M. Wimmer, A. R. Akhmerov, J. P. Dahlhaus, and C. W. J. Beenakker, New J. Phys. **13**, 053016 (2011).
[20] V. Mourik, K. Zuo, S. M. Frolov, S. R. Plissard, E. P. A. M. Bakkers, and L. P. Kouwenhoven, Science **336**, 1003 (2012).
[21] A. Das, Y. Ronen, Y. Most, Y. Oreg, M. Heiblum, and H. Shtrikman, Nat. Phys. **8**, 887 (2012).
[22] M. T. Deng, C. L. Yu, G. Y. Huang, M. Larsson, P. Caroff, and H. Q. Xu, Nano Lett. **12**, 6414 (2012).
[23] J. Liu, A. C. Potter, K. T. Law, and P. A. Lee, Phys. Rev. Lett. **109**, 267002 (2012).
[24] D. I. Pikulin, J. P. Dahlhaus, M. Wimmer, H. Schomerus, and C. W. J. Beenakker, New J. Phys. **14**, 125011 (2012).
[25] M. F. Crommie, C. P. Lutz, and D. M. Eigler, Science **262**, 218 (1993).
[26] S. Fölsch, P. Hyldgaard, R. Koch, and K. H. Ploog, Phys. Rev. Lett. **92**, 056803 (2004).
[27] N. Nilius, T. M. Wallis, and W. Ho, Science **297**, 1853 (2002).
[28] L. Yu, Acta Phys. Sin. **21**, 75 (1965).
[29] H. Shiba, Prog. Theor. Phys. **40**, 435 (1968).
[30] A. I. Rusinov, Sov. Phys. JETP **29**, 1101 (1969).
[31] A. V. Balatsky, I. Vekhter, and J.-X. Zhu, Rev. Mod. Phys. **78**, 373 (2006).

[32] A. Yazdani, B. A. Jones, C. P. Lutz, M. F. Crommie, and D. M. Eigler, Science **275**, 1767 (1997).

[33] S.-H. Ji, T. Zhang, Y.-S. Fu, X. Chen, X.-C. Ma, J. Li, W.-H. Duan, J.-F. Jia, and Q.-K. Xue, Phys. Rev. Lett. **100**, 226801 (2008).

[34] M. E. Flatté and J. M. Byers, Phys. Rev. Lett. **78**, 3761 (1997).

[35] M. I. Salkola, A. V. Balatsky, and J. R. Schrieffer, Phys. Rev. B **55**, 12648 (1997).

[36] S. Loth, S. Baumann, C. P. Lutz, D. M. Eigler, and A. J. Heinrich, Science **335**, 196 (2012).

[37] M. Menzel, Y. Mokrousov, R. Wieser, J. E. Bickel, E. Vedmedenko, S. Blügel, S. Heinze, K. von Bergmann, A. Kubetzka, and R. Wiesendanger, Phys. Rev. Lett. **108**, 197204 (2012).

[38] P. D. Sacramento, V. K. Dugaev, and V. R. Vieira, Phys. Rev. B **76**, 014512 (2007).

[39] See Supplemental Material at http://link.aps.org/supplemental/10.1103/PhysRevB.88.020407 for more information about details of the calculation.

[40] D. K. Morr and N. A. Stavropoulos, Phys. Rev. B **67**, 020502 (2003).

[41] T. Soda, T. Matsuura, and Y. Nagaoka, Prog. Theor. Phys. **38**, 551 (1967).

[42] D. K. Morr and J. Yoon, Phys. Rev. B **73**, 224511 (2006).

[43] J. Alicea, Y. Oreg, G. Refael, F. von Oppen, and M. P. A. Fisher, Nat. Phys. **7**, 412 (2011).

[44] B. I. Halperin, Y. Oreg, A. Stern, G. Refael, J. Alicea, and F. von Oppen, Phys. Rev. B **85**, 144501 (2012).

[45] B. van Heck, A. R. Akhmerov, F. Hassler, M. Burrello, and C. W. J. Beenakker, New J. Phys. **14**, 035019 (2012).