Two-dimensional $p$-wave superconducting states with magnetic moments on a conventional $s$-wave superconductor

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(Dated: May 7, 2014)

Unconventional superconductivity induced by the magnetic moments in a conventional spin-singlet $s$-wave superconductor is theoretically studied. By choosing the spin directions of these moments, one can design spinless pairing states appearing within the $s$-wave superconducting energy gap. It is found that the helix spins produce $p_x + p_y$-wave state while the skyrmion crystal configuration $p_x + ip_y$-wave like state. Nodes in the energy gap and the zero energy flat band of Majorana edge states exist in the former one, while the chiral Majorana channels along edges of the sample and the zero energy Majorana bound state at the core of the vortex appear in the latter case.

PACS numbers: 74.45.+c, 74.20.-z, 74.78.-w

Introduction.— Unconventional superconducting states are one of the most important issues in current condensed matter physics.$^{1-3}$ Although most of the superconductors show the conventional spin-singlet $s$-wave pairing, strongly correlated materials sometimes show unconventional pairing since the on-site pairing is suppressed by the repulsive interaction. However, the discovery of the unconventional pairings relies on serendipity to some degree, and their theoretical designs and artificial fabrications are highly desired. Especially, recent intensive interest in the topological superconductivity and consequent Majorana fermions enhance the importance of this topics since Majorana fermions are the leading candidate for the platform of the quantum computation.$^{4-9}$

A promising proposal for realization of a topological superconducting state is the combined system of semiconducting nanowire with $s$-wave superconductor under an external magnetic field. The spin-orbit interaction and the magnetic field reduce the degrees of freedom of electrons concerning superconducting states, and effectively generate spinless $p$-wave superconductor.$^{10-14}$ As for one-dimensional system, signals suggesting Majorana fermions at the ends of the nanowire have been observed in some experimental setups.$^{15-18}$ There are other routes for creating topological superconductors; spin-singlet superconductor deposited on the topological insulator,$^{19,20}$ superfluid of cold atoms with laser-generated effective spin-orbit interaction,$^{21}$ aligned quantum dots connected by $s$-wave superconductors,$^{22}$ and magnetic moments in $s$-wave superconductors$^{23-26}$ or nodal superconductors.$^{27}$ The last ones are significantly distinct in that they don’t explicitly require spin-orbit interaction in the system. With respect to the cooperation between magnetic moment and superconductivity, it has been known that the bound states are created around the impurities with the energy inside the bulk superconducting gap (not necessarily zero energy).$^{28-30}$ The modulation of the local density of states by a single magnetic impurity has been observed in the experiment.$^{31}$ The authors of Refs 24 and 26 considered the one-dimensional array of the magnetic impurities, and studied the possibility of Kitaev state with the Majorana bound states at the ends of the array. The influence of magnetic moments on a superconductor by the proximity effect has been intensively studied albeit in different interests.$^{32-34}$ On the other hand, it has been recognized that the spin-orbit interaction at the interface results in Rashba type interaction and hence non-collinear spin configuration is organized.\footnote{Especially, the skyrmion crystal state is observed at the interface of Fe and Ir.\cite{36}} Therefore, the magnetic proximity effect of non-collinear moments to a superconductor becomes a realistic and important issue.

In this paper, we propose a generic principle to design unconventional superconductivity in terms of non-collinear/non-coplanar configurations of magnetic moments on the surface of an $s$-wave superconductor. We derive an effective model constituted from the bound states around magnetic moments. The effective pair potentials as well as transfer integrals in the effective model depend on the directions of two neighboring moments. We show that a $p_x + p_y$-wave pairing state with nodes in the energy gap is generated by a non-collinear helical spin configuration, and moreover, we design a topological $p_x + ip_y$-wave like state by means of a non-coplanar skyrmion crystal configuration of moments, as evidenced by chiral Majorana channels along the edges of the system and zero energy Majorana bound states at the cores of vortices.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig1.png}
\caption{(a) Schematic illustration for the formation of an effective lattice model from the bound states localized around magnetic moments on the surface of $s$-wave superconductor (see Eq. (3)). \(b\) Energy levels of quasiparticles obtained by a tight binding model calculation with a single moment with $\Delta_0/t = 0.7$ in Eq. (1). $J$ is the coupling constant between electrons and magnetic moment and $S$ is the magnitude of the spin moment. The solid (blue) curve shows the analytical solution $E_0$ for the continuum model (see the main text).}
\end{figure}
Model.— Figure 1 (a) shows a schematic illustration of the present model. We analyze the following tight-binding Hamiltonian describing double exchange model with the superconducting order parameter defined on a square lattice

\[
H = - \sum_{\langle ij \rangle \sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} - \sum_i \mu_i c_{i\sigma}^\dagger c_{i\sigma} + \sum_i \Delta_0 \left( c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger + \text{H.c.} \right) - \sum_i JS_i \cdot \sigma_{\alpha \beta} c_{i\alpha}^\dagger c_{i\beta}.
\]

(1)

The first three terms describe a conventional spin-singlet s-wave superconductor with the transfer integral \(t\), the chemical potential \(\mu\), and the pairing potential \(\Delta_0\). In addition, electrons couple with magnetic moments located at sites \(i\)'s with the strength \(J\) through double exchange mechanism. This model can describe the interface between a bulk s-wave superconductor and a magnetic material. We assume that the pairing potential is not affected by magnetic moments, which are supposed to be solidly ordered. Below we construct unconventional superconducting states with some particular structures of magnetic moments. We derive an effective model in the aim of choosing appropriate magnetic order for intended unconventional states before directly solving Eq. (1). First, we start with the case of a single moment in a superconductor. The Bogoliubov-de Gennes equations are given by

\[
(\xi_k - E)u_k^\dagger - \frac{J S}{V} \sum_i u_i^\dagger + \Delta_0 v_k^\dagger = 0,
\]

\[(\xi_k + E)v_k^\dagger - \frac{J S}{V} \sum_i v_i^\dagger - \Delta_0 u_k^\dagger = 0,
\]

(2)

where we set the origin at the site of moment, \(h = 1\), and \(\xi(k) = -2t(\cos k_x + \cos k_y) - \mu\) is the tight-binding dispersion. The numerical result of energy level is shown in Fig. 1 (b). The dispersion can be approximated in the continuum limit as \(\xi(k) = \frac{k^2}{2m} - \mu - 4t\) with \(m = (2t)^{-1}\). We can find solutions with energy \(\pm E_0 = \pm \Delta_0 \frac{1}{2} \sqrt{1 - (\pi JS N_0/2)^2} / (1 + (\pi JS N_0/2)^2}\), where \(N_0\) is the density of states in the normal phase \((1 - \Delta_0)/\Delta_0\) and within the bulk superconducting energy gap. The corresponding wave functions are real and asymptotically given for \(r \to \infty\) as

\[
u_\uparrow(r) \sim \frac{\sin(p_F r - \delta_+)}{p_F r} \exp \left[-\frac{r}{\xi_0} \left| \sin(\delta_+ - \delta_-) \right| \right],
\]

\[
u_\downarrow(r) \sim \frac{\sin(p_F r - \delta_-)}{p_F r} \exp \left[-\frac{r}{\xi_0} \left| \sin(\delta_- - \delta_) \right| \right],
\]

(3)

where we define some quantities; \(\tan \delta_{\pm} = \pm \pi JS N_0 / 2\), \(p_F\) is the Fermi momentum, \(v_F = p_F / m\) is the Fermi velocity, and \(\xi_0 = v_F / (\pi \Delta)\). When the moments are aligned in a lattice, we expect that the bound state around each moment has overlap with neighboring bound states. The overlap causes effective transfer integrals and pair potentials among the bound states. The low energy properties, i.e., in the bulk superconducting gap, can be described by an effective BdG lattice model constructed from these bound states. One can find similar arguments in Refs. 24–26.

Design of p-wave superconducting states.— We propose a principle to design the superconducting states appearing within the gap of the host spin-singlet s-wave superconductor. It will be shown that configurations of magnetic moments play the essential role for the emergence of unconventional superconducting states. In the last section, we assume the magnetic moment parallel to +z-direction. Here, we introduce a unitary transformation for the description of general directions of moments. The coupling term with magnetic moments in Eq. (1) can be transformed as

\[
\psi^\dagger \alpha \sigma S \cdot \sigma_{\alpha \beta} \psi_\beta = (U \psi)^\dagger U S \cdot \sigma \psi^\dagger U \psi = \widetilde{\psi} \sigma \psi
\]

by the unitary matrix

\[
U = \begin{pmatrix}
\cos \frac{\theta}{2} & -e^{-i\phi} \sin \frac{\theta}{2} \\
e^{i\phi} \sin \frac{\theta}{2} & \cos \frac{\theta}{2}
\end{pmatrix}
\]

(5)

where \(\theta\) and \(\phi\) are the polar coordinates such that \(S = S(\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta)\). The wave functions for arbitrary spin directions are obtained by operating \(U^\dagger\) on Eqs. (3). Then, the electron operators are expressed for the low energy sector as

\[
u_\uparrow = \sum_i \left[ \cos \frac{\theta_i}{2} u^\dagger_i (r - r_i) \alpha_i - e^{-i\phi_i} \sin \frac{\theta_i}{2} v^\dagger_i (r - r_i) \alpha^\dagger_{i}\right],
\]

\[
u_\downarrow = \sum_i \left[ e^{i\phi_i} \sin \frac{\theta_i}{2} u^\dagger_i (r - r_i) \alpha_i + \cos \frac{\theta_i}{2} v^\dagger_i (r - r_i) \alpha^\dagger_{i}\right],
\]

(6)

where \(\alpha_i\) is the annihilation operator of the bound state around the moment located at site \(i\). By substituting Eqs. (6) into the original Hamiltonian Eq. (1), we obtain

\[
H_{\text{eff}} = \sum_i E_0 \alpha^\dagger_i \alpha_i + \sum_{\langle ij \rangle} \left[\tilde{t}_{ij} \alpha^\dagger_i \alpha_j + (\tilde{\Delta}_{ij} \alpha^\dagger_i \alpha^\dagger_j + \text{H.c.})\right],
\]

(7)

where \(\tilde{t}_{ij}\) and \(\tilde{\Delta}_{ij}\) are effective transfer integrals and pair potentials for the nearest neighbor sites \(\langle i, j \rangle\) in the present low energy Hamiltonian. We keep them up to the nearest neighboring sites. Here, we define

\[
\tilde{\xi}_i = \begin{pmatrix}
\cos \frac{\theta_i}{2} \\
e^{i\phi_i} \sin \frac{\theta_i}{2}
\end{pmatrix},
\]

(8)

which represents the spin as \(S_i = S \tilde{\xi}_i^\dagger \sigma \tilde{\xi}_i\). The effective transfer integrals and pair potentials are represented by

\[
\tilde{t}_{ij} = \tilde{\xi}_i^\dagger \tilde{\xi}_j \tilde{t}_{0},
\]

\[
\tilde{\Delta}_{ij} = \tilde{\xi}_i^\dagger i \sigma_3 \tilde{\xi}_j^\dagger \tilde{\Delta}_{0},
\]

(9)

(10)

with \(t_0 = \int dr \left[ (u_i \xi(r) u_j - v_i \xi(r) v_j) + \Delta_0 (u_i u_j + v_i v_j) \right]\), \(\Delta_0 = \int dr \left[ (u_i \xi(r) u_j + v_i \xi(r) v_j) + \Delta_0 (u_i u_j - v_i v_j) \right]\).
We consider following two cases; \( p_x + p_y \)-wave pairing for the opposite direction (\( \theta = \pm \pi \)). This is well known as chiral \( p \)-wave superconductor. We always choose the phases of the pairing order parameter \( \Delta_{ij} \) as real by appropriate gauge transformation once the moments lie in a plane. Then we need to consider non-coplanar spin configurations. Here we study the case of skyrmion crystal state (Fig. 3 (a)) recently observed experimentally.\(^{35,36}\) In this case, moments obviously have a non-coplanar configuration. The parameters in the effective model calculated by Eqs. (9) and (10) are given in Supplemental Material A (Fig. S2). We have confirmed the following properties of the system, and based on them we conclude that it has the same topological nature as chiral \( p \)-wave superconducting states while the transfer integrals and pair potentials are not uniform with this configuration. The characteristic properties of chiral \( p \)-wave superconductors are (i) the full gap nature, (ii) the existence of edge modes and currents, and (iii) the emergence of zero energy states at the cores of vortices.\(^{37}\) First we have confirmed that the system has an energy gap in the whole Brillouin zone by the same calculation as Fig. 2 (b), which indicates the complex value of the pair potential because the system is essentially spinless. Figure 3 (b) shows the energy dispersion of quasiparticles with the open boundaries. One can see two linearly dispersing bands crossing at \( k_x = \pm \pi \), which are localized at the edges of the system.\(^{34}\) Here the Fermi surface in the normal state is hole-like, then chiral edge modes cross at \( k_x = \pm \pi \) not \( k_x = 0 \). The fact that these modes yield edge current is manifested by directly calculating current density

\[
\mathcal{J}_i = \sum_{k_x, \sigma} 2t \sin k_x \alpha_i^{\dagger} (k_x) \alpha_i (k_x). 
\]

The result is shown in Fig. 3 (c). At \( J S \sim 2.4 \) the clear signal appears indicating the topological quantum phase transition. We also confirmed that zero energy Majorana bound states appear at the cores of vortices (Fig. 3 (d)). We conclude that
the resulting superconducting state is in the same topological phase as the chiral $p$-wave superconductor based on these observations. As another example of the non-coplanar spin configuration, we study the double spiral structure in Supplemental Material B, and found the similar $p_x + ip_y$-wave like state.

Discussion and conclusions.— In this paper, we have proposed a new way of creating effective two-dimensional unconventional superconductivity by local moments on the conventional singlet $s$-wave superconductor. The non-collinear configurations of moments are essential to induce $p$-wave pairing. There is a hierarchical structure in energy scale, i.e., the original $s$-wave energy gap and that of the induced $p$-wave superconductivity. Andreev bound states by a topological origin appear within the latter energy gap. Even the chiral $p_x + ip_y$-wave like pairing is realized by the non-coplanar configuration of moments, which shows the chiral Majorana edge channel with linear dispersion and zero energy Majorana bound states at the vortex cores. Moreover it indicates that we can create various kinds of superconducting states by choosing appropriate configurations of moments. For example, by changing the distance between the moments, one can tune the magnitudes of effective transfer integrals and pair potentials. Then, the anisotropy $|t_x/t_y|$ can be controlled to obtain the rich topological phases discussed in Ref. 45. Here we briefly discuss the effect of self-energy correction and spin fluctuation for legitimizing our approach and results. The self-energy correction due to the dynamical quantum fluctuation of spins can be estimated as $Re\Sigma(\varepsilon) \sim \lambda \varepsilon$ and $Im\Sigma(\varepsilon) \sim \lambda^2 \varepsilon^2$, where $\lambda = J^2 S/(I \varepsilon_F)$ is the dimensionless coupling constant with $I$ being the exchange coupling between spins in the magnet, and $\varepsilon_F$ the Fermi energy of the superconductor. This correction is tiny at small electron energy $\varepsilon$, and does not change the mini-gap structure. Also we have confirmed numerically the robustness of the induced gap structure against the small (static) spin fluctuation as shown in Fig. S6 in Supplemental Material C. Though our model will simulate the interface of bulk superconductors and magnetic materials, we end with an account of another experimental realization of these proposals. To create intended patterns of magnetic moments, we can use atomic manipulation techniques using scanning tunneling microscopy.\textsuperscript{46,47} The spin structure in organized magnetic impurities is also observed,\textsuperscript{48,49} although it is antiferromagnetic and cannot be utilized for our proposal.

ACKNOWLEDGMENTS

Acknowledgment.— S. N. was supported by Grant-in-Aid for JSPS Fellows. This work was supported by Grant-in-Aid for Scientific Research (S) (Grant No. 24224009); the Funding Program for World-Leading Innovative RD on Science and Technology (FIRST Program); Strategic International Cooperative Program (Joint Research Type) from Japan Science and Technology Agency; Innovative Areas “Topological Quantum Phenomena” (Grant No. 22103005) from the Ministry of Education, Culture, Sports, Science, and Technology of Japan.

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Supplemental Material for  
“Two-dimensional \(p\)-wave superconducting states with magnetic moments on a conventional \(s\)-wave superconductor”

Appendix A: \(\bar{t}_{ij}\) and \(\bar{\Delta}_{ij}\)

**FIG. S1.** Spin configuration and parameters in the effective model for coplanar spin helix configuration (corresponding to \(p_x + p_y\)-wave pairing states). \(\bar{t}_x\) and \(\bar{t}_y\) are measured in the unit of \(\bar{t}_0\) while \(\bar{\Delta}_x\) and \(\bar{\Delta}_y\) in the unit of \(\bar{\Delta}_0\) defined below Eq. (10) in the main text. \(\vec{n} = \vec{S}/S\) shows the direction of the moment at each site.

**FIG. S2.** Spin configuration and parameters in the effective model for skyrmion lattice (corresponding to \(p_x + ip_y\)-wave like pairing states). Here the spin configuration is given in a graphical way, which is identical to Fig. 3 (a). The arrows, circles with x (into the paper) and filled circle (out of the paper) inside indicate the directions of the moments. Broken lines on right side show the magnetic unit cell. We take the same units as in Fig. S1.

We gave three particular spin configurations shown in Figs. 2 (a), 3 (a), and S4 (a). Here we show the explicit values of the effective parameters calculated from Eqs. (9) and (10). Figures S1, S2, and S3 (for coplanar spin helix, skyrmion crystal, and non-coplanar spin helix, respectively) show following information; (i) direction \(\vec{n}\) of the moment at each site in a unit cell, (ii)
effective transfer integrals $\bar{t}$ and in the unit of $\bar{t}_0$, and (iii) effective pair potentials $\bar{\Delta}$ in the unit of $\bar{\Delta}_0$. The directions of moments are given by $\vec{n} = (n_x, n_y, n_z)$ in Figs. S1 and S3, and in a graphical way in Fig. S2. The unit cell is $3 \times 3$ block for both spin helix configurations, and skyrmion crystal contains 8 atomic sites in a unit cell. $\bar{t}_0$ and $\bar{\Delta}_0$ are defined just below Eq. (10) in the main text.

FIG. S3. Spin configuration and parameters in the effective model for non-coplanar spin helix configuration (corresponding to $p_x + ip_y$-wave like pairing states). We take the same units as in Fig. S1.

Appendix B: Non-coplanar helical spin configuration

In the main text, we discuss the realization of the $p_x + ip_y$-wave like state by means of the skyrmion structure. Here in Supplemental Material we consider another non-coplanar configuration of magnetic moments. It is shown in Fig. S4 (a). This can be seen as follows; we have sequential spin helix stripes along $x$-direction, but the planes on which spins rotate are tilted along $y$-direction. Describing in more detail, we start from the moment at the origin pointing along $+s_z$-direction, we rotate it by $2\pi/3$ within $s_x s_z$-plane along $x$-direction. Now we have a row of moments extended in $x$-direction. Then we rotate the plane where the moments lie by $2\pi/3$ around $s_x$-axis along $y$-direction. After three successive rotations, the plane comes back to the original one, i.e., $s_x s_z$-plane as shown in Fig. S4 (a) right side. It is expected that the former rotation gives real $\bar{\Delta}_{ij}$'s in Eq. (10) while the latter imaginary ones. The resulting $\bar{t}_{ij}$ and $\bar{\Delta}_{ij}$ are explicitly given in Fig. S3. In fact, $\bar{t}_{i+y,i} = \frac{1}{2} \bar{t}_0$ and $\bar{\Delta}_{i+y,i} = \frac{\sqrt{3}}{2} \bar{\Delta}_0$, which are consistent with the invariance of them under common rotation of two spins. On the other hand, along $y$-direction the moments have finite $s_y$ component, and hence complex $\bar{\Delta}_{i+y,i}$ results. Actually, they have pure imaginary values while $\bar{t}_{i+y,i}$ are not necessarily real. Note that any coplanar configurations of moments are transformed onto $s_x s_z$-plane by a common rotation, and all $\bar{t}_{ij}$ and $\bar{\Delta}_{ij}$ are essentially real. To obtain complex $\Delta_{ij}$'s, the non-coplanar configurations of moments are indispensable. While the transfer integrals and pair potentials in the effective model are not uniform with this configuration (see Fig. S3), it has the same topological nature as chiral $p$-wave superconductors as we will discuss below in the completely same ways as we do in the main text for the skyrmion structure.

First, the system described by the Hamiltonian in Eq. (1) has an energy gap in the whole Brillouin zone, which suggests complex value of pair potential. Figure S4 (b) shows the energy dispersion of quasiparticles with the periodic (open) boundary condition along $x$- ($y$-)direction. The magnitude of $JS$ is chosen to be $2t$ so that the energy of the bound state around a single moment is about zero energy (see Fig. 1). There are two one-dimensional bands as chiral Majorana edge channels localized at the open boundaries in the energy gap. To confirm the emergence of edge modes, we also calculate current density along $x$-direction with site indices $i$'s along $y$-direction. The result is given in Fig. S4 (c), which clearly shows the presence of the edge current. It also shows that the signature of the topological quantum phase transition at $JS = (JS)_c \sim 2.7t$. Namely, the system enters into a trivial phase for $JS > (JS)_c$ where the edge modes and current vanish. We have also confirmed that zero energy Majorana bound state appears at the cores of a vortices, which is consistent with chiral $p$-wave superconductors. We
FIG. S4. (a) Spin configuration producing effective chiral $p$-wave pairing. They have a non-coplanar structure. The moments along $x$-direction rotate by $2\pi/3$ within the planes in the spin space schematically shown on the right side. This plane is rotated along the $y$-direction by $2\pi/3$ around the $s_z$-axis indicated by the arrows. Therefore $3 \times 3$ sites constitute a unit cell. (b) Energy spectrum of quasiparticles with the periodic (open) boundary conditions along $x$-($y$-)direction. (c) Current density calculated with the configuration given in (a) with the width $N_y = 24$. The other parameters are the same as in (b). There are finite chiral current density at the edges.

Insert vortices into the pair potential of the original $s$-wave superconductor. To avoid the effect of the boundary which may cause in-gap states, we impose the periodic boundary condition for both $x$- and $y$-directions. For the consistency of the phase, we introduce two vortices with winding number 1 and other two anti-vortices with winding number -1. The four-fold zero energy states appear in the induced gap corresponding to the four vortices in total, and the probability of one of their wave functions in the real space shows localized distribution around the vortices as shown in Fig. S5. These results are the same as those in the case of the genuine chiral $p$-wave superconductor.

FIG. S5. (a) Energy levels of quasiparticles obtained by a tight binding model calculation with vortices. The horizontal axis shows the indices of energy eigenvalues. The system size is set $48 \times 48$ with periodic boundary condition, and $t = \Delta_0 = 1.0$. The zero energy states are four-fold degenerate. (b) Distribution of a wave function of one of the zero energy states. It has peaks at the positions of vortex cores.

In addition we study the effect of a defect. Here we use “defect” in the meaning of taking away one magnetic moment from the suite of aligned magnetic moments. In the tight binding picture, there is a lattice site for the original $s$-wave superconductor at the defect point. In the conventional $s$-wave superconductor, the non-magnetic defect does not produce any in-gap state. In sharp contrast, we find that new states appear inside the lower energy gap. Note that the energy is not necessarily zero. This property is characteristic to unconventional superconductors.

We employ the rotation angle $2\pi/3$ in the coplanar and non-coplanar spin helix structure for the sake of numerical calculation. However, the properties discussed above obviously hold when we consider other angles as long as it is not equal to 0 or $\pi$. 

Appendix C: Robustness against fluctuation

As stated in the main text, we assume the configuration of magnetic moments are strictly fixed all through the calculations. Here we examine the influence of spin fluctuation. It is shown that the results obtained above are qualitatively unaffected. To take into account the effect of spin fluctuation, we mimic it by modulating directions of the moments with random magnitude about 7% from the static configuration (Fig. 3 (a)). In Fig. S6 the edge modes still connect occupied and unoccupied states even though they are slightly modified by the fluctuation.

FIG. S6. Energy spectrum with random modulation of directions of magnetic moments. The lines near energy 0 (blue ones) are edge modes. They remain crossing at $k_x = \pm \pi$ and separated from the bulk states.