Spin anisotropy and quantum Hall effect in the *kagomé* lattice: Chiral spin state based on a ferromagnet

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A ferromagnet with spin anisotropies on the two-dimensional (2D) *kagomé* lattice is theoretically studied. This is a typical example of the flat-band ferromagnet. The Berry phase induced by the tilting of the spins opens the band gap and quantized Hall conductance $\sigma_{xy}=\pm e^2/h$ is realized. This is the most realistic chiral spin state based on the ferromagnetism. We also discuss the implication of our results to the anomalous Hall effect observed in the metallic pyrochlore ferromagnets $R_2Mo_2O_7$ ($R=$Nd, Sm, Gd).

The spin Berry phase plays an important role in the quantum transport of strongly correlated electronic systems. Consider an electron hopping from site i to j coupled to a spin at each site with Hund's coupling J_H.[1] The Hamiltonian is expressed by the double-exchange model

$$H=\sum_{NN} t_{ij}\psi^{\dagger}_{i\sigma}\psi_{j\sigma}-J_H\sum_{i} \psi^{\dagger}_{i\alpha}\vec{\sigma}_{\alpha\beta}\cdot\vec{S}_i\psi_{i\beta}, \tag{1}$$

where $\psi^{\dagger}_{i\sigma}$ is the spin σ electron creation operator, and $\vec{S}_i$ is the localized spin on site i, which we assumed to be classical. When J_H is strong enough the spin of the hopping electron is forced to align parallel to $\vec{S}_i$ and $\vec{S}_j$ at each site, with the spin-wave function being $|\chi_i\rangle$ and $|\chi_j\rangle$, respectively. The spin wave function is explicitly given by

$$|\chi_i\rangle={}^t\left[e^{ib_i}\cos\frac{\theta_i}{2},e^{i(b_i+\phi_i)}\sin\frac{\theta_i}{2}\right], \tag{2}$$

where we have introduced the polar coordinates as $\langle\chi_i|\vec{S}_i|\chi_i\rangle=\frac{1}{2}(\sin\theta_i\cos\phi_i,\sin\theta_i\sin\phi_i,\cos\theta_i)$. The overall phase b_i corresponds to the gauge degrees of freedom and does not appear in physical quantities. Therefore, the effective transfer integral t^{eff}_{ij} is given by[1]

$$\begin{aligned}t^{eff}_{ij}&=t\langle\chi_i|\chi_j\rangle\\&=te^{i(-b_i+b_j)}\left[\cos\frac{\theta_i}{2}\cos\frac{\theta_j}{2}+e^{i(-\phi_i+\phi_j)}\sin\frac{\theta_i}{2}\sin\frac{\theta_j}{2}\right]\\&=te^{ia_{ij}}\cos\frac{\theta_{ij}}{2},\end{aligned} \tag{3}$$

where θ_{ij} is the angle between the two spins $\vec{S}_i$ and $\vec{S}_j$. The phase a_{ij} is the vector potential generated by the spin, and corresponds to the Berry phase felt by the hopping electron. Let us consider an electron hopping along a loop $1\rightarrow2\rightarrow3\rightarrow1$. The total phase that the electron obtains is the gauge flux by a_{ij}, which corresponds to one half of the solid angle subtended by the three spins $\vec{S}_i$ $(i=1,2,3)$. This is called the spin chirality and is one of the key concepts in the physics of strongly correlated electronic systems.[2–7] One can easily see that the spin chirality is absent for collinear and coplanar spin alignment, and the spin chirality has been intensively discussed in the context of the quantum spin liquid where the spins and hence a_{ij} fluctuate quantum mechanically.[2–7] This a_{ij} is the leading actor in the gauge theory of strongly correlated electronic systems.[3,6]

Among them the proposal of chiral spin state with broken time-reversal symmetry in a triangular lattice[2] and the *kagomé* lattice,[7,8] and later the anyon superconductivity[4] attracted great interest at the early stage of the high-T_c research. Wen *et al.*[5] constructed a mean-field theory for a chiral spin liquid on a square lattice. They start from the π-flux state, and break the time-reversal symmetry by introducing the next-nearest-neighbor hopping with a phase. However, it turned out to be rather difficult to find physical realization of the (chiral) spin liquid in real materials, even in frustrated lattices.

The spin Berry phase has been discussed also in the context of the anomalous Hall effect (AHE) in manganites.[9] It is proposed that the spin-orbit interaction H' leads to the coupling between the magnetization M and the spin chirality, i.e., the gauge flux, b as expressed by $H'=\lambda bM$. At finite temperature T, Skyrmions are thermally excited and the balance between the positive and negative chiralities is broken by H' to give rise to a finite average $\langle b\rangle$. This $\langle b\rangle$ gives an additional ''magnetic field'' and hence leads to the anomalous Hall effect proportional to the coupling constant λ and Skyrmion density $\sim e^{-\Delta/T}$, where Δ is the excitation energy of the Skyrmion. This mechanism is the one coming from the Berry phase of the spins compared with the conventional skew-scattering mechanism.[10–12] However, it shares a feature with these conventional theories, namely the AHE vanishes in the zero-temperature limit, which is the case in the conventional ferromagnetic metals experimentally.[10] It is related to the fact that the spin chirality is zero in the ground state. However, it is noted that a recent work proposes the staggered flux state as the ground state of the double exchange model on a cubic lattice with doping.[13]

On the other hand, recent transport experiments on ferromagnetic pyrochlores $R_2Mo_2O_7$ ($R=$Nd, Sm, Gd) revealed that the AHE increases as T is lowered and approaches to the saturated value.[16,17] This behavior is qualitatively different from the conventional one.[10] One clue to explain this anomalous feature is that the pyrochlore structure has geometrical frustration.[14] It consists of corner-sharing tetrahedrons and the antiferromagnetic interactions between nearest-neighbor spins are frustrated. It was recently pointed out that even the ferromagnetic interaction is frustrated, if the spin easy axis points to the center of the tetrahedron.[15] In this case, because the spin configuration becomes noncoplanar, we expect that the spin chirality appears and affects the quantum transport of electrons, especially the transverse conductivity σ_{xy}. However, it is a nontrivial issue whether the spin chirality really contributes to σ_{xy} when the spins form a periodic structure.

Motivated by these pyrochlore compounds, we study in this paper the two-dimensional *kagomé* lattice, which is the cross section of the pyrochlore lattice perpendicular to the (1,1,1) direction.[14] We show that the chiral spin state is realized in an *ordered* spin system on the *kagomé* lattice, when the spin anisotropy is introduced. When the Fermi energy is in the gap, the system shows a quantized Hall effect. Implications of our results to these pyrochlore compounds are also discussed especially on the AHE which does not vanish at low temperatures.

We consider the double-exchange ferromagnet on the *kagomé* lattice shown in Fig. 1. Here the triangle is the one face of the tetrahedron, and the easy axis of the spin anisotropy points to the center of each tetrahedron and has an out-of-plane component. In this situation the three spins on sites A, B, and C in Fig. 1 have different directions and the spin chirality emerges.[18]

The effective Hamiltonian for the hopping electrons strongly Hund-coupled to these localized spins is given by

$$H=\sum_{NN} t_{ij}^{eff}\psi_i^\dagger\psi_j, \tag{4}$$

with t_{ij}^{eff} being given in Eq. (3). We set the flux originated from the spin chirality per triangle as ϕ, which satisfy $e^{i\phi}=e^{i(a_{AB}+a_{BC}+a_{CA})}$. The flux penetrating one hexagon is determined as -2ϕ. We take the gauge, in which the phase of t_{ij}^{eff} is the same for all the nearest-neighbor pairs with the

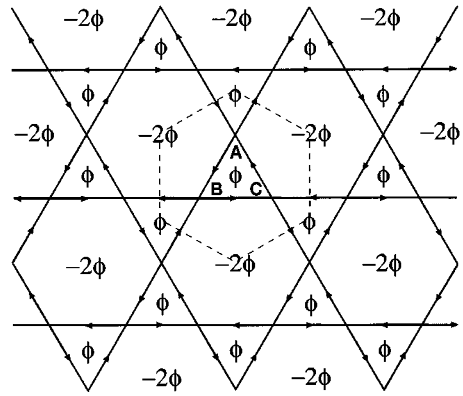

FIG. 1. *kagomé* lattice. The dotted line represents the Wigner-Seitz unit cell, which contains three independent sites (A,B,C). It is assumed that each site has a different spin anisotropy axis. The arrows on bonds mean the sign of the phases of the transfer integral t_{ij}.

direction shown by the arrows in Fig. 1.[18] Note that the net flux through a unit cell vanishes due to the cancellation of the contribution of two triangles and a hexagon. It should be also noted that time-reversal symmetry is broken except for the case of $\phi=0,\pi$.

From now on we choose the unit of $t\cos(\theta_{ij}/2)=1$, and set the length of each bond as unity. We define three vectors $\vec{a}_1=(-1/2,-\sqrt{3}/2)$, $\vec{a}_2=(1,0)$, and $\vec{a}_3=(-1/2,\sqrt{3}/2)$, which represent the displacements in a unit cell from A to B site, from B to C site, from C to A site, respectively. In this notation, the Brillouin zone (BZ) is a hexagon with the corners of $\vec{k}=\pm(2\pi/3)\vec{a}_1, \pm(2\pi/3)\vec{a}_2, \pm(2\pi/3)\vec{a}_3$, two of which are independent.

To diagonalize the Hamiltonian, we rewrite the Hamiltonian in the momentum space as $H=\Sigma_{\vec{k}}\psi^\dagger(\vec{k})h(\vec{k})\psi(\vec{k})$, where $\psi(\vec{k})={}^t(\psi_A(\vec{k}),\psi_B(\vec{k}),\psi_C(\vec{k}))$ and $h(\vec{k})$ is a 3×3 matrix:

$$h(\vec{k})=\begin{pmatrix} 0 & 2\cos(\vec{k}\cdot\vec{a}_1)e^{-i\phi/3} & 2\cos(\vec{k}\cdot\vec{a}_3)e^{i\phi/3} \\ 2\cos(\vec{k}\cdot\vec{a}_1)e^{i\phi/3} & 0 & 2\cos(\vec{k}\cdot\vec{a}_2)e^{-i\phi/3} \\ 2\cos(\vec{k}\cdot\vec{a}_3)e^{-i\phi/3} & 2\cos(\vec{k}\cdot\vec{a}_2)e^{i\phi/3} & 0 \end{pmatrix}. \tag{5}$$

After diagonalization, we obtain eigenvalues E_i and eigenvectors $|\psi_i(\vec{k})\rangle=[a_i(\vec{k})\psi_A^\dagger(\vec{k})+b_i(\vec{k})\psi_B^\dagger(\vec{k})+c_i(\vec{k})\psi_C^\dagger(\vec{k})]|0\rangle$, which satisfy $h(\vec{k})|\psi_i(\vec{k})\rangle=E_i(\vec{k})|\psi_i(\vec{k})\rangle$. There are three bands with dispersion relations

$$E_{\rm upper}(\vec{k})=4\sqrt{\frac{1+f(\vec{k})}{3}}\cos\frac{\theta(\vec{k})}{3},$$

$$E_{\rm middle}(\vec{k})=4\sqrt{\frac{1+f(\vec{k})}{3}}\cos\frac{\theta(\vec{k})-2\pi}{3},$$

$$E_{\rm lower}(\vec{k})=4\sqrt{\frac{1+f(\vec{k})}{3}}\cos\frac{\theta(\vec{k})+2\pi}{3}, \tag{6}$$

where $\theta(\vec{k})(0\leqslant\theta(\vec{k})\leqslant\pi)$ is defined by

$$\theta(\vec{k})=\arg\left[f(\vec{k})\cos\phi+i\sqrt{4\left(\frac{1+f(\vec{k})}{3}\right)^3-[f(\vec{k})\cos\phi]^2}\right], \tag{7}$$

and $f(\vec{k})$ is given by $f(\vec{k})=2\cos(\vec{k}\cdot\vec{a}_1)\cos(\vec{k}\cdot\vec{a}_2)\cos(\vec{k}\cdot\vec{a}_3)$.

As special cases, the energy dispersions for $\phi=0,\pi/3$ are shown in Fig. 2. The spectra have some characteristic fea-

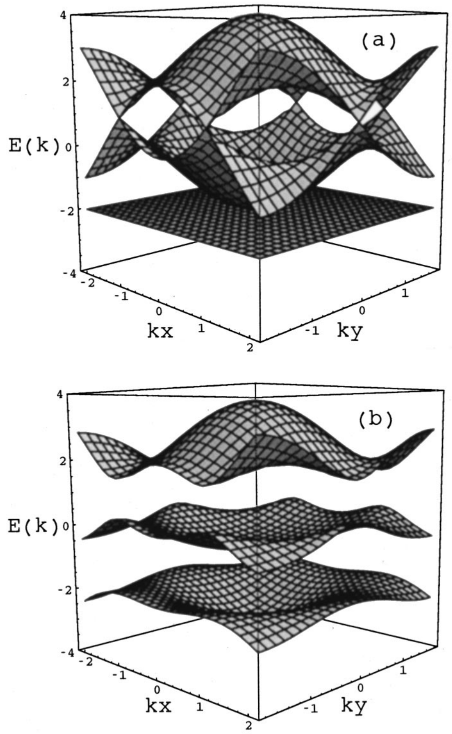

FIG. 2. The energy spectra [Eq. (6)] in the case of (a) $\phi=0$ and (b) $\phi=\pi/3$.

tures. The relation $E_{\rm lower}(\vec{k})\le E_{\rm middle}(\vec{k})\le E_{\rm upper}(\vec{k})$ is always satisfied, and the equality is achieved only when the system is time-reversal symmetric, i.e., $\phi=0,\pi$. When $\phi=0$, the lower band becomes dispersionless [$E_{\rm lower}(\vec{k})=-2=\text{const}$], which is the reflection of the fact that the *kagomé* lattice is a line graph of the honeycomb structure.[19] This flat band touches at the center of the BZ ($\vec{k}=0$) with the middle band, whose dispersion relation around it is $E_{\rm middle}(\vec{k})\propto\vec{k}^2$. The middle band and the upper band touch at two independent corners of the BZ. Around each of the two corners, the dispersion is expressed by a massless Dirac fermion. The spectrum of $\phi=\pi$ is a particle-hole conjugate of that of $\phi=0$; therefore, the upper band becomes flat with an eigenvalue of 2. Generally the energy spectra has no particle-hole symmetry except for the case of $\phi=\pm\pi/2$, in which the middle band becomes dispersionless: $E_{\rm middle}(\vec{k})=0$.

We now calculate the Hall conductance of this system. It is clear that the Hall conductance σ_{xy} is equal to zero ($\sigma_{xy}=0$) in the time-reversal symmetric cases $\phi=0,\pi$. Therefore, we focus on the case of $\phi\neq0,\pi$. In this case there is an energy gap between each band, and we first assume that the Fermi energy is lying in the gap. The Hall conductance is given by the summation of that for each band below the Fermi energy: $\sigma_{xy}=\Sigma_{E_i\le E_F}\sigma^i_{xy}$, and the Hall conductance is generally quantized, i.e., $\sigma_{xy}=\nu e^2/h$ (ν: integer).[21] The contribution to the Hall conductance from an ith band is written as

$$\sigma^i_{xy}=\frac{e^2}{h}\frac{1}{2\pi i}\int_{BZ}d^2k\hat{z}\cdot\nabla_{\vec{k}}\times\vec{A}_i(\vec{k})=\frac{e^2}{h}C_i, \tag{8}$$

where $\vec{A}_i(\vec{k})$ is the vector potential defined with the ith Bloch wave function as

$$\vec{A}_i(\vec{k})=(a_i(\vec{k}),b_i(\vec{k}),c_i(\vec{k}))^*\cdot\nabla_{\vec{k}}{}^t(a_i(\vec{k}),b_i(\vec{k}),c_i(\vec{k})), \tag{9}$$

and C_i is the so-called first Chern number. This value is invariant under gauge transformation $|\psi'_i(\vec{k})\rangle=e^{ig(\vec{k})}|\psi_i(\vec{k})\rangle,\vec{A}'_i(\vec{k})=\vec{A}_i(\vec{k})+i\nabla_{\vec{k}}g(\vec{k})$, where $g(\vec{k})$ is an arbitrary smooth function of $\vec{k}$. To calculate the Hall conductance explicitly, we fix the gauge, for example by setting $a_i(\vec{k})$ to be real. If this gauge choice is applicable in the whole region of the BZ, the evaluation of Eq. (8) leads to $\sigma^i_{xy}=0$. However, generally speaking, there might be some points where the amplitude of $a_i(\vec{k})$ becomes zero. We call these points as the center of vortices. At the center of the vortices, our previous choice of the gauge is ill defined, and we have to choose another gauge, for example, $b_i(\vec{k})$ is real around them. It is this phase mismatch between patches in the BZ that contributes to the nonzero Hall conductance.

In our model, we can calculate the Hall conductance of each band analytically. We take the lower band as an example and we will omit the band index in this paragraph. We choose the gauge of real $a(\vec{k})$, and rewrite the eigenvector as $(a(\vec{k}),b(\vec{k}),c(\vec{k}))=(a'(\vec{k}),b'(\vec{k})e^{-i\xi_b(\vec{k})},c'(\vec{k})e^{-i\xi_c(\vec{k})})$, where $a'(\vec{k})>0,b'(\vec{k})>0,c'(\vec{k})>0,\xi_b(\vec{k}),\xi_c(\vec{k})$ are real numbers. This gauge choice is ill defined at the point $\vec{k}=(0,\pi/\sqrt{3})$; therefore, we take the gauge of real $b(\vec{k})$ around it. The first Chern number is written as

$$C=\frac{1}{2\pi}\oint_\Gamma d\vec{k}\cdot\nabla_{\vec{k}}\xi_b(\vec{k}), \tag{10}$$

where the integral is over the closed loop Γ around the vortex. An explicit calculation leads to $C_{\rm lower}=-\text{sgn}(\sin\phi)$. In a similar way, we can calculate the contribution from the middle and the upper band, and the results are $C_{\rm middle}=0,C_{\rm upper}=\text{sgn}(\sin\phi)$. This means that the quantum Hall effect with zero total flux in the unit cell is realized in the present model.[22]

It is noted here that an infinitesimal tilting of spin and hence the spin chirality ϕ opens the gap, and the bands obtain chiralities. Although this situation is similar to the chiral spin liquid,[5] still there are crucial differences between these two cases. In the present model, both the spin direction on each site and the flux through a plaquette are ordered. This is in sharp contrast to the chiral spin liquid where only the flux through a plaquette is ordered, and the direction of spin on each site is fluctuating. Furthermore, in the present case, the physical observable σ_{xy} is nonvanishing and quantized while σ_{xx} is zero. In the chiral spin liquid, on the other hand, σ_{xy} and σ_{xx} always vanish because the charge degree of freedom is missing there. Even when carriers are doped and the anyon superconductivity occurs,[4] the Meissner term in the action, i.e., $\rho_s\vec{A}\cdot\vec{A}$, is dominant and detection of σ_{xy} through the electric Hall effect is difficult.

Up to now, we have concentrated on the ferromagnet represented by the double-exchange model. Our theory is also applicable to the ferromagnet based on the Hubbard model, because in the mean-field level the Hamiltonian is expressed by the double-exchange model [Eq. (1)], where we identify $\vec{S}_i$ with the classical $(i\omega_n=0)$ component of the Stratonovich-Hubbard field. It is proved that the ground state of the Hubbard model on the *kagomé* lattice is a ferromagnet if the flat band is half-filled,[19] and this flat-band ferromagnetism is robust under introduction of a small dispersion to the dispersionless band.[20] Furthermore the spin-orbit coupling gives the spin anisotropies, which are different for three crystallographically independent sites. This introduces the tilting of the spins from the perfect ferromagnetic alignment, as was assumed in Eq. (4). Therefore, from the theoretical point of view, we can strongly expect that once the electron density is 1/3 per atom on the *kagomé* lattice, the chiral spin state presented here is realized and Hall conductance is quantized as $\sigma_{xy}=\pm e^2/h$.

Finally, we discuss the recent experiments on $R_2Mo_2O_7$ ($R=$Nd, Sm, Gd),[16,17] which are itinerant ferromagnets on the verge of a Mott transition on the pyrochlore lattice. The spin polarization is almost perfect,[16] and the tight-binding model Eq. (4) is the appropriate one for these spin-polarized electrons. Although the spin structure of these materials are not yet determined, we can expect that easy-axis spin anisotropy produces the spin chirality by the symmetry consideration. These compounds show metallic behaviors, which means that the Fermi energy is not in the band gap, and the above argument is not straightforwardly applicable to discuss the large nonvanishing AHE at zero temperature. However, our results show that each band contributes to the Hall conductance as a whole in the ground state, and nonvanishing anomalous Hall conductance is expected to be realized even when the Fermi energy is lying inside the band, which is qualitatively consistent with the experiment. In this case, the magnitude of σ_{xy} depends on band dispersion and also the lifetime of the quasiparticles. Thus, the quantitative discussion is beyond the scope of our present analysis. Considerations of these issues as well as the extension to three-dimensional systems[23] are left for future studies.

In summary, we studied the chiral spin state realized in the flat-band ferromagnet with spin anisotropy on the two-dimensional *kagomé* lattice. If the Fermi energy is lying in the gap, we expect quantized Hall conductance $\sigma_{xy}=\pm e^2/h$. In other cases, the system behaves as an itinerant ferromagnet with finite Hall conductance at zero temperature. This feature is qualitatively in good accordance with recent experiments on the pyrochlore oxides $R_2Mo_2O_7$ ($R=$Nd, Sm, Gd).

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[1] P. W. Anderson and H. Hasegawa, Phys. Rev. **100**, 675 (1955).

[2] V. Kalmeyer and R. B. Laughlin, Phys. Rev. Lett. **59**, 2095 (1987).

[3] G. Baskaran and P. W. Anderson, Phys. Rev. B **37**, 580 (1988).

[4] R. B. Laughlin, Science **242**, 525 (1988).

[5] X. G. Wen, F. Wilczek, and A. Zee, Phys. Rev. B **39**, 11 413 (1989).

[6] P. A. Lee and N. Nagaosa, Phys. Rev. B **46**, 5621 (1992).

[7] Kun Yang, L. K. Warman, and S. M. Girvin, Phys. Rev. Lett. **70**, 2641 (1993).

[8] J. N. Reimers and A. J. Berlinsky, Phys. Rev. B **48**, 9539 (1993).

[9] Jinwu Ye *et al.*, Phys. Rev. Lett. **83**, 3737 (1999); P. Matl, N. P. Ong, Y. F. Yan, Y. Q. Li, D. Studebaker, T. Baum, and G. Doubinina, Phys. Rev. B **57**, 10 248 (1998); S. H. Chun *et al.*, Phys. Rev. Lett. **84**, 757 (2000).

[10] C. M. Hurd, *The Hall Effect in Metals and Alloys* (Plenum Press, New York, 1972).

[11] R. Karplus and J. M. Luttinger, Phys. Rev. **95**, 1154 (1954).

[12] J. Kondo, Prog. Theor. Phys. **27**, 772 (1962).

[13] M. Yamanaka, W. Koshibae, and S. Maekawa, Phys. Rev. Lett. **81**, 5604 (1998).

[14] A. P. Ramirez, Annu. Rev. Mater. Sci. **24**, 453 (1994); M. J. Harris and M. P. Zinkin, Mod. Phys. Lett. B **10**, 417 (1996).

[15] M. J. Harris *et al.*, Phys. Rev. Lett. **79**, 2554 (1997); S. T. Bramwell and M. J. Harris, J. Phys.: Condens. Matter **10**, L215 (1998); R. Moessner, Phys. Rev. B **57**, R5587 (1998).

[16] Y. Taguchi and Y. Tokura, Phys. Rev. B **60**, 10 280 (1999).

[17] T. Katsufuji, H. Y. Hwang, and S-W. Cheong, Phys. Rev. Lett. **84**, 1998 (2000).

[18] Even when the atom on top (bottom) of each triangle is missing, the spin-orbit interaction H_{SO} produces the similar gauge flux distribution. The spin-orbit interaction is given by $H_{SO}=(e\hbar/4m^2c^2)(\vec{\sigma}\times\nabla V)\cdot\vec{p}=(e/mc)\vec{A}_{SO}\cdot\vec{p}$, where V is the periodic potential, $\vec{\sigma}$ are the Pauli spin matrices, and $\vec{p}$ is the momentum operator. In the ferromagnetic state, the vector potential $A_{SO}=(\hbar/4mc)(\vec{\sigma}\times\nabla V)$ produces the nonuniform distribution of the internal gauge flux $\vec{B}_{SO}=\nabla\times\vec{A}_{SO}$. By symmetry, its pattern is exactly the same as given in Fig. 1.

[19] A. Mielke, J. Phys. A **24**, L73 (1991); **24**, 3311 (1991); **25**, 4335 (1992).

[20] K. Kusakabe and H. Aoki, Phys. Rev. Lett. **72**, 144 (1994).

[21] D. J. Thouless, M. Kohmoto, M. P. Nightingale, and M. den Nijs, Phys. Rev. Lett. **49**, 405 (1982); M. Kohmoto, Ann. Phys. (N.Y.) **160**, 343 (1985).

[22] The quantum Hall effect with zero total flux through a unit cell was discussed by F. D. M. Haldane [Phys. Rev. Lett. **61**, 2015 (1988)], based on the tight-binding model with the complex transfer integral between next-nearest-neighbor sites in the honeycomb lattice. However, it is not so easy to realize Haldane's model in real materials, because the introduction of appropriate flux is technically difficult.

[23] G. Montambaux and M. Kohmoto, Phys. Rev. B **41**, 11 417 (1990); M. Kohmoto, B. Halperin, and Y.-S. Wu, *ibid.* **45**, 13 488 (1992).