Anomalous Hall Effect and Spontaneous Orbital Magnetization in Antiferromagnetic Weyl Metal

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We study the anomalous Hall effect and the orbital magnetization in chiral antiferromagnets, constructing a simple tight-binding model on a stacked Kagome lattice structure with spin-orbit coupling and the exchange interaction between the localized spins and itinerant electrons. It is shown that the chiral antiferromagnet with spin-orbit coupling is an orbital ferromagnet with the easy-plane anisotropy. The relation between the orbital magnetization and the configuration of the Weyl points are discussed.

KEYWORDS: anomalous Hall effect, orbital magnetization, chiral antiferromagnet, Weyl semimetal

Introduction — The anomalous Hall effect is observed in ferromagnetic materials with spin-orbit coupling. It is known that the anomalous Hall effect is originated from extrinsic scattering by spin-orbit coupled scatterers or intrinsic contribution from the spin-orbit coupled electronic band structure. In most cases the Hall resistivity is expressed in the following form

$$\rho_{xy} = R_0 B_z^{\text{ext}} + R_M M_{\text{spin}}^z,$$

where $B_z^{\text{ext}}$ is an external magnetic field and $M_{\text{spin}}^z$ is the spin magnetization. At zero field, the Hall conductivity of a ferromagnetic metal is proportional to the perpendicular component of the spin magnetization,

$$\sigma_{ij}^{\text{AHE}} \propto \epsilon_{ijk} M_{\text{spin}}^{k}.$$

Because of this relation, the anomalous Hall effect is used to detect the magnetization in ferromagnetic materials. In magnetic materials with noncoplanar spin configurations a finite scalar spin chirality acts as a fictitious magnetic field in real space for the conduction electrons and contributes to the anomalous Hall effect even without spin-orbit coupling.

The anomalous Hall effect in antiferromagnets has been theoretically studied. Recently, the anomalous Hall effect was experimentally observed at room temperature in non-collinear antiferromagnets $\text{Mn}_3\text{Z}$, where $Z = \text{Sn, Ge, and Ir}$. The anomalous Hall conductivity is as large as that in conventional ferromagnetic metals such as Iron and Cobalt even though the net spin magnetization is negligibly small. $\text{Mn}_3\text{Z}$ has the layered hexagonal lattice structure. Inside a layer, Mn atoms form a Kagome-type lattice with mixed triangular and hexagonal (Sn, Ge, and Ir) atoms are located at the center of these hexagons. All Mn moments are arranged inside the Kagome plane forming triangular spin structures, referred to chiral antiferromagnets (CAF). Since the scalar spin chirality is zero in antiferromagnets, the mechanism of anomalous Hall effect is essentially different from that in magnetic materials with noncoplanar spin structures.

Electronic structures in chiral antiferromagnets have been studied using first principle calculation, and the existence of multiple Weyl points has been observed. It has been also shown that the mechanism of the anomalous Hall effect in $\text{Mn}_3\text{Z}$ can be characterized by the cluster extension of octupole moments in the same manner as that in ferromagnets by the magnetization of dipole moment. Up to now, however, a simple tight-binding model has not been studied in detail. In this paper we construct an effective tight-binding Hamiltonian with the exchange interaction and spin-orbit coupling on a stacked Kagome lattice. We show that the system has a spontaneous orbital magnetization even though net spin magnetization is zero. The anomalous Hall conductivity, $\sigma_{xy}$, and $\sigma_{yz}$, and $\sigma_{zx}$ are computed using the Kubo formula and connected with the orbital magnetization. The existence of Weyl points plays an important role in the anomalous Hall effect. We discuss the relation between the orbital magnetization and the configuration of the Weyl points.

Model Hamiltonian — In the following we construct a single-orbital tight-binding model on the layered hexagonal lattice (the stacked Kagome lattice structure) of Mn atoms, neglecting electronic degrees of freedom on Z sites, as shown in Fig. 1 (a). We start from the hopping term

$$H_0 = -\sum_{\langle i,j \rangle} t_{ij} c_{i\sigma}^\dagger c_{j\sigma},$$

where $c_{i\sigma}$ creates an electron with spin $\sigma (= \uparrow \text{ or } \downarrow)$ at the $i$th site of the stacked Kagome layers, and $\langle i, j \rangle$ denotes nearest neighbors. As Fig. 1 shows, a unit cell of the crystal consists of six atoms located at $A = (0, 0, 0)$, $B = (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$, $C = (-\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$, $B' = (-\frac{1}{2}, \frac{1}{2}, -\frac{1}{2})$, $C' = (\frac{1}{2}, -\frac{1}{2}, -\frac{1}{2})$ in another layer. Here $a$ and $c$ are lattice spacing intralayer and interlayer, respectively. The intralayer nearest-neighbor vectors are given by $a_1 = (-\frac{1}{\sqrt{3}}, 0, 0)$, $a_2 = (a, 0, 0)$, $a_3 = (-\frac{1}{\sqrt{3}}, 0, 0)$, and the interlayer nearest-neighbor vectors are $c_1 = (-\frac{1}{\sqrt{3}}, -\frac{2}{\sqrt{3}}, 0)$, $c_2 = (0, -\frac{\sqrt{3}}{2}, -\frac{\sqrt{3}}{2})$, and $c_3 = (\frac{\sqrt{3}}{2}, -\frac{\sqrt{3}}{2}, -\frac{\sqrt{3}}{2})$ as shown in Fig. 1. In the following we set $t_{ij} = t_0$ (between nearest neighbor, otherwise zero) and $a = c = 1$ for simplicity.

Next we introduce spin-dependent nearest-neighbor hopping which is one of ingredients for the anomalous Hall effect. In the stacked Kagome lattice inversion symmetry is locally broken. In a process of nearest neighbor hopping an electron feels an electric field perpendicular to the direction of hopping that gives rise to the spin-orbit coupling term of the form

$$H_{so} = it_{so} \sum_{<i,j>} \mathbf{n}_{ij} \cdot \sigma_{ij}^{\dagger} \mathbf{a}_{\sigma\tau} c_{j\tau},$$

where $\mathbf{n}_{ij}$ is a unit vector. This term does not affect the anomalous Hall conductivity, because it is a local term that comes from the spin-orbit coupling.
where $t_{so}$ is the strength of spin-orbit coupling and $n_i = (-n_j)$ is the unit vectors perpendicular to the directions of hopping and the local electric fields. In a Kagome layer $n_{BA} = n_{CB} = n_{AC} = n_{B'A'} = n_{C'B'} = n_{AC'} = (0, 0, 1)$, while $n_{A'B'} = n_{B'A'} = 2b_1 \times e_1 = (\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}})$ along $c_1$, $n_{C'B'} = n_{C'B'} = 2b_2 \times c_2 = (0, \frac{\sqrt{3}}{2}, \frac{\sqrt{3}}{2})$ along $c_2$, and $n_{AC} = n_{AC} = 2b_3 \times e_3 = (\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0)$ along $e_3$, where $b_1 = (-\frac{1}{\sqrt{2}}, -\frac{\sqrt{3}}{2}, 0)$, $b_2 = (\frac{1}{\sqrt{2}}, 0, 0)$, $b_3 = (-\frac{1}{\sqrt{2}}, \frac{\sqrt{3}}{2}, 0)$ as shown in Fig. 1(b). All unit vectors, $n_i$, are illustrated in Fig. 1(c).

The interaction between itinerant electron spins and localized spins is described by the exchange coupling term

$$H_{exc} = -J \sum_i m_i \cdot c_i^{\dagger} \sigma_{\alpha \beta} c_{i \alpha \beta},$$

where $m_i$ is the direction unit vector of the localized magnetic moment at $i$th site. We focus on two cases with spin textures under the magnetic fields along the $x$ and $y$ directions, referred to CAF1 and CAF2, respectively, as shown in Fig. 2 (a) and (b). In terms of the Fourier components of the creation and annihilation operators, $c_{k\alpha} = \frac{1}{\sqrt{N}} \sum_{\mathbf{R}} c_{\alpha \mathbf{R}} e^{ik \cdot \mathbf{R}}$, the total Hamiltonian is represented in the form of

$$H = H_0 + H_{so} + H_{exc} = \sum_k c_{k\sigma}^\dagger H(k) c_{k\sigma},$$

The energy eigenvalues, obtained by diagonalizing $H(k)$, are shown along high-symmetry lines in Fig. 3 for (a) CAF1 and (b) CAF2 configurations. Here we set $t_{so} = 0.2t_0$ and $J = 1.7t_0$. These parameters have been estimated from the first principle calculation in Ref. 7 for MnIr. We checked that qualitative behaviors shown below remain unchanged as the parameters change.

Anomalous Hall conductivity—Using the Kubo formula the anomalous Hall conductivity $\sigma_{ij}$ ($i \neq j$) from the intrinsic mechanism is given by

$$\sigma_{ij} = \frac{e^2}{h} \sum_{ij} \int_{BZ} \frac{d^3k}{(2\pi)^3} \Omega_{ij}(k)(E_{nk} - \mu),$$

where $\Omega_{ij}(k) = \nabla_k \times A \sigma_{ij}$ is the Berry curvature and $A \sigma_{ij}$ is the Berry connection, $\mu$ being the Bloch state obtained by solving the eigen equation $H(k)|\mu\rangle = E_{nk}|\mu\rangle$. The anomalous Hall conductivities are shown as a function of the Fermi energy $E$ in Fig. 3 for (c) CAF1 and for (d) CAF2. In the CAF1 configuration $\sigma_{xz}$ is finite, while $\sigma_{xy} = 0$. In the CAF2 configuration, on the other hand, $\sigma_{xy}$ is finite, while $\sigma_{xz} = 0$. These results are consistent with experiments.

Orbital magnetization—Next we consider the orbital magnetization which is obtained by the following equation:

$$M^{\text{orb}} = \frac{e}{2h} \sum_{ij} \int_{BZ} \frac{d^3k}{(2\pi)^3} f(E_{nk} - \mu) \times i \left[ \frac{\partial \mu}{\partial k} \times (2\mu - E_{nk} - H(k)) \frac{\partial \mu}{\partial k} \right],$$

and discuss the relation with the anomalous Hall effect. Here $\mu$ is the Fermi energy. The orbital magnetization $M^{\text{orb}} = (M_x, M_y, M_z)$ is shown in Fig. 4 (a) for CAF1 and (b) for CAF2 as a function of the Fermi energy $E$. In CAF1 $M_x$ is finite, while $M_y = M_z = 0$. In CAF2, on the other hand, $M_y$ is finite, while $M_x = M_z = 0$. These results show that the ground state of the our tight-binding Hamiltonian under the fixed local spin magnetizations (CAF1 and CAF2) possesses a finite orbital magnetization contrary to the fact that the net spin magnetization is zero. In the presence of a magnetic field $B$ pointing in the Kagome plane, the orbital magnetization couples with the field via $-B \cdot M^{\text{orb}}$. When $B$ points in the $x$ direction, the CAF1 configuration with $M^{\text{orb}}$ pointing in the $x$ direction is energetically favored. Similarly, when $B$ points in the $y$ direction, the CAF2 configuration with $M^{\text{orb}}$ pointing in the $y$ direction is favored, consistent with experiments.

Here we study the anisotropy of the orbital magnetization. We first consider the case where the local magnetiza-
The anomalous Hall conductivity as a function of the orbital magnetization $M_{\text{orb}}$ for (a) CAF1 and (b) CAF2, respectively. The anomalous Hall conductivity is given as

$$\sigma_{\text{AHE}} = \frac{\langle M_{\text{orb}} \rangle}{\mathcal{N}}$$

where $M_{\text{orb}}$ is the orbital magnetization, $\mathcal{N}$ is the number of unit cells, and $f(E_f)$ is the Fermi-Dirac distribution function. Figure 5 (c) shows the angle dependence of the orbital magnetization $M_{\text{orb}}(\phi, \theta)$, where $\phi$ is the in-plane tilting angle and $\theta$ is the out-of-plane tilting angle. Figure 5 (d) shows the total energy of electrons as a function of $\phi$ and $\theta$.

To study the anisotropy of the orbital magnetization, we decompose the Hall conductivity into two terms

$$\sigma_{\text{AHE}} = \sigma_{\text{AHE}}^{(I)} + \sigma_{\text{AHE}}^{(II)}$$

where $\sigma_{\text{AHE}}^{(I)} = \langle M_{\text{orb}} \rangle / \mathcal{N}$ and $\sigma_{\text{AHE}}^{(II)} = -e/\hbar \sum_{ijkl} v_{ij} G^{ik} v_{kl}$, with $G^{ik} = (\mu \pm i0 - \mathcal{H})^{-1}$ and $v_{ij} = \partial^2 \mathcal{H}/\partial p_i \partial p_j$. Near the peaks of the anomalous Hall conductivity, these quantities are close each other.

Weyl points—Finally, we study the Weyl points in the spec-
Here we consider the case where the energy dispersion is isotropic for simplicity. The Weyl points appear as pairs with opposite chiralities: the sign in the right hand side of eq. (11). $Q^{(o)}$ is the position of the Weyl point of $\alpha$th pair with the positive chirality, and $Q^{(e)}$ is that with the negative chirality. The separation of the Weyl points $\Delta Q^{(o)} = Q^{(o)} - Q^{(e)}$ can be realized when time-reversal and/or inversion symmetries are broken. When time-reversal symmetry is broken, the anomalous Hall effect occurs. In an ideal Weyl semimetal where all Weyl points appear at the same energy, say $\mu = 0$, the anomalous Hall conductivity is given by the sum of contributions from pairs of Weyl points separated by $\Delta Q^{(o)}$,

$$\sigma_{ij}^{\text{Weyl}} = \epsilon_{ijk} \frac{e^2}{2\pi\hbar} \sum \Delta Q_{k}^{(o)},$$  \hspace{1cm} (12)

at $\mu = 0.18,19$ In terms of decomposition of the anomalous Hall conductivity eq. (9), $\sigma_{ij}^{(o)} = 0$ because there is no finite Fermi surface at $\mu = 0$, vanishing the density of states. On the other hand, eq. (10) connects the Hall conductivity and the orbital magnetization, leading the relation$^{20}$

$$\mathbf{M}^{\text{orbital}} = -\frac{e\mu}{2\pi\hbar} \sum \Delta Q^{(o)}$$  \hspace{1cm} (13)

at the Fermi level $\mu$.

In our model the band dispersions are bent as shown in Fig. 6 so that hole pockets appear when the Fermi level resides at the Weyl point. The anomalous Hall conductivity and the orbital magnetizations are not as simple as eqs. (12) and (13). Nevertheless, qualitative behaviors such as the relation between the directions of the orbital magnetization, the anomalous Hall conductivity tensors, and the configurations of the Weyl points are the same as those. Indeed, the position of the Weyl points shown in Fig. 6 (a) are $\alpha^{-1}(\pm0.5341, \pm0.8948, \pm2.110)$ and $\alpha^{-1}(\pm1.948, \pm3.434, \pm3.565)$, and the sum of the relative displacements of all pairs, $\sum \Delta Q^{(o)} = \alpha^{-1}(0, 8.71, 0)$, point the $y$ direction. Thus, eq. (12) indicates that $\sigma_{xy}^R \neq 0$ and $\sigma_{yx} = \sigma_{xy}^E = 0$, and eq. (13) indicates that $M_x \neq 0$ and $M_y = M_z = 0$, consistent to the results shown in Figs. 3 and 4. The estimated value $\sigma_{xy}^R = 1.39 [e^2/ha]$ and $\partial M_y / \partial \mu = -1.39 [e/ha]$, from eq. (12) and eq.(13) respectively, are in reasonable agreement with the anomalous Hall conductivity $\sigma_{xy}^R = 1.21 [e^2/ha]$ and $\partial M_y / \partial \mu = -1.16 [e/ha]$ at $E = -1.96t_0$ in the lattice model shown in Figs. 3 and 4.

Conclusion— In this work we studied the anomalous Hall effect and the spontaneous orbital magnetization in chiral antiferromagnets. We showed that the single-band tight-binding Hamiltonian indicates an orbital ferromagnetic order with the easy-plane anisotropy. The symmetry relation between the anomalous Hall conductivity and the local spin configuration is characterized by the Weyl points and is consistent with experiments.

While we were finalizing the paper, a preprint Ref. 24 appeared. While we focus on itinerant electrons on Mn atoms, Ref. 24 focuses on $Z$ atoms in Mn$_3$Z where $Z$=Sn or Ge.

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Fig. 6. (a) Positions of Weyl points in momentum space. The sign $\pm$ corresponds to the chiralities of the Weyl points. (b) Direction of the Berry curvature around the Weyl points. Dotted circles indicate the positions of the Weyl points. (c)-(h) Energy dispersions around the Weyl points WP1 and WP2.

Weyl semimetals and Weyl metals are characterized by the presence of nondegenerate band-touching points (Weyl points) which appear as separated pairs in momentum space. In terms of the Berry curvature, Weyl points are synthetic magnetic monopoles, and thus contribute to the anomalous Hall conductivity. Here we focus on the Weyl points appearing between fourth band and fifth band in CAF2, where the anomalous Hall conductivity $\sigma_{xy}$ takes a maximum value around $E / t_0 = -2$ in Fig. 3 (d). The model Hamiltonian $\mathcal{H}(k)$ with parameters shown above has 16 Weyl points between fourth and fifth bands in the first Brillouin zone as shown in Fig. 6 (a). Figure 6 (b) shows the Berry curvature$^{11}$ of the fourth band in the vicinity of the Weyl point WP2 noted in Fig. 6 (a). By examining whether the Berry flux is inward or outward, the chirality of the Weyl points can be assigned by the sign $\pm$ in Fig. 6 (a). Figures 6 (c)-(h) show energy spectra near the Weyl points.

We now present a qualitative argument showing the relation between the directions of the orbital magnetization, anomalous Hall conductivity tensor, and the positions of the Weyl points. In a Weyl semimetal the low-energy excitations are described by the Weyl Hamiltonian$^{18,19}$

$$\mathcal{H}^{\alpha\beta}_{\text{Weyl}}(k) = \pm i\hbar v_F \sigma \cdot (k - Q^{(\alpha)}).$$  \hspace{1cm} (11)

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