Orbital ferromagnetism and anomalous Hall effect in antiferromagnets on distorted fcc lattice

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The Berry phase due to the spin wavefunction gives rise to the orbital ferromagnetism and anomalous Hall effect in the non-coplanar antiferromagnetic ordered state on face-centered-cubic (fcc) lattice once the crystal is distorted perpendicular to (1,1,1) or (1,1,0)-plane. The relevance to the real systems \(\gamma\)-FeMn and NiS\(_2\) is also discussed.

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It has been recognized for a long term that the chirality plays important roles in the physics of frustrated spin systems \cite{1-6}. These degrees of freedom are distinct from the (staggered) magnetization, and could show phase transition without magnetic ordering \cite{1,2}. Especially since the discovery of the high-T\(_c\) cuprates, the spin chirality mechanism \cite{12-15}. Proposed for example, in the charge transfer (CT) interaction ever observed \cite{24}. In particular the phenomenological Ginzburg-Landau theory for the 4-spin exchange interaction is given as \(H_4 = J_4 \sum_{a \neq b} (\vec{S}_a \cdot \vec{S}_b)^2\) \cite{19}. With positive \(J_4\), the ground state configuration is given by \(\vec{S}_1 = (\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}})\), \(\vec{S}_2 = (\frac{1}{\sqrt{3}}, -\frac{1}{\sqrt{3}}, -\frac{1}{\sqrt{3}})\), \(\vec{S}_3 = (-\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, -\frac{1}{\sqrt{3}})\), \(\vec{S}_4 = (-\frac{1}{\sqrt{3}}, -\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}})\), where each direction corresponds to the four corners from the center of a tetrahedron. This non-coplanar spin structure gives the scalar chirality in eq.(1) locally. For the itinerant system \(\gamma\)-FeMn, a recent band structure calculation \cite{20} concludes the stability of the triple-Q spin structure, in agreement with experiment \cite{7}.

In this paper we explore the chiral spin state in the ordered antiferromagnet (AF) on the three-dimensional face-centered-cubic (fcc) lattice. The AF on the fcc lattice is a typical frustrated system, and nontrivial spin structure with the finite spin chirality in eq.(1) is expected. For example, in the charge transfer (CT) insulator NiS\(_2\) \cite{18} and in the metallic alloy \(\gamma\)-FeMn \cite{17} the non-coplanar spin structure (so-called triple-Q structure shown in Fig. 1a) has been observed. A theoretical explanation for this structure is the following. Let us consider the case where the lattice points are divided into 4-sublattices as shown in Fig. 1a. Denoting the (classical) spin moment at each sublattice as \(\vec{S}_a\) \((a = 1, 2, 3, 4)\), the 2-spin exchange interaction energy is written as \(H_2 \propto (\sum_{a=1,4} \vec{S}_a)^2\). Therefore the condition of the lowest energy \(\sum_{a=1,4} \vec{S}_a = \vec{0}\) does not determine the spin structure and leaves many degenerate lowest energy configurations. Then the interactions which lift this degeneracy such as the 4-spin exchange interaction become important \cite{8,19}. Experimentally anomalous behaviors in the fcc AF are often observed. For example there occurs mysterious weak ferromagnetism (WF) in NiS\(_2\) below the second AF transition temperature \(T_{N2}\) \cite{21}. The Hall effect in this material is also large and strongly temperature dependent \cite{22}. In Co(S\(_3\)S\(_{1-x}\))\(_2\), the AHE is enhanced in the intermediate \(x\) region, where the nontrivial magnetism is realized \cite{23} and CeSb shows the largest Faraday rotation ever observed \cite{24}.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig1}
\caption{(a) Triple-Q spin structure on fcc lattice. (b) Relation of the 4-spin moments \(\vec{S}_a\) \((a = 1, 2, 3, 4)\). (c) Triangle lattice as a cross section of the fcc lattice perpendicular to \([1,1,1]\)-direction.}
\end{figure}

\begin{table}
\centering
\begin{tabular}{|c|c|}
\hline
Structure & Description \\
\hline
1:1 & \(\text{Basic unit cell of fcc lattice}\) \\
1:2 & \(\text{Sublattice division}\) \\
1:3 & \(\text{Interactions}\) \\
2:1 & \(\text{Energy terms}\) \\
2:2 & \(\text{Ground state configuration}\) \\
2:3 & \(\text{Chirality mechanism}\) \\
\hline
\end{tabular}
\caption{Summary of the chiral spin state in the ordered antiferromagnet (AF) on the three-dimensional face-centered-cubic (fcc) lattice.}
\end{table}
As shown below, the triple-Q AF state (Fig. 1a) on the distorted fcc lattice gives the orbital ferromagnetism accompanied by the AHE and even the realization of the three-dimensional quantum Hall liquid [28] without the external magnetic field.

The Hubbard on-site repulsive interaction $U$ can be decomposed in terms of the Stratonovich-Hubbard transformation as

$$U \frac{\phi_i^2}{2} - U \phi_i \cdot e^\dagger_{\alpha} \sigma_{\alpha\beta} e^{i\beta},$$

(2)

where $\sigma$ are the Pauli matrices and $\phi_i$ is the spin fluctuation field. This field acts as the local effective magnetic field for the electron, which can be regarded as the effective spin in the mean field approximation for the magnetically ordered state. The symmetry properties of the ground state is captured by this approximation, and the quantized Hall effect discussed below is stable against the fluctuation of the $\phi$-field as long as the gap does not collapse. Therefore we can consider this system as the free electron model in the background of the static field $U\phi_i$. In particular when this field $U|\phi_i|$ is much stronger than the transfer integrals $t_{ij}$'s, we can map the model into that of spinless fermions $H = -\sum_{ij} t_{ij}^\text{eff} f_i^\dagger f_j$ with the effective transfer integral

$$t_{ij}^\text{eff} = t_{ij}(|\chi_i|)$$

$$= t_{ij}(\cos \frac{\theta_i}{2} \cos \frac{\theta_j}{2} + \sin \frac{\theta_i}{2} \sin \frac{\theta_j}{2} e^{-i(\phi_i - \phi_j)}),$$

(3)

where $|\chi_i| = [\cos \frac{\theta_i}{2}, \sin \frac{\theta_i}{2} e^{i\phi_i}]^t$ is the spin wavefunction and $\theta_i$ and $\phi_i$ are the polar coordinates of the spin direction. The phase factor appearing in $t_{ij}^\text{eff}$ can be regarded as the gauge vector potential $a_\mu(r')$, and the corresponding gauge flux is related to $\chi_{ijk}$ in eqs. [30]. However, it should be noted here that the effective magnetic flux vanishes when averaged over the unit cell because of the periodicity of the vector potential $a_\mu(r') = a_\mu(r' + T_i)$ ($T_i$: primitive vector). Therefore, the net effect of the gauge flux comes from the fact that there are more than two atoms and/or orbitals in the unit cell and the resultant multiband structure. Then each band is characterized by the Chern number [26]. The Chern number appears as a multiband structure. Then each band is characterized by the Chern number [26]. The Chern number appears as a moment.

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where ± correspond to right- and left-handed chirality [8]. Here we consider the mass of the Dirac fermions at the edges of the BZ. For \( d > 0 \), the mass of the (2+1)D fermion along the \( k_y \)-axis is positive for every \( k_\mu \), while that changes sign at \( k_y = \pm D \) for \( d < 0 \).

Based on this observation, the transverse conductivity can be calculated in terms of the formula in [20]

\[
\sigma_{xy} = \sum_{n=1}^{4} \int \frac{d k_z}{2 \pi} \int_{[-\pi,\pi]^2} \frac{d k_y}{2 \pi i} f(\varepsilon_n(\vec{k})) \langle \nabla_{\vec{k}} \times \hat{A}_n(\vec{k}) \rangle_z
\]

where \( f(\varepsilon) \) is the Fermi distribution function, and \( \hat{A}_n(\vec{k}) = (n\vec{k})\nabla_{\vec{k}} |n\vec{k}\rangle \) is the vector potential created by the Bloch wavefunction \(|n\vec{k}\rangle\). Let us consider \( \mu = 0 \) case, i.e. quarter filled case. \( \sigma_{xy}(k_z) \) is the Hall conductance in (2+1)D system with fixed \( k_z \), which is determined by the parity anomaly caused by the Dirac fermions along the edge of the BZ. Explicit calculation shows at \( T = 0 \)K, \( \sigma_{xy}(k_z) = -\frac{e^2}{h} \text{sign}(f_2(k_z) \cdot d) \) where \( f_2(k_z) = (4 - 2d) \cos(k_z^2) + 2d \sin(k_z^2) \). For \( d > 0 \), \( \sigma_{xy}(k_z) = -\frac{e^2}{h} \) for all \( k_z \), while \( \sigma_{xy}(k_z) = \frac{e^2}{h} \) for \( k_z = (-D, D) \) and \( \sigma_{xy}(k_z) = -\frac{e^2}{h} \) for \( k_z = [-\pi, -D) \) and \( [D, \pi] \) in the case of negative \( d < 0 \). Integrating over \( k_z \), we obtain \( \sigma_{xy} = -\frac{e^2}{h} \) for \( d > 0 \) and \( \sigma_{xy} = \frac{e^2}{h} \left[ \frac{\arcsin(\sqrt{\frac{1-2d}{4d}})}{\pi} - 1 \right] \) for \( d < 0 \), while \( \sigma_{xy} \) vanish for \( d = 0 \).

One can easily confirm that \( \sigma_{xy} = \sigma_{yz} = \sigma_{zx} = \sigma_H \), and that the sign of \( \sigma_H \) changes when all the spins \( \hat{S}_a \) are inverted \( (\hat{S}_a \rightarrow -\hat{S}_a) \). One can confirm analytically in eq. (4) that the cancellation between the contributions from the two \( \vec{k} \)-points related by the parity \( \text{P} \) symmetry, e.g. \((k_x, k_y, k_z)\) and \((-k_x, k_y, k_z)\), occurs and \( \sigma_{xy} \) is zero for the undistorted fcc lattice. This remains true even when we modify \( \hat{S}_a \) from those given in Fig. 1b. For example even with finite magnetization \( (\sum_{a=1}^{4} \hat{S}_a \neq 0) \), \( \sigma_{xy}(\omega) = 0 \) for any \( \omega \) on the undistorted fcc lattice. In short, P-symmetry is not broken while T-symmetry is broken in the undistorted fcc lattice, where finite \( \sigma_H \) is forbidden. An distortion along \([1,1,1]-\text{direction does break this P-symmetry and produces finite } \sigma_H \).

Next we turn to the half filled case. When the chemical potential is in the Mott gap, i.e. Mott insulator, the d.c. \( \sigma_H \) vanishes. However the optical \( \sigma_H(\omega) \) can be finite, which corresponds to the Faraday and/or the Kerr rotation. In order to calculate \( \sigma_H(\omega) \), we have to take into account optical transitions between the lower and the upper Hubbard bands. In the mean field picture, this corresponds to the two splitted bands due to the effective magnetic field \( U_i \hat{\sigma}_i \) in eq.(2). Diagonalizing the tight-binding Hamiltonian with this local “magnetic field”, we can calculate \( \sigma_H(\omega) \). \( \sigma_H(\omega) \) shown in Fig. 2 is for \( d = -0.1, U_i |\hat{\sigma}_i| = 5 \).

![FIG. 2. \( \sigma_H(\omega) \) for \( d = -0.1, U_i |\hat{\sigma}_i| = 5 \)](image)

Now we turn to the orbital ferromagnetism induced by the distortion. Orbital magnetization \( M \) is given by

\[
M = \lim_{B \to 0} \int_{-\infty}^{\epsilon_F} \frac{\partial N(B, \mu)}{\partial B} d\mu.
\]

In terms of the Středa formula [29], i.e. \( \sigma_{xy} = \frac{\sigma_{xy}^I|\mu| + ec \frac{\partial N(B, \mu)}{\partial B}}{\sigma_{xy}^I|\mu|} \) with \( \sigma_{xy}^I|\mu| = \frac{1}{2m} \text{Tr}[J_i G^+(\mu) J_i G^-(\mu)] \), we estimate the integrand in eq.(4) from \( \sigma_{xy}|\mu \) and \( \sigma_{xy}^I|\mu \).

![FIG. 3. Magnetization \( M \) as a function of \( d \), where \( U_i |\hat{\sigma}_i| = 5 \) (we set \( \frac{\delta}{\delta t_{\text{intra}}} = 1 \'))](image)

Shown in Fig. 3 is the orbital magnetization \( M \) as a function of the distortion \( d \) for the half filled case. The sign of orbital magnetization \( M \) changes when all the spins are inverted. (Magnetization depicted in Fig. 3 corresponds to the triple-Q structure in Fig. 1a,b.) Note that \( M \) is finite even though the d.c. \( \sigma_H = 0 \) in this case, because the former is determined by the integral over the occupied states.

In real materials, the configuration with all the spins being inverted (which means that the chirality is also inverted) has the same energy. Thus it is expected that the
domain structure of these two chirals is formed. In order to align this chiral domain, we must cool down into AF order phase by applying external strain and external magnetic field, which couples to the orbital magnetization and prefers one of the chiral domain. (For $d > 0$, the magnetic field in [1,1,1]-direction prefers the triple-Q structure as in Fig. 1a,b.) Lastly it is noted here that the distortion along [1,1,0] or other three equivalent directions produces the similar effect as discussed above, while that along [1,0,0] etc. does not. This also offers a way to test this idea experimentally.

Now we discuss the experimental relevance of these results. One of the most promising materials for this spin chirality mechanism is the itinerant AF $\gamma$-Fe$_2$Mn$_{1-x}$Al alloy as mentioned above [17]. In this material, the triple-Q structure is observed for $0.35 < x < 0.8$. This material remains metallic even below $T_N$. Because the crystal structure is the undistorted fcc, one needs to apply uniaxial pressure to produce $\sigma_H$ of the order of $e^2/\hbar a \approx 14000 d^{-1} c^{-1}$ for $a = 3.6 \AA$ when the chiral domains are aligned by the field cooling.

Another candidate is the CT insulator AF NiS$_2$. In this material the valence of Ni is $2+$, and the angular orbital moment is quenched with $d^8$ configuration. Thus spin-orbit interaction is expected to be small, and this material is an ideal laboratory to study the spin chirality mechanism. It shows two successive magnetic phase transitions at $T_{N1} = 40$K and $T_{N2} = 30$K. Between $T_{N1}$ and $T_{N2}$, the magnetic structure is given by Fig. 1a,b (type I AF state). At $T_{N2}$ the type II AF structure appears in addition to the type I structure. This is accompanied by the rhombohedral distortion and with the mysterious WF [21]. This lattice distortion ($d > 0$) lifts the quasi-degeneracy of type I and type II structures [22]. This brings about finite orbital ferromagnetism, which can be detected by hysteresis in the magnetization curve under the magnetic field. Therefore the present results give a possible scenario for the WF in NiS$_2$. Even in the temperature range between $T_{N1}$ and $T_{N2}$, where lattice is not distorted spontaneously, suppression towards [1,1,1] or [1,1,0]-direction is predicted to bring about an orbital ferromagnetism. (The compressibility of this material is of the order of $10^{-3}$ bar$^{-1}$ [23] and we need $\sim 140$kbar uniaxial pressure to produce $d = -0.1$ for example.) Although the d.c. $\sigma_H(\omega)$ is zero at $T = 0$K, the optical $\sigma_H(\omega)$ is expected to be finite, as shown in Fig. 2. As for other fcc AF such as Co(S$_2$Se$_1$)$_2$, detailed studies on the spin structure by neutron scattering are highly desirable, with which the mechanism of the Hall effect can be dictated.

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