Non-topological Anomalous Hall Effect in States with zero Magnetic Moment per unit-cell

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We show that a finite Hall effect in zero field for partially filled bands can occur in time-reversal violating states with zero net flux per unit-cell for parameters in the effective one-particle Hamiltonian such that the states are not topological.

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I. INTRODUCTION

A Faraday rotation of the polarization of photons in transmission or a Kerr effect in reflection must accompany a state which has a non-zero off-diagonal conductivity $\sigma_{xy}$. A Kerr effect with unusual properties has been discovered in underdoped cuprates\(^\text{2}\) below a temperature which in two families of cuprates coincides with the so-called pseudogap temperature $T^*$ deduced through several transport and thermodynamic measurements\(^\text{3}\). Within some uncertainty, this is also the temperature in which evidence for a state with broken time-reversal has been presented in these compounds by polarized neutron scattering\(^\text{4}\). The symmetry of the state is consistent with the prediction of a state with orbital current loops in each unit-cell with opposite chirality, which breaks both time-reversal and inversion and preserves their product and conserves translational invariance (A magneto-electric (ME) state)\(^\text{5}\). This ME state cannot have a finite $\sigma_{xy}$, i.e. a Kerr effect in zero applied magnetic field. But as discussed in a recent paper\(^\text{6}\), a state with an anomalous Hall effect (AHE) must be induced in the ME state in the presence of perturbations which independently break the reflection symmetries of the lattice. The induced state has the current pattern in a unit-cell exhibited in Fig. 1 and has been called a Magneto-Chiral (MC) state\(^\text{6}\)\(^\text{7}\). The discussion in Ref. \(^\text{8}\) was done for a three band model with parameters such that they are an extension of the topological state discussed by Haldane\(^\text{9}\) for a two band model.

The purpose of this paper is not so much to dwell further on the Kerr effect in the cuprates but to discuss a general feature of AHE for states which have zero magnetic moment per unit-cell but are not topological states. To this end, we do however continue the discussion in the context of the three orbital model already treated but with more general parameters than in Reference \(^\text{8}\). The general point we wish to make is that in a time-reversal violating state a current is carried by each eigenstate $\mathbf{k}$ of any of the bands. Additional symmetries may make the sum of states up to the chemical potential add up to 0 in many cases, but this is not true always. In that case there is a finite $\sigma_{xy}$. Orenstein\(^\text{10}\) has also discussed symmetry of various magneto-electric states with zero total magnetic moment per unit-cell in which a finite $\sigma_{xy}$ must exist. Nonzero $\sigma_{xy}$ is also found for systems which break handedness but not time reversal as in a solid made up of chiral molecules\(^\text{11}\) and recently invoked\(^\text{12}\). Variants of the ME state with chirality in going form one plane to the other have also been recently invoked for the phenomena observed in the cuprates\(^\text{13}\). Our result can be understood as a special case of the intrinsic anomalous Hall effect\(^\text{14}\) where the Hall conductivity is written as

$$\sigma_{xy} = \frac{e^2}{\hbar} \sum_n \int \frac{dk}{(2\pi)^2} F_z(k) f(\varepsilon_n(h)) \tag{1}$$

where $F(k) = \nabla_k \times A(k)$ is the Berry curvature and $A(k)$ is the Berry phases in momentum space. The intrinsic anomalous Hall effect can also be understood semi-classically by the appearance of the “anomalous velocity” $\mathbf{v}_{\text{anom}} = -\frac{e}{\hbar} \mathbf{E} \times \mathbf{F}(k)$ in the formula for the velocity $\mathbf{v}(k) = \frac{1}{\hbar} \frac{\partial \mathbf{E}(k)}{\partial \mathbf{k}} + \mathbf{v}_{\text{anom}}(k)\(^\text{15}\). Equation (1) is most commonly applied to the case where there is time reversal symmetry breaking by a uniform magnetization as in a ferromagnet but it is clear that $\sigma_{xy}$ can be nonzero as long as $F_z$ is nonzero in some part of the Brillouin zone. Furthermore, in the case of partially filled bands, whether the band has nonzero Chern number or not should not play an important role. In this paper we work this out in detail for a model where time reversal is broken but the net moment in a unit cell is zero.
II. MODEL

Several different translation preserving time-reversal breaking states through orbital currents are possible in the three band model of the cuprates. The proposed state with AHE has two current loops in a unit-cell as shown in Fig. 1. Such states may in general be called Magneto-Chiral (MC). In the model for graphene, Haldane showed the limits in parameters in which the state is topological, i.e. the state has an integral value of \( \sigma_{xy} \) in units of \( e^2/h \) or an integral Chern number for one band filled and another totally unfilled as well as described a metallic state which has unquantized Hall effect under the same circumstances. The condition on the parameters is related to the occurrence of degeneracy for states in the two bands which can be discussed as leading to a topological charge or a monopole somewhere in the Brillouin zone. In an earlier paper, Haldane’s ideas were implemented in the three-band model for cuprates with a partially filled band. But the condition in which the complete band has a finite Chern number, i.e. the state is topological are rather restrictive. We show here that a finite \( \sigma_{xy} \) occurs in far less restrictive conditions than required for a non-zero Chern number for any of the bands. This is shown in the context of the three band model of cuprates but it will be clear that the results are more general.

We consider the loop current model depicted in Fig. 1, with the current flowing between the oxygen atoms. In the space of the three orbitals, \( d \) for Cu, \( p_x \) and \( p_y \) for the two Oxygens in each unit-cell, a general Hamiltonian is

\[
H = \sum_{bfk} H_k, \text{ with }
\]

\[
H_k = \begin{pmatrix}
E_d & it s_x & is y \\
itos_x & E_p & t_p s_x s_y + irc x c_y \\
its_y & t_p s_x s_y - irc x c_y & E_p
\end{pmatrix}
\]

(2)

with \( s_x = \sin(k_x/2) \) and \( c_x = \cos(k_x/2) \), etc. Previously we considered only the case \( E_d = E_p \) in which the state is topological. We consider here the more general situation \( E_d \neq E_p \).

In (2), it does not matter if we subtract a constant matrix as well as make it traceless. We can make the problem even simpler, by taking \( t_p = 0 \). As long as \( t_p \) is not too big, there is no band crossing when \( t_p \) decreases to 0. So \( t_p = 0 \) leads to no qualitative difference in the calculated properties. Therefore we consider the simpler Hamiltonian (where we have taken \( t = 1 \) for convenience):

\[
H = \begin{pmatrix}
\frac{2}{3} E_d & is x & is y \\
-its_x & -\frac{1}{3} E_d & irc x c_y \\
-its_y & -irc x c_y & -\frac{2}{3} E_d
\end{pmatrix}
\]

(3)

A. Change in Chern number as \( E_d \) increases from 0 to \( \infty \)

For the two band model, there is a relation between Chern number and winding number which provides an analytical result for the Chern number. The 3-band model is too complicated to find a analytical formula for the Chern number directly in this manner. We will instead use an indirect way to find its Chern numbers.

When \( E_d = 0 \), we know that the Chern numbers are \(-1, 0, 1\) from the top to the bottom bands. Now we show that when \( E_d \) increases from 0 to \( \infty \), band degeneracy between the top and the middle band only occurs at \( E_d = r \) and the Chern number of any band is non-zero only for \( E_d < r \).

The band energies are determined from

\[
\det(H - \lambda I) = \lambda^3 + p \lambda + q = 0
\]

(4)

\[
p = -E_d^3/3 - c_x^2 r^2 - s_x^2 - s_y^2
\]

\[
q = E_d/27 (-2 E_d - 9 s_x^2 - 9 s_y^2 + 18 r^2 c_x^2 s_y^2)
\]

The discriminant of the above equation is

\[
\Delta = 4 p^2 + 27 q^3 = A_1 + A_2 + A_3 + A_4
\]

\[
A_1 = -4r^2 c_x^2 s_y (E_d^2 - c_x^2 s_y^2)^2
\]

\[
A_2 = -12 r^4 c_x^2 c_y^2 (s_x^2 + s_y^2)
\]

\[
A_3 = -(s_x^2 + s_y^2)^2 [E_d^2 + (s_x^2 + s_y^2)]
\]

\[
A_4 = -4 r^2 c_x^2 c_y^2 (5 E_d^2 + 3 s_x^2 + s_y^2) (s_x^2 + s_y^2)
\]

It is easy to see that \( A_i \leq 0 \) for \( i = 1, \ldots, 4 \). From \( A_{2,3,4} = 0 \), we find that \( s_x = s_y = 0 \) or \( k_x = k_y = 0 \). From \( A_1(k_x = 0, k_y = 0) = -4r^2 (r^2 - E_d^2)^2 \), we find \( E_d = r \). Therefore the only degeneracy point is located at \( k_x = k_y = 0 \) with \( E_d = r \). In the parameter space \( k_x, k_y, E_d \) this point can be thought as a monopole, as discussed earlier. When \( E_d \) passes from less than \( r \) to greater than \( r \), there is a jump of Chern numbers for both the top and the bottom bands. But the sum of the Chern numbers of these two bands is the same as before. The change of Chern number of top band equals...
the monopole charge or the Berry curvature flux through a small sphere enclosing the monopole. To see this we expand the Hamiltonian around \( k_x = k_y = 0 \) and \( E_d = r \).

\[
H = \begin{pmatrix}
\frac{2}{3}(r + \epsilon/\sqrt{2}) & -ik_x/2 & ik_y/2 \\
-ik_x/2 & -\frac{1}{3}(r + \epsilon/\sqrt{2}) & ir \\
-ik_y/2 & -ir & -\frac{1}{3}(r + \epsilon/\sqrt{2})
\end{pmatrix}
\]

To the first order in \( k_x, k_y \) and \( \epsilon \), we find the eigenstate of the top band

\[
\psi = \frac{1}{\sqrt{4R(R - \epsilon)}} \begin{pmatrix} \sqrt{2}(k_x - ik_y) \\ i(\epsilon - R) \\ \epsilon - R \end{pmatrix}
\]

Here \( R = \sqrt{\epsilon^2 + k_x^2 + k_y^2} \). It is easy for this case to calculate the Berry phase and Berry curvature,

\[
A_{x,y} = -i\psi^\dagger \frac{\partial}{\partial x_{x,y}} \psi, \quad F = \frac{\partial}{\partial k_x} A_y - \frac{\partial}{\partial k_y} A_x
\]

Then we find that the \( 1/2\pi \) times the integral of the Berry curvature over the Brillouin zone is equal to 1. We can then show that the Chern number of the top band increases by 1 and of the middle band decreases by 1 as \( E_d \) goes across the degeneracy point \( E_d = r \). We will verify this below by a numerical calculation. This leads to the conclusion that for \( t_p \) not too large, the Chern number of the top band is

\[
c_1 = -1 \quad \text{for} \quad 0 < E_d < r
\]

\[
c_1 = 0 \quad \text{for} \quad E_d > r
\]

Although the top band has zero Chern number for \( E_d > r \), the Berry phase and the Berry curvature are not identically zero. By taking a fixed \( \epsilon > 0 \), we can see that \( F > 0 \) around \( k_x = k_y = 0 \). We must have \( F < 0 \) in the rest of the BZ in order to cancel the positive contribution from around \( k_x = k_y = 0 \). Then for fully filled top band \( c_1 = 0 \). To evaluate \( \sigma_{xy} \) for arbitrary filling of the bands however requires a numerical calculation.

### III. NUMERICAL RESULT FOR \( \sigma_{xy} \)

In the last section, we expanded the Hamiltonian around \( k_x = k_y = 0 \), and obtained only the formula of Berry phase and curvature around this region. In the general case, the wave function of the top band is

\[
\psi = C_N \left( \begin{array}{c} is_y(E_d + E_1) - rs_x c_x c_y \\
rs_x s_y - ir c_x c_y (2E_d - E_1) \\
(2E_d - E_1) - s_x^2 \end{array} \right)
\]

Here \( C_N \) is the normalization factor to make \( \psi^\dagger \psi = 1 \). \( E_1 \) is the largest root of cubic equation Eq. (4). Thus \( E_1 \) is an implicit function of \( k_x \) and \( k_y \). As \( k_x, k_y \) vary, the order in energy of the 3 roots may change; therefore we do not have an explicit formula for \( E_1 \). We can only symbolically write it as

\[
E_1 = \max_{n=0,1,2} \omega n \left\{ \sqrt{\frac{q^2}{2} + \frac{p^2}{27}} + \omega n \sqrt{\frac{q^2}{2} + \frac{p^2}{27}} \right\}
\]

Here \( p, q \) are defined under Eq. (4), and \( \omega = \frac{-i\sqrt{3}}{\epsilon} \). We can compute \( dE_1/dk_x \), etc, but the result is too lengthy to write here. Similarly directly plugging in Eq. (10) into the expressions for the Berry Phase and Berry curvature generates a very complicated result. So we pursue an alternate strategy suggested by Hatsugai et al.\textsuperscript{12}

It is much easier to take the Brillouin zone for a discrete lattice and find out the eigenstates at each point numerically. Let \((i, j)\) label lattice sites. Then \( k_x = \frac{2\pi i}{N} \), \( k_y = \frac{2\pi j}{N} \) for \( i, j = 0, 1, \ldots, N \). At site \((i, j)\), numerically diagonalize \( H \) and find the top band eigenvector \( \psi(i, j) \). Then we can define Berry phase as the phase difference of two eigenvector located at the neighboring sites of each links of the lattice,

\[
U_x(i, j) = \frac{\psi(i, j) \cdot \psi(i + 1, j)}{|\psi(i, j) \cdot \psi(i + 1, j)|}, \quad U_y(i, j) = \frac{\psi(i, j) \cdot \psi(i + 1, j)}{|\psi(i, j) \cdot \psi(i + 1, j)|}
\]

The \( \psi(i, j) \) and \( U_x(i, j) \) defined this way are gauge dependent and contain an arbitrary gauge factor. If we take a product of link variables \( U \) around a closed loop, then the arbitrary phase factor cancels out. Therefore we can define the gauge invariant Berry curvature for each plaquette as

\[
F(i, j) = -i \ln \left[ U_x(i, j) U_y(i + 1, j) \right] \times U_x^{-1}(i, j + 1) U_y^{-1}(i, j)
\]

Here \( F \) is just the phase angle of the quantity inside the bracket; as a convention we assume \( -\pi < F < \pi \). Then the Chern number is

\[
c = \frac{1}{2\pi} \sum_{i,j} F(i, j)
\]

All the above are standard definitions of vector field and field strength in lattice gauge field theory. Hatsugai et al.\textsuperscript{12} point out that this method provides a very efficient way to compute Chern number numerically.\textsuperscript{15} Even for a very small lattice such as 4 by 4, it generates the correct Chern number. The following results are obtained by this method.

Now we show the numerical results of the partially filled band conductance \( \sigma_{xy} \) in figure (2). In Figure (2), we take \( t = 1, t_p = 0.5, r = 0.1 \) and \( E_d = 0.15 \). In the left panel, we plot \( \sigma_{xy} \) as a function of filling factor. In
the right panel we plot $\sigma_{xy}$ as a function of the chemical potential $\mu$. Since the energy minima of the top band is located at $k_x = k_y = 0$, the fermions first fill the region around $k_x = k_y = 0$. In this region the Berry curvature is positive; therefore $\sigma_{xy}$ is positive at first. When the fermi energy or the filling factor increases, we integrate an increasingly larger area such that we begin to get a negative contributions from the points far away from $k_x = k_y$. When the filling approaches 1, $\sigma_{xy}$ gradually approaches 0.

In the above discussion $r$ is fixed and $E_d$ is changed. This is equivalent to fixing $E_d$ and sweeping $r$. In figure 3, we take $t = 1$, $t_p = 0.5$ and $E_d = 0.1$, and plot $\sigma_{xy}$ at half-filling as a function of $r$. From Eq. (14), we can see that around BZ center ($k_x = k_y = 0$), $F > 0$ for $E_d > r$ and $F < 0$ for $E_d < r$. In both cases, the band bottom is at BZ center. For half filling, the filled region is roughly a circle enclosing the BZ center, thus $\sigma_{xy} > 0$ for $E_d > r$ and $\sigma_{xy} < 0$ for $E_d < r$. This is why there is a jump when $r$ passing through $E_d$. For $r < E_d$, at half filling, the physical point is that time-reversal with net zero moment per unit-cell has finite current carried by each $k$ state. If the symmetry is such that a given $k$ state does not have a degenerate partner under reflection or inversion carrying current in the opposite direction, there is a finite $\sigma_{xy}$.

For the experimental effects which led to the original investigation, the present more general results lead only to a small modification in the magnitude of the Kerr effect.

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