

Berry phase and anomalous Hall effect in a three-orbital tight-binding Hamiltonian

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We consider the anomalous Hall (AH) state induced by interactions in a three-orbital per unit-cell model. To be specific, we consider a model appropriate for the copper-oxide lattice to highlight the necessary conditions for time-reversal breaking states which are AH states and which are not. We compare the singularities of the wave functions of the three-orbital model, which are related to the nonzero Berry curvature, and their variation with a change of gauge to those in the two-orbital model introduced in a seminal paper by Haldane. Explicit derivation using wave functions rather than the more powerful abstract methods may provide additional physical understanding of the phenomena.

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I. INTRODUCTION

In asking the question whether a quantized Hall effect may exist, in principle, without an applied magnetic field, Haldane¹ introduced an effective one-electron model on the two-orbital per unit-cell hexagonal crystal with complex next nearest transfer integrals. This has turned out to be a fecund contribution. It further augmented the topological arguments of Thouless and collaborators² for the quantum Hall effect. It also introduced the general discussion of the topological features of band structures in two dimensions and in particular led through further imaginative work to the suggestion and discovery of topological insulators.³⁻⁶ Haldane's model also showed the connection of topological properties to the time-reversal-violating states due to orbital current loops in the lattice without changing translational invariance; see Fig. 1.

Orbital current loops without changing translational symmetry were predicted to arise as broken symmetry states due to interactions in a three-orbital per unit cell model for underdoped cuprates⁷⁻⁹ and have been discovered in several families of cuprates.¹⁰⁻¹² These loop-current states, however, do not lead to the quantized anomalous Hall effect (QAHE) or “Chern insulator” discussed by Haldane. The difference is that the loop-current states violate both time reversal \mathcal{R} and inversion \mathcal{I} but preserve their product \mathcal{I} . It was pointed out by Fradkin and Sun¹³ that there is no QAHE effect when $\mathcal{R}\mathcal{I}$ symmetry is present; they also pointed out that a QAHE state for the three-orbital cuprate model is possible, in principle, through a state with symmetry different from that observed.

In this paper, we elaborate on the work of Fradkin and Sun by deriving the Berry phase responsible for the QAHE state and also how the singularities of the wave functions vary with the choice of gauge. When the topologically active band (i.e., the one with nonzero Chern number or TKNN integer²) is partially rather than completely filled, the Berry phase will still contribute to a nonquantized intrinsic anomalous Hall effect.¹⁴⁻¹⁷ For comparison, we also rederive wave functions for the two-orbital case. The physics of the three-orbital model is not surprising in the context of previous general work on topological effects in noninteracting lattice models; we hope that we have discussed it in a new fashion which will be useful to nonexperts and that the particular model explains

how topological effects might appear in three-band materials. Whenever possible we seek to explain the value of a Berry-phase calculation geometrically rather than simply stating the result. We also work with explicit wave functions rather than more powerful abstract methods, although a few comments are provided regarding the latter.

II. ANOMALOUS HALL STATES IN THE CU-O MODEL

Consider the two-dimensional lattice with the structure of the copper oxides; see Fig. 2. There are three orbitals per unit cell—the d orbital on the copper atom and the p_x and p_y orbitals on the oxygens. The minimal kinetic energy operator with a choice of gauge such that the d orbital, p_x orbital and the p_y orbital are purely real imaginary is

$$H_{\text{KE}} = it d_{\mathbf{k}}^{\dagger} (s_x p_{x,\mathbf{k}} + s_y p_{y,\mathbf{k}}) - t' s_x s_y p_{x,\mathbf{k}}^{\dagger} p_{y,\mathbf{k}} + \text{H.c.} \quad (1)$$

with $s_x = \sin(k_x/2)$ and $s_y = \sin(k_y/2)$ for a lattice constant taken to be 1. For simplicity, let the fermions be spinless. Consider only the interaction between the p orbitals,

$$H_{\text{int}} = \sum_{(i,j)} V n_{p,i} n_{p,j}. \quad (2)$$

Following the procedure with which some time-reversal violating states were derived for the cuprates, we use the operator identity (for spinless fermions),

$$n_i n_j = -\frac{1}{2} (|j_{ij}|^2 + n_i + n_j), \quad (3)$$

where j_{ij} is the self-adjoint operator,

$$j_{ij} = i(c_i^{\dagger} c_j - c_j^{\dagger} c_i). \quad (4)$$

Decomposing [In general the diagonal in spin indices part of $n_i n_j$ gives Eq. (3); the nondiagonal can be written in terms of products of spin currents with which mean-field theory gives the possibility of symmetry breaking topological spin-current states. [The decompositions of the operator may also be done without the i in Eq. (3) from which various Pomeranchuk instabilities may be derived for symmetry breaking in various irreducible representations for spin and charge densities.] the interaction term in Eq. (2), by defining

$$(V/2) \langle j_{ij} \rangle = ir, \quad (5)$$

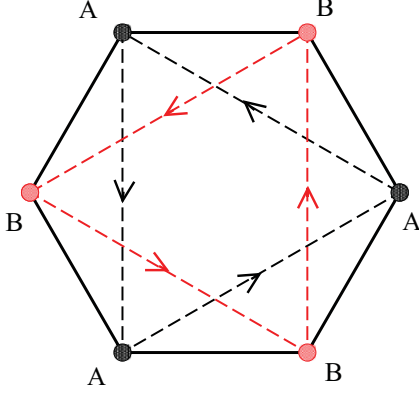


FIG. 1. (Color online) Schematic figure of loop currents connecting the A sub-lattice and the B sub-lattice within the unit-cells of a hexagonal lattice which preserves inversion about the center of the hexagonal cell. A state which such loop currents has an anomalous Hall effect.

and doing a mean-field calculation, one finds an additional kinetic-energy term,

$$H'_{\text{int}} = i r c_x c_y p_{x,\mathbf{k}}^\dagger p_{y,\mathbf{k}} + \text{H.c.} \quad (6)$$

If $r \neq 0$ is a stable state, it describes loop currents flowing clockwise (or counterclockwise) around the oxygens in each unit cell as shown in Fig. 2. This is one of the five possible loop-current states with nonoverlapping loops in the Cu-O lattice, all of which preserve translational symmetry.¹⁸ In Eq. (2), the flux has one sign in the square formed by the nearest-neighbor oxygens which surround a Cu and another sign in the square formed by the nearest-neighbor oxygens which do not surround a Cu. As pointed out by Fradkin and Sun,¹³ such a time-reversal violating state, which does not change translational symmetry or break inversion symmetry, satisfies all the conditions of a Haldane state for the Cu-O lattice. The other four loop-current states do not. One of those is just the photon on a lattice and cannot order. The other three can order and indeed order consistent with the symmetry of two of them (in different domains) is observed in underdoped cuprates. So, our consideration of states such as those in Fig. 2 is only a specific example to illustrate the nature of anomalous Hall (AH) states in three-orbital models.

We will consider the Haldane state (quantized anomalous Hall effect) of the Cu-O model and therefore the singularities of the model with the Hamiltonian $H = H_{\text{KE}} + H'_{\text{int}}$. Before we do that, let us consider the simpler case of two orbitals per unit cell.

III. TWO-BAND MODELS

A general Hamiltonian in the space of two orbitals per unit cell may be written as, ignoring an overall shift of the energy that does not affect the Berry phase and assuming that there is no basis of the Bravais lattice,

$$H = \mathbf{R}(\mathbf{k}) \cdot \boldsymbol{\sigma} = \begin{pmatrix} R_3 & R_1 - i R_2 \\ R_1 + i R_2 & -R_3 \end{pmatrix}. \quad (7)$$

Here R_i for $i = 1, 2, 3$ are some smooth functions of k_x and k_y with period 2π . For now, we do not need the detailed

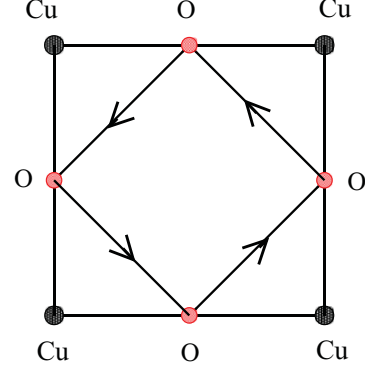


FIG. 2. (Color online) Schematic figure of a loop current state in the Cu-O lattice, which has an anomalous Hall effect. This is not the state which is realized in the Cuprates but is discussed in this paper for its interest as a simple model for possible anomalous Hall effect in a three band model.

form of these functions. It is easy to diagonalize the above Hamiltonian to find that there are two bands, $E = \pm R$, with $R = \sqrt{R_1^2 + R_2^2 + R_3^2}$.

Consider the lower band, $E = -R(\mathbf{k})$. The eigenstate can be written in two ways corresponding to two different choices of gauge (the point of studying apparent consequences of the choice of gauge will be clear in a later section of the paper):

$$|\psi^A\rangle = \frac{1}{\sqrt{2R(R-R_3)}} \begin{pmatrix} R_3 - R \\ R_1 + i R_2 \end{pmatrix}, \quad (8)$$

$$|\psi^B\rangle = \frac{1}{\sqrt{2R(R+R_3)}} \begin{pmatrix} R_1 - i R_2 \\ -R - R_3 \end{pmatrix}. \quad (9)$$

They are connected by a $U(1)$ gauge transformation

$$|\psi^B\rangle = e^{i\phi} |\psi^A\rangle, \quad \text{with } e^{i\phi} = \frac{-R_1 + i R_2}{\sqrt{R_1^2 + R_2^2}}, \quad \phi = -\arctan\left(\frac{R_2}{R_1}\right). \quad (10)$$

Then the *Berry phase*, A_μ , is also gauge dependent, given for the two choices respectively by

$$A_\mu^A \equiv -i \langle \psi^A | \nabla_\mu | \psi^A \rangle = -\frac{1}{2R(R-R_3)} \left(R_2 \frac{\partial R_1}{\partial k_\mu} - R_1 \frac{\partial R_2}{\partial k_\mu} \right), \quad (11)$$

$$A_\mu^B \equiv -i \langle \psi^B | \nabla_\mu | \psi^B \rangle = \frac{1}{2R(R+R_3)} \left(R_2 \frac{\partial R_1}{\partial k_\mu} - R_1 \frac{\partial R_2}{\partial k_\mu} \right). \quad (12)$$

A_μ 's are also connected by a $U(1)$ gauge transformation:

$$A_\mu^B = A_\mu^A + \nabla_\mu \phi, \quad \nabla_\mu \phi = \frac{1}{R^2 - R_3^2} \left(R_2 \frac{\partial R_1}{\partial k_\mu} - R_1 \frac{\partial R_2}{\partial k_\mu} \right). \quad (13)$$

The *Berry curvature* is gauge invariant and given by

$$F_{xy} = \frac{\partial A_y}{\partial k_x} - \frac{\partial A_x}{\partial k_y} = \frac{1}{2R^3} \epsilon_{abc} R_a \frac{\partial R_b}{\partial k_x} \frac{\partial R_c}{\partial k_y} = \frac{1}{2} \epsilon_{abc} \hat{R}_a \frac{\partial \hat{R}_b}{\partial k_x} \frac{\partial \hat{R}_c}{\partial k_y}. \quad (14)$$

Here $\hat{\mathbf{R}} = \mathbf{R}/R$ is a unit vector. If we integrate over the entire Brillouin zone, we find

$$c = \frac{1}{2\pi} \int d^2k F_{xy} = \frac{1}{4\pi} \int d^2k \epsilon_{abc} \hat{R}_a \frac{\partial \hat{R}_b}{\partial k_x} \frac{\partial \hat{R}_c}{\partial k_y}. \quad (15)$$

This is the well-known result¹⁹ that the Chern number of a two-band model is equivalent to the winding number of the mapping from a two-dimensional (2D) Brillouin zone which is 2D torus (T^2) to the 2D unit sphere (S^2). This mapping can be understood by taking spherical coordinates $\mathbf{R} = R(\sin\theta \cos\phi, \sin\theta \sin\phi, \cos\theta)$. The wave function can be written as $|\phi\rangle = [-\sin(\theta/2), \cos(\theta/2)e^{i\phi}]$, which is a two-component spinor. The unit sphere is just the Bloch sphere $\hat{\mathbf{R}} = -\langle\phi|\sigma|\phi\rangle$ associated with this spinor.

The Berry phase \mathbf{A} is a vector field defined on the momentum space or the torus. Since the torus is mapped to a sphere, one can also think of the Berry phase as defined on this sphere. In spherical coordinates, we have

$$\mathbf{A}^A = \frac{1 + \cos\theta}{2 \sin\theta} \hat{\phi}, \quad \mathbf{A}^B = -\frac{1 - \cos\theta}{2 \sin\theta} \hat{\phi}. \quad (16)$$

This is just the vector potential of the Wu-Yang monopole²⁰ on a unit sphere. The magnetic field is $\mathbf{B} = \nabla \times \mathbf{A} = \frac{1}{\sin\theta} \frac{\partial}{\partial\theta} (A_\phi \sin\theta) \hat{\mathbf{r}} = -\frac{1}{2} \hat{\mathbf{r}}$. The magnetic field is like that of a monopole with charge $g = -2\pi$. Furthermore, this implies that a monopolelike singular point is located at the center of the sphere $R_1 = R_2 = R_3 = 0$, which is also the point at which the two bands become degenerate.

The winding number is easier to compute than the Chern number, since it is directly written in terms of matrix elements of the Hamiltonian and does not require computing the eigenvectors. If R_1, R_2 , and R_3 are independent of each other, and each of them can take both positive and negative values at the point where the other two components are zero, then $\hat{\mathbf{R}}$ will sweep out the whole unit sphere which encloses the singular point inside it. Then the winding number or the Chern number is nontrivial. But in general it is also possible that $\hat{\mathbf{R}}$ winds the sphere twice in opposite directions and cancels out or comes back to a given point as \mathbf{k} is varied over all its values without sweeping the entire sphere. Then the Chern number is zero.

As a specific example,²¹ take $\mathbf{R} = (\sin k_x, \sin k_y, m + \cos k_x + \cos k_y)$. For $0 < m < 2$, there is always a gap between the two bands and it is easy to see that $\hat{\mathbf{R}}$ sweeps the whole sphere. One can also directly verify that

$$c = - \int \frac{d^2k}{4\pi} \frac{\cos k_x + \cos k_y + m \cos k_x \cos k_y}{[\sin^2 k_x + \sin^2 k_y + (m + \cos k_x + \cos k_y)^2]^{\frac{3}{2}}} = 1. \quad (17)$$

Consider next the Haldane model.¹ It has a staggered flux inside each unit cell. The Hamiltonian is

$$H = t_1 \left(\sum_i \cos(\mathbf{k} \cdot \mathbf{a}_i) \sigma^1 + \sum_i \sin(\mathbf{k} \cdot \mathbf{a}_i) \sigma^2 \right) + \left(M - 2t_2 \sin\phi \sum_i \sin(\mathbf{k} \cdot \mathbf{b}_i) \right) \sigma^3. \quad (18)$$

The maximum of $\sum_i \sin(\mathbf{k} \cdot \mathbf{b}_i)$ is $3\sqrt{3}/2$; thus for $|M/t_2| < 3\sqrt{3} |\sin\phi|$, $\hat{\mathbf{R}}$ will cover the whole sphere. Indeed, for $\phi > 0$, one can directly verify that $c = 1$ in this case.

The condition on M is simply the necessary condition for the AH state that the monopole singularity exist which requires that $R_3(\mathbf{k})$ go through zero at some point \mathbf{k} and change sign as that point is crossed.

Fradkin and Sun¹³ pointed out that if both time reversal \mathcal{R} and inversion \mathcal{I} are broken but the product $\mathcal{R}\mathcal{I}$ conserved, there can be no anomalous Hall state: the diagonal components of the Berry vector potential must vanish. Note that $(\mathcal{R}\mathcal{I})R_3\sigma_3(\mathcal{R}\mathcal{I}) = -R_3\sigma_3$. Therefore, if $\mathcal{R}\mathcal{I}$ is conserved, $R_3(\mathbf{k}) = 0$ for all \mathbf{k} . Then the sphere $\hat{\mathbf{R}}(\mathbf{k})$ turns to a circle and no singularity can be defined.

In contrast to this is the θ_{II} type loop-current states realized in the three-orbital model for cuprates.¹⁰⁻¹² Its mean-field Hamiltonian in the same basis as Eq. (1) is

$$H = \begin{pmatrix} 0 & its_x + irc_x & its_y + irc_y \\ -its_x - irc_x & 0 & t's_x s_y \\ -its_y - irc_y & t's_x s_y & 0 \end{pmatrix}. \quad (19)$$

If we define $id^\dagger = \tilde{d}^\dagger$, then the Hamiltonian in the new basis is a real matrix. Actually, if $\mathcal{R}\mathcal{I}$ is invariant, then the Hamiltonian (in momentum space) can always be written as a real matrix and the phase of all eigenvectors are constant. Therefore, such a state, though violating time reversal, cannot have an AH state.

IV. THREE-BAND LOOP-CURRENT MODEL WITH AH

A. Chern number and winding number

Now we turn back to the three-orbital copper-oxygen model given by Hamiltonian $H = H_{\text{KE}} + H'$, which in the space of d, p_x, p_y is

$$H = \begin{pmatrix} 0 & its_x & its_y \\ -its_x & 0 & t's_x s_y + irc_x c_y \\ -its_y & t's_x s_y - irc_x c_y & 0 \end{pmatrix}, \quad (20)$$

with $s_x = \sin(k_x/2)$ and $c_x = \cos(k_x/2)$, etc. Note that even though the matrix elements as a function of k_x and k_y do not have the period 2π , the energy dispersion as a function of k_x and k_y does have a period 2π . As commented on below, the Hamiltonian for a tight-binding model with a basis is not strictly periodic when \mathbf{k} is translated by a reciprocal lattice vector \mathbf{G} , but rather is transformed by the unitary matrix $\exp(i\mathbf{G} \cdot \mathbf{a}_i)$, where \mathbf{a}_i is the location of the i th site in the unit cell.

To diagonalize the above Hamiltonian, one has to solve a cubic equation to find out the eigenvalues. Since the Chern number is topological invariant, if we deform the Hamiltonian without the bands crossing, the Chern number will stay the same. We can therefore simplify the problem by dropping the $t's_x s_y$ term and come back later to ensure that this simplification is valid. The simplified Hamiltonian is

$$H' = \begin{pmatrix} 0 & its_x & its_y \\ -its_x & 0 & irc_x c_y \\ -its_y & -irc_x c_y & 0 \end{pmatrix}. \quad (21)$$

This Hamiltonian can be written as $H = \mathbf{R} \cdot \mathbf{L}$ with $R_1 = ts_x$, $R_2 = -ts_y$, $R_3 = rc_xc_y$ and L_x, L_y, L_z are the spin 1 representation of the $SU(2)$ generators in contrast to the spin-1/2 representation of the $SU(2)$ generators for the two-band case.

We will discuss the location of singular points in simple gauges for model H' of Eq. (4). They should be qualitatively similar to model H of Eq. (3). It is easy to find the eigenvalues $E = 0, \pm R$ with $R = \sqrt{R_1^2 + R_2^2 + R_3^2}$. Let us focus on the lowest band $E_1 = -R$; the corresponding eigenvector can be written in two different ways labeled by A, B ,

$$|\psi_1^A\rangle = \frac{1}{\sqrt{2(R^2 - R_3^2)}R} \begin{pmatrix} R^2 - R_3^2 \\ -R_2R_3 + iRR_1 \\ -R_1R_3 - iRR_2 \end{pmatrix}, \quad (22)$$

$$|\psi_1^B\rangle = \frac{1}{\sqrt{2(R^2 - R_1^2)}R} \begin{pmatrix} -R_1R_3 + iRR_2 \\ -R_1R_2 - iRR_3 \\ R^2 - R_1^2 \end{pmatrix}. \quad (23)$$

These two wave functions are related by a $U(1)$ gauge transformation,

$$|\psi_1^B\rangle = e^{i\phi}|\psi_1^A\rangle, \quad e^{i\phi} = \frac{-R_1R_3 + iRR_2}{\sqrt{(R^2 - R_1^2)(R^2 - R_3^2)}}, \quad (24)$$

$$\phi = -\arctan\left(\frac{RR_2}{R_1R_3}\right).$$

The Berry phase is given by

$$A_\mu^A = -i\langle\psi^A|\nabla_\mu|\psi^A\rangle$$

$$= -\frac{R_3}{R(R^2 - R_3^2)}\left(R_2\frac{\partial R_1}{\partial k_\mu} - R_1\frac{\partial R_2}{\partial k_\mu}\right), \quad (25)$$

$$A_\mu^B = -i\langle\psi^B|\nabla_\mu|\psi^B\rangle$$

$$= -\frac{R_1}{R(R^2 - R_1^2)}\left(R_3\frac{\partial R_2}{\partial k_\mu} - R_2\frac{\partial R_3}{\partial k_\mu}\right). \quad (26)$$

They are also connected by a $U(1)$ gauge transformation,

$$A_\mu^B = A_\mu^A + \nabla_\mu\phi. \quad (27)$$

The Berry curvature is given by

$$F_{xy} = \frac{\partial A_y}{\partial k_x} - \frac{\partial A_x}{\partial k_y} = -\frac{1}{R^3}\epsilon_{abc}R_a\frac{\partial R_b}{\partial k_x}\frac{\partial R_c}{\partial k_y}$$

$$= -\epsilon_{abc}\hat{R}_a\frac{\partial\hat{R}_b}{\partial k_x}\frac{\partial\hat{R}_c}{\partial k_y}. \quad (28)$$

Note there is a factor of 2 difference compared to the two-band model. The Chern number is the integral of the Berry curvature in the Brillouin zone (BZ),

$$c = \frac{1}{2\pi} \int d^2k F_{xy} = -\frac{1}{2\pi} \int d^2k \epsilon_{abc} \hat{R}_a \frac{\partial \hat{R}_b}{\partial k_x} \frac{\partial \hat{R}_c}{\partial k_y}$$

$$= \frac{1}{2\pi} \int d^2k \frac{t^2 r (c_x^2 + s_x^2 c_y^2)}{4[(ts_x)^2 + (ts_y)^2 + (rc_xc_y)^2]^{3/2}}. \quad (29)$$

In this model, $R_3 = rc_xc_y$ takes only positive values and $R_1 = ts_x$ and $R_2 = -ts_y$ continuously vary from $-t$ to t and do not go back. Thus $\hat{\mathbf{R}}$ only sweeps half of the unit sphere. Thus the

surface integral $\int d^2k \hat{\mathbf{R}}(\partial_x \hat{\mathbf{R}} \times \partial_y \hat{\mathbf{R}}) = 2\pi$ and Chern number $c = 1$.

We have obtained the relation between the Chern number and winding number for the spin-1/2 and spin-1 representations of $SU(2)$ algebra. Actually, we can generalize this relation to any spin- $n/2$ representation of $SU(2)$ for integer n . The Hamiltonian is given by

$$H = R_1 J_x + R_2 J_y + R_3 J_z. \quad (30)$$

Here J_a for $a = x, y, z$ are $n \times n$ matrices and satisfy $[J_a, J_b] = i\epsilon_{abc}J_c$. Then the eigenvalues are $E_i/R = -n/2, -(n/2 - 1), \dots, n/2 - 1, n/2$. Then, for the i th band, we have

$$c = \frac{1}{2\pi} \int d^2k F_{xy} = \frac{E_i}{R} \frac{1}{2\pi} \int d^2k \epsilon_{abc} \hat{R}_a \frac{\partial \hat{R}_b}{\partial k_x} \frac{\partial \hat{R}_c}{\partial k_y}. \quad (31)$$

To prove the above result, it is better to consider $H/R = \hat{\mathbf{R}} \cdot \mathbf{J}$, which has the same Chern number as H . Since $\hat{\mathbf{R}}$ is a unit vector, it can be parametrized by spherical coordinates $\hat{\mathbf{R}} = (\sin\theta \cos\phi, \sin\theta \sin\phi, \cos\theta)$. Here θ, ϕ are functions of k_x and k_y .

To be specific, we take J_z as a diagonal matrix $J_z = \text{diag}\{n/2, (n/2 - 1), \dots, -n/2 - 1, -n/2\}$. We can make a rotation to diagonalize H/R as

$$e^{i\theta J_y} e^{i\phi J_z} \hat{\mathbf{R}} \cdot \mathbf{J} e^{-i\phi J_z} e^{-i\theta J_y} = J_z. \quad (32)$$

For the i th band, we have the eigenvector

$$\psi_i = e^{-i\phi J_z} e^{-i\theta J_y} \mathbf{n}_i, \quad \mathbf{n}_i(0, \dots, 1, \dots, 0)^T. \quad (33)$$

In the above vector, only i th component is 1 and all others are zero. The Chern number can also be written in terms of differential forms as

$$c = -\frac{i}{2\pi} \int d^2k \left(\frac{\partial \psi^\dagger}{\partial k_x} \frac{\partial \psi}{\partial k_y} - \frac{\partial \psi^\dagger}{\partial k_y} \frac{\partial \psi}{\partial k_x} \right)$$

$$\equiv -\frac{i}{2\pi} \int d\psi^\dagger \wedge d\psi. \quad (34)$$

It is easy to find

$$d\psi = (-iJ_z e^{-i\phi J_z} e^{-i\theta J_y} d\phi - i e^{-i\phi J_z} e^{-i\theta J_y} J_y d\theta) \mathbf{n}_i,$$

$$d\psi^\dagger = \mathbf{n}_i^T (i e^{i\theta J_y} e^{i\phi J_z} J_z d\phi + i J_y e^{i\theta J_y} e^{i\phi J_z} d\theta).$$

Using the above in Eq. (34), we find

$$c = -\frac{i}{2\pi} \int \mathbf{n}_i^T (J_y e^{i\theta J_y} J_z e^{-i\theta J_y} d\theta \wedge d\phi$$

$$+ e^{i\theta J_y} J_z e^{-i\theta J_y} J_y d\phi \wedge d\theta) \mathbf{n}_i$$

$$= -\frac{i}{2\pi} \int \text{Tr}[e^{i\theta J_y} (J_y J_z - J_z J_y) e^{-i\theta J_y} \cdot (\mathbf{n}_i \mathbf{n}_i^T)] d\theta \wedge d\phi$$

$$= \frac{1}{2\pi} \int \text{Tr}[e^{i\theta J_y} J_x e^{-i\theta J_y} \cdot (\mathbf{n}_i \mathbf{n}_i^T)] d\theta \wedge d\phi$$

$$= \frac{1}{2\pi} \int \text{Tr}[(\cos\theta J_x + \sin\theta J_z) \cdot (\mathbf{n}_i \mathbf{n}_i^T)] d\theta \wedge d\phi. \quad (35)$$

The matrix $(\mathbf{n}_i \mathbf{n}_i^T)$ has 1 as its i th diagonal element, and all other elements are zero. Thus for any $n \times n$ matrix A , we have $\text{Tr}[A(\mathbf{n}_i \mathbf{n}_i^T)] = A_{ii}$. Since J_x only has off-diagonal elements,

only the second term of Eq. (35) contributes. Therefore,

$$c = \frac{(J_z)_{ii}}{2\pi} \int \sin \theta d\theta \wedge d\phi = \frac{E_i}{R} \frac{1}{2\pi} \int \sin \theta d\theta \wedge d\phi. \quad (36)$$

On the other hand, the winding number integral in terms of spherical coordinates can be written as

$$\begin{aligned} \int d^2k \epsilon_{abc} \hat{R}_a \frac{\partial \hat{R}_b}{\partial k_x} \frac{\partial \hat{R}_c}{\partial k_y} &= \frac{1}{2} \int \epsilon_{abc} \hat{R}_a dR_b \wedge dR_c \\ &= \int \sin \theta d\theta \wedge d\phi. \end{aligned} \quad (37)$$

Combining the above two equations, we find the desired results.

There is a subtle point about this loop-current model's behavior when \mathbf{k} is shifted by a lattice vector. Recall that $R_1 = t \sin(k_x/2)$, $R_2 = -t \sin(k_y/2)$, $R_3 = r \cos(k_x/2) \cos(k_y/2)$ and they are functions of k_x and k_y with period 4π not 2π . Thus the Hamiltonian is not invariant under changes $k_x \rightarrow k_x + 2\pi$ and $k_y \rightarrow k_y + 2\pi$. This happens generally if the lattice contains a basis. It is easy to see that the eigenstates are also not invariant under 2π shift. However, if we rewrite the wave function in real space, we find

$$\psi_1^A \propto \sum_i e^{i\mathbf{k}\cdot\mathbf{r}_i} \begin{pmatrix} R^2 - R_3^2 \\ -\left(\frac{tr}{2} \sin k_y - itR\right) \sin(k_x/2) e^{ik_x/2} \\ -\left(\frac{tr}{2} \sin k_x + itR\right) \sin(k_y/2) e^{ik_y/2} \end{pmatrix}. \quad (38)$$

Since R and $R_{1,2,3}^2$ has period 2π , the above wave function is invariant under 2π shift as one expected.

If we define the torus to be $-\pi < k_{x,y} < \pi$, then R_3 is always positive and the torus is mapped to half of a unit sphere by $\hat{\mathbf{R}}$. It might seem that, in this case, the monopole singular point is not enclosed by the half surface; therefore, the Chern number need not to be quantized and may have no topological meaning. But if we look at the vector potential in Eq. (26), they are invariant under 2π shift, and thus are well defined on the whole torus. Therefore, according to Dirac's arguments, the integral of field strength on this closed surface should give a quantized topological invariant. In the mapping $\hat{\mathbf{R}}(k_x, k_y)$, the boundary of BZ is mapped to the equator of the sphere. As discussed above, the wave functions are the same at the two points like $(-\pi, k_y)$ and (π, k_y) on the boundary of BZ. These two points are mapped to $(-\frac{1}{1+s_y^2}, s_y, 0)$ and $(\frac{1}{1+s_y^2}, s_y, 0)$ on the equator. These two points should be identified, and then the boundary of the half sphere is glued together to make a closed surface which is topologically equivalent to a sphere. In this loop-current model, we have wound over this closed surface once.

B. Singular points of wave functions and their gauge dependence

We now discuss the singular points of wave functions inside the BZ for the three-orbital case. One can see that ψ_1^A is well defined for all possible values of $R_{1,2,3}$ except when $R_3 = \pm R$ or $R_1 = R_2 = 0$. So this is the singular point of ψ_1^A . It corresponds to $k_x = k_y = 0$ in the BZ. Similarly, ψ_1^B has

singular points when $R_1 = \pm R$ or $R_2 = R_3 = 0$. It correspond to $k_x = \pm\pi, k_y = 0$ in the BZ. Therefore, the location of singular points depends on the choice of gauge.

The reason that any gauge has singular points is simply that the Chern number being nonzero implies no continuous gauge can cover the whole Brillouin zone. It is easiest to understand the connection of these two by thinking of a spherical rather than toroidal Brillouin zone. If a single gauge covered the whole sphere, then we could apply Stokes' theorem to relate the Chern number, which is the integral of the Berry curvature over the whole sphere, to the integral of the Berry connection around a tiny circle, which must be zero. In the same way, a nonzero Chern number is an "obstruction" to having continuously defined wave functions over the whole Brillouin zone.

Each form of wave function is valid only on one patch of the torus and the two are connected by $U(1)$ gauge transformation on the boundaries. This is exactly the same as for the Wu-Yang monopole. ψ_1^A and ψ_1^B define a $U(1)$ bundle on the torus. Let U^A be the open set which covers the torus without the point $k_x = k_y = 0$. Let U^B be the open set which covers the torus without the point $k_x = \pm\pi, k_y = 0$. Then ψ_1^A is well defined on U^A and ψ_1^B is well defined on U^B . Both ψ_1^A and ψ_1^B are well defined on the overlap $U^A \cap U^B$ and they are related by $U(1)$ gauge transformation $\psi_1^A = e^{i\phi} \psi_1^B$. We can take a closed loop as the boundary of U^A and U^B ; then we find a mapping from this closed loop to $U(1)$. Then the Chern number is just the winding number of this mapping.

We can make this connection more explicit by taking a small closed loop as $c: k_x^2 + k_y^2 = \epsilon^2$ with small positive ϵ to enclose the singular point of ψ_1^A . Making a small \mathbf{k} expansion, we find $R_{1,2} \approx k_{x,y}/2$, $R_3 \approx 1$, and $R \approx 1$. Then we have

$$\phi \approx -\arctan \frac{k_y}{k_x}, \quad \nabla_\mu \phi \approx \left(\frac{k_y}{k_x^2 + k_y^2}, -\frac{k_x}{k_x^2 + k_y^2} \right). \quad (39)$$

Thus the Chern number can also be obtained as a line integral around this small loop,

$$\begin{aligned} c &= \frac{1}{2\pi} \oint_c (\mathbf{A}^B - \mathbf{A}^A) \cdot d\mathbf{l} = \frac{1}{2\pi} \oint_c \nabla_\mu \phi \cdot d\mathbf{l}_\mu \\ &= \frac{1}{2\pi} \oint_c \frac{k_y dk_x - k_x dk_y}{k_x^2 + k_y^2} = 1. \end{aligned} \quad (40)$$

Even without detailed calculation, one can see that as the momentum goes around this loop, the phase difference ϕ of Eq. (24) also goes around one circle. Thus the winding number is -1 , which agrees with the previous calculation.

The Chern number can also be defined as a line integral $c = \frac{1}{2\pi} \oint_C A_\mu dl_\mu$, where integral path C is the boundary of the BZ. Since the Berry vector potential depends on the gauge choice, to get a correct answer for the Chern number, one has to choose a gauge such that the wave function has no singular point inside the loop. In the Cu-O model, we should use A_μ^B . It is easy to see that $A_x^B = 0$ for $k_y = \pm\pi$ and $-\pi \leq k_x \leq \pi$ and $A_y^B = 0$ for $k_x = \pm\pi$ and $-\pi \leq k_y \leq \pi$. Thus we find loop integral $\oint A_\mu dl_\mu = 0$. But since there are two singular points $k_x = \pm\pi, k_y = 0$ on the boundary, we should choose an integral path with a small semicircle to circumvent the two singular points. Expanding A_μ^B around $k_x = \pm\pi, k_y = 0$, we

find

$$A_\mu^B(\pm\pi + k_x, k_y) = \frac{1}{k_x^2 + k_y^2}(k_x, -k_y). \quad (41)$$

Let ϵ denote the small circle around the singular point; then

$$c = \frac{1}{2\pi} \oint_C A_\mu dl_\mu = -\frac{1}{2\pi} \oint_\epsilon \frac{k_x dk_y - k_y dk_x}{k_x^2 + k_y^2} = 1. \quad (42)$$

This result agrees with the Chern number calculated from the Berry curvature.

For the middle band $E = 0$ and the wave function is $|\psi_2\rangle = \frac{1}{R}(R_3, R_2, R_1)$, which is always real in the BZ. Clearly this band is topologically trivial and Chern number $c = 0$. The sum of the Chern numbers of all bands is always zero. Thus for the top band we have $c = -1$.

Now we come back to the original Hamiltonian H . We show that if t' is not too large, there is no band crossing so the result stays the same as H' . Let $R_4 = t s_x s_y$; the eigenvalues are the roots of cubic equation

$$E^3 - (R_4^2 + R^2)E + 2R_4 R_1 R_2 = 0. \quad (43)$$

The condition for degeneracy is $-[(R_4^2 + R^2)/3]^3 + (R_4 R_1 R_2)^2 = 0$. It can be rewritten as

$$\begin{aligned} & -[(\hat{R}_4^2 + 1)/3]^3 + (\hat{R}_4 \hat{R}_1 \hat{R}_2)^2 \\ & \leq -[(\hat{R}_4^2 + 1)/3]^3 + \hat{R}_4^2/4 = 0, \end{aligned}$$

with $\hat{R}_4 = R_4/R$. The last equality of the above is satisfied only for $\hat{R}_4^2 = 1/2$. In our model, for simplicity, we take $r = t$; then the maximum value of \hat{R}_4 is $\frac{t'}{2t}$ at $k_x = k_y = \pi$. Thus, as long as $t' < t$, there is no band crossing and the Chern numbers stay the same as H' .

It follows from the discussion above that if the band is only partially filled, i.e., there is a Fermi surface, there can be no topologically protected currents. Nor can there be any singular properties of the Fermi liquid coming from the physics of the (nonquantized) anomalous Hall effect because one can always move the singularities of the wave functions away from the Fermi surface by a suitable choice of gauge. The intrinsic contribution to the anomalous Hall effect can be calculated by integrating the Berry curvature over the Fermi surface volume. This procedure is best carried out numerically by writing the Chern number in terms of the projection operator²² onto the occupied subspace, $P_k = |\psi_k\rangle\langle\psi_k|$, as this object is manifestly gauge-invariant.

V. CONCLUSIONS AND REMARKS ON THREE-DIMENSIONAL MATERIALS

We have discussed the calculation of Berry phases and the contribution to the Hall effect in a three-band model motivated by the copper-oxygen planes of the high-temperature superconductors. There are two topologically active bands (i.e., with nonzero Chern number ± 1) separated by a middle band with Chern number zero. We have neglected interaction effects, but there is considerable recent interest in the possibility of fractional quantum Hall phases when a band of nonzero Chern number is partly occupied. Bands with Chern number ± 2 or larger are particularly interesting as, while these are formally equivalent to bilayer quantum Hall systems, it has been argued that they are likely to support novel fractional quantum Hall states because the nature of interactions is modified.²³ That work proposed creating the Chern number ± 2 bands via an oxide heterostructure, and this technique might also enable the PT -breaking model described here to be realized at the interface between a cuprate and another material.

In closing, it may be useful to mention another topological property enabled when a model has three bands rather than two; the CP violation enabled by the 3×3 Cabibbo-Kobayashi-Maskawa matrix in the standard model provides a well-known example of how 3×3 matrices allow additional subtleties. The orbital contribution to the linear magnetoelectric effect, i.e., the polarization induced by a magnetic field dP_i/dB_j or magnetization by an electric field dM_i/dE_j , has recently been a subject of active study.^{21,24–26} The topological part of this effect is the scalar diagonal part (“axion electrodynamics”), computed by the Chern-Simons integral over the Berry connection,²¹ which vanishes in a purely 2D model such as that considered here.

In a 3D model, either P or T symmetry quantizes the scalar diagonal part to only two possible values, corresponding to ordinary and topological insulators. Without these symmetries, in a 3D model with only two bands, the Chern-Simons integral is quantized and computes the “Hopf invariant” of the band structure, viewed as a mapping to the sphere.²⁷ Three bands are required in order to generate generic values of the scalar magnetoelectric coupling. The computation for a single occupied band, in which case the Chern-Simons integral is Abelian, has been recently discussed.²⁸ We hope that the results of this paper lead to further study of the consequences of wave function topology for transport and magnetism of oxide materials.

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