Quantum spin Hall effect in a three-orbital tight-binding Hamiltonian

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Abstract
We consider the quantum spin hall (QSH) state in a three-orbital model, with a certain spin loop current order which is induced by spin-dependent interactions. This type of order is motivated by the loop current model, which was proposed long ago to describe the pseudogap phase of cuprates. It is shown that this model has nontrivial Chern parity by directly counting the zeros of the Pfaffian of the time reversal operator. By connecting to the second Chern number, we explicitly show the property of singularities of the wave-functions, and also their dependance on the gauge choices. Also it is shown that the Berry phase of the QSH state can be mapped to a non-Abelian instanton.

Keywords: quantum spin Hall, quantum anomalous Hall, loop current order

1. Introduction

In recent years, a lot of interest has arisen around the topological properties of band structures, such as quantum anomalous Hall (QAH) and quantum spin Hall (QSH) effects. All these topological nontrivial states are inspired by the integer Quantum Hall effects, in which it is shown that quantized Hall conductance is also the Chern number of the underlying band structure [1]. Later, Haldane introduced a complex next-nearest-neighbor hop in a 2D lattice model to give rise to a nonzero Chern number without applying an external magnetic field [2]. This has led to extensive study of QAH [3, 4]. It has also been shown that the Chern number is the only topological invariant which characterizes the non-interacting time-reversal-breaking Hamiltonian [5].

In our previous paper [6], we noted that Haldane’s model can be realized in a lattice model with a special time reversal breaking loop current order, due to the nearest neighbor interaction. Loop current ordered states which don’t change translational symmetry, were originally thought to arise as broken symmetry states due to interactions in a three-orbital model for underdoped cuprates [7–9], and have been discovered in several families of cuprates [10–12]. These observed loop-current states, however, do not lead to the quantized anomalous Hall effect (QAHE) or nonzero Chern number because they preserve the product of time reversal and spatial inversion symmetry. But other possible types of loop current order will lead to QAH. Also, in [6] the discussion of singularities in the wave function helps to reveal topological obstruction in QAH states.

In this paper we generalize these results to include spin degrees of freedom and consider ordered spin loop current states due to nearest-neighbor interaction. This will restore the time reversal symmetry and also make the Chern number trivially zero. Although the first order Chern number is zero, it has been pointed out that the time reversal invariant Hamiltonian is characterized by the second Chern number [13]. Many years later, in a seminal paper [14], Kane and Mele introduced the $\mathbb{Z}_2$ invariant to classify the two dimensional time reversal invariant model, which also led to the suggestion of 2D and 3D topological insulators [15–17]. These two classifications of a time reversal invariant model seem to be contradictory. This contradiction can be resolved using the dimensional reduction method, as discussed in [18]. Another more geometric method to connect the Chern parity to the second Chern number can be found in [19]. This argument is very similar to the one used in Witten’s $SU(2)$ global anomaly [20]. In this way, the topological obstruction meaning of the $\mathbb{Z}_2$ invariant is more apparent. For the two-band time reversal breaking Hamiltonian, it is well-known that the $U(1)$ Berry
phase configuration is the same as Wu–Yang’s magnetic monopole solution [21]. Similarly, for the two band time reversal invariant Hamiltonian, we found that, after some suitable coordinate transformations, the SU (2) Berry phase configuration can be mapped to the self-adjoint instanton solution of Non-abelian gauge theory.

The rest of the paper is organized as follows. The spin loop current ordered states are discussed in section 2. Then, in section 3, we follow Kane and Mele’s method to construct the $Z_2$ invariant directly and show that the zeros of Pfaffian is coincidental with the singular points of the eigenfunction. In section 4, we connect the $Z_2$ invariant to the second Chern number and analyze the singular points of the wave function of a two-band model example in detail, just as in the QAH case [6]. In section 5, the three orbital Cu−O lattice model will be discussed. Again we will directly construct the $Z_2$ invariant to verify it is a QSH state. We conclude in section 6.

2. Spin loop current states in a copper-oxygen lattice model

We consider a two-dimensional lattice with the structure of a copper oxide lattice, as shown in figure 1. There are three orbitals per unit cell, which are the $d_{xy}$, and $p_x$, $p_y$ orbitals on the oxygen atoms. The minimal kinetic energy operator, with a choice of gauge such that the $d$ orbital is purely real and the $p_x$ and $p_y$ orbitals are purely imaginary, is

$$H_{kk'} = i t \sum_{\alpha} (s_x p_{\alpha, k} + s_y p_{\alpha, k'}) - t' s_x s_y p_{\alpha, k} p_{\beta, k} + \text{h.c.}$$  \hfill (1)

Here $s_x = \sin(k_x / 2)$ and $s_y = \sin(k_y / 2)$ and the lattice constant is taken to be 1.

In the pseudogap phase of the loop current model, one usually only considers the charge channel; so, it is equivalent to consider spinless fermions. To consider spin Hall effects, we also need to decompose the interaction term in the spin channel. As we know from the previous paper, the only topological nontrivial state is obtained by considering the interaction between the $p$ orbitals as

$$H_{int} = \sum_{i,j,\sigma,\sigma'} V n_{p_i,\sigma} n_{p_j,\sigma'}.$$  \hfill (2)

Here $i, j$ labels the lattice sites and $\sigma, \sigma'$ labels the spin.

In the spinless case, the above interaction term can be decomposed by using the operator identity $n_i n_j = -\frac{1}{2} (J_{ij}^2 - n_i - n_j)$ with charge current operator $J_{ij} = i (c_{ij}^+ c_{ji} - c_{ij}^+ c_{ji})$. In the mean field theory, one of currents in the current interaction term can be replaced by its expectation as $\langle V(2) \rangle J_{ij} = i r$. Thus, one finds an interaction induced kinetic energy term

$$H_{int'} = i r c_{ij} p_{\alpha, k}^\dagger p_{\alpha, k} + \text{h.c.}$$  \hfill (3)

If $r \neq 0$ is a stable state, it describes loop currents flowing clockwise (or anti-clockwise) around the oxygen in each unit cell, as shown in figure 1. This is one of the five possible loop-current states, with non-overlapping loops in the Cu−O lattice, all of which preserve translational symmetry. In figure 1, the flux has one sign in the square formed by the nearest neighbor oxygens which surround a Cu, and the opposite sign in the square formed by the nearest neighbor oxygens which do not surround a Cu. Therefore the total flux is zero.

For the spinful fermions, the above operator can be trivially generalized to interaction terms which are diagonal in the spin indices. Following a similar method, the density coupling can be rewritten as the spin current coupling by the operator identity $n_i,\sigma n_j,\sigma = -\frac{1}{2} \langle J_{ij,\sigma}^2 - n_i,\sigma - n_j,\sigma \rangle$ where the spin current is

$$J_{ij,\sigma} = \langle c_{ij,\sigma}^+ c_{ji,\sigma} - c_{ij,\sigma}^+ c_{ji,\sigma} \rangle.$$  \hfill (4)

For interaction terms which are off-diagonal in the spin indices, such as $n_i,\sigma n_j,\sigma + n_j,\sigma n_i,\sigma$, the decomposition is more complicated. We can begin with the product of the spin current of two different spins.

$$J_{ij,\sigma} J_{ji,\sigma'} = -c_{ij,\sigma}^+ c_{ji,\sigma} c_{ij,\sigma'}^+ c_{ji,\sigma'} + c_{ij,\sigma}^+ c_{ji,\sigma} c_{ij,\sigma'}^+ c_{ji,\sigma'} + c_{ij,\sigma}^+ c_{ji,\sigma} c_{ij,\sigma'}^+ c_{ji,\sigma'}$$  \hfill (5)

Here $S_\sigma = c_{ij,\sigma}^+ c_{ji,\sigma}$ and $S_{\sigma'} = \frac{1}{2} (n_i,\sigma - n_j,\sigma)$ form the spin $SU(2)$ algebra, and $T_\sigma^+ = c_{ij,\sigma}\dagger c_{ji,\sigma}$ and $T_\sigma = \frac{1}{2} (n_i,\sigma + n_j,\sigma - 1)$ form the charge $SU(2)$ algebra. Making use of the following identities

$$S_\sigma S_{\sigma'} = \frac{1}{2} (S_\sigma^+ S_{\sigma'}^+ + S_{\sigma'}^+ S_\sigma^+) + S_{\sigma}^+ S_{\sigma'}^+$$  \hfill (6)

we find the following decomposition.

$$n_i,\sigma n_j,\sigma + n_j,\sigma n_i,\sigma = J_{ij,\sigma} J_{ji,\sigma'} - 2 (S_{\sigma} S_{\sigma'} - T_\sigma^+ T_{\sigma'}^- + T_{\sigma'}^- T_{\sigma}^+) + \frac{1}{2} (n_i,\sigma + n_j,\sigma)$$  \hfill (7)

Other than the spin current couplings, there are also more complicated terms like spin and charge operator interaction between neighboring sites. Since we only want to consider current order here, these spin and charge interaction terms will be ignored. As before, in the mean field level, the current can be replaced by its expectations, so we find a new kinetic term
If the expectations of spin up and spin down currents are opposite, this loop current ordered system is time-reversal invariant again and it is possible to give rise to a QSH state.

In the rest of the paper, we will consider the QSH state of this spin current ordered three-orbital Cu–O model, with the Hamiltonian $H = H_{\text{KE}} + H_{\text{int}}$, and also determine the singularities of its eigenfunctions. Before we do that, let us first consider the simpler case of a two-band model.

### 3. A two-band model with spin

In [6], we discussed a simple two-band Hamiltonian on a square lattice from a wave function point of view.

$$H = \mathbf{R} \cdot \sigma.$$  \hspace{1cm} (9)

This Hamiltonian breaks time reversal. For $0 < m < 2$ or $-2 < m < 0$, the Chern number is $+1$ or $-1$ respectively for the lower band. In the two-band model, the Chern number simply equals to the winding number of the mapping $\mathbf{R}/|\mathbf{R}|$ from a 2D torus $T^2$ to a 2D sphere $S^2$. In this case, the geometric meaning of the Chern number is quite clear. If we change one of the $R_i$ to be $-R_i$, then the orientation of the above mapping is reversed and the Chern number will change signs.

Now we can introduce spin degrees of freedom to enlarge the above Hamiltonian to become a 4-band model and restore the above Hamiltonian to become a 4-band model and restore.

$$H = \mathbf{R} \cdot \sigma.$$  \hspace{1cm} (10)

Here $\sigma_i$ is the $i$ component of spin. To be specific, we assume that $-2 < m < 0$ and only consider the top band. For this band, the Chern number equals to $1$ for $s_z = 1$ or spin up and equals to $-1$ for $s_z = -1$ or spin down. Here we also insert an arbitrary constant $a$, in order to lift the degeneracy of the spin up and down bands. In matrix form, the model is

$$H = H_1 + H_2.$$  \hspace{1cm} (11)

Here $H_1$ and $H_2$ are Pauli matrices and $I$ is 2 by 2 identity matrix, $R_1 = m + \cos k_x + \cos k_y$ and $R_2 = \sin k_x$.

The spin up and spin down two-bands are still degenerate at $k_z = 0$, $\pm \pi$. So one cannot distinguish the Chern number between the spin up and spin down bands. The total Chern number is zero. But for a certain choice of parameters, there is also the $Z_2$ topological invariant. There are several different ways to get this $Z_2$ invariant. Here we use the approach proposed in Kane and Mele's original proposal [14]. In this method, we define the Pfaffian $P(\mathbf{k}) = \text{Pf}[(\langle u_1(\mathbf{k}) | \Theta | u_2(\mathbf{k}) \rangle)]$ where $\Theta = I \otimes (i, 0, 0, 0)$ is the time reversal operator and $K$ is the operator to take a complex conjugate. The zeros of $P(\mathbf{k})$ always come in pairs, if $\mathbf{k}$ is a zero point, so does $-\mathbf{k}$. Since two pairs can annihilate each other even the number of pairs is topologically trivial; an odd number of pairs is the QSH state.

In our model, the Pfaffian is simply $P(\mathbf{k}) = \langle u_1(\mathbf{k}) | \Theta | u_1(\mathbf{k}) \rangle$. Here $u_{\uparrow, \downarrow}$ are the eigenstates of spin up and spin down for the lower two bands. For concreteness, we take $m = -1$, let $\ell \ll 1$ and define $R_{1, \uparrow} = a + \sin k_x$, $R_{3, \uparrow} = a - \sin k_x$ and $R_{1, \downarrow} = (R_{1, \uparrow}^2 + R_{2, \uparrow}^2 + R_{3, \uparrow}^2)^{1/2}$. Since $\Theta$ will always change spin up to spin down, we can omit the spin part of the wave function and only need to write out its orbital part explicitly.

We already know the eigenfunctions of this model from [6]. One way to write them is

$$\langle u_{\uparrow} \rangle = \frac{1}{\sqrt{2R_1(R_1 - R_{3, \uparrow})}} \begin{pmatrix} R_{1, \uparrow} - R_1 \\ R_1 + iR_2 \\ R_1 - iR_2 \\ -R_{3, \uparrow} - R_1 \end{pmatrix}$$  \hspace{1cm} (12)

The above wave functions are well defined if $R_1$ and $R_2$ are not equal to zero at the same time.

First we consider a special case $R_1 = R_2 = 0$. We will show that if $R_1 = R_2 = 0$, then $|P(\mathbf{k})| = 0$. But since $R_1 = R_2 = 0$ only happens for $k_z = 0$ and $k_y = \pm \pi$. At these two points, equation (12) may be ill-defined. In this case, it is easy to find the eigenstates if we go back to the Hamiltonian. The Hamiltonians for spin up and spin down at these points are actually diagonal matrices

$$H_1 = \begin{pmatrix} (a + \sin k_y) & 0 \\ 0 & -(a + \sin k_y) \end{pmatrix}$$

$$H_2 = \begin{pmatrix} (a - \sin k_y) & 0 \\ 0 & -(a - \sin k_y) \end{pmatrix}$$  \hspace{1cm} (13)

At point $k_z = 0$, $k_y = \pi$, we find $|u_{\uparrow}| = (0, 1)$ and $|u_{\downarrow}| = \left(1, 0 \right)$. Thus, we clearly have $P(\mathbf{k}) = 0$ at this point. A similar thing also happens at $k_z = 0$, $k_y = -\pi$.

So far we have found one pair of zeros. Now we want to show that there are no other zeros: this is the only pair of zeros, the number is odd—and, therefore, we have the QSH state. Since we are only looking for zeros, we can drop the normalization factors. For cases other than $R_1 = R_2 = 0$, equation (12) is well defined. Thus, we find the Pfaffian to be

$$\langle u_{\uparrow} | \Theta | u_{\uparrow} \rangle \propto (R_1 + iR_2, -R_{1, \uparrow} - R_1, R_1 + iR_2, R_{1, \uparrow} + R_1)$$

$$= R_0(R_{1, \uparrow} - R_1 - R_{1, \downarrow} + iR_2(R_1 + R_{1, \uparrow} - R_{1, \downarrow} + R_1))$$  \hspace{1cm} (14)

Now we show that, if we assume $\langle u_{\uparrow} | \Theta | u_{\uparrow} \rangle = 0$ then it will lead to some contradictions. We can distinguish three different cases. Note that we always have the following identity

$$R_1^2 - R_2^2 = R_{1, \uparrow}^2 - R_{1, \downarrow}^2$$  \hspace{1cm} (15)

First, if $R_1 = 0$ and $R_2 = 0$, then $\langle u_{\uparrow} | \Theta | u_{\uparrow} \rangle = 0$ implies $R_1 = 0 = R_{1, \uparrow} = R_{1, \downarrow}$. Combining this with equation (15), we find $R_1 = R_{1, \uparrow} = R_{1, \downarrow}$. But since $R_2 = 0$, we should have $|R_{1, \uparrow}| > |R_{1, \downarrow}|$ and $|R_{1, \uparrow}| > |R_{1, \downarrow}|$, which leads to a contradiction.

Similarly, if $R_1 = 0$ and $R_2 = 0$, then $\langle u_{\downarrow} | \Theta | u_{\downarrow} \rangle = 0$ implies $R_1 = R_{1, \downarrow} = R_{1, \uparrow}$. Combining with equation (15), we find $R_1 = R_{1, \uparrow} = R_{1, \downarrow}$. Again, since $R_1 = 0$, we should have $|R_{1, \uparrow}| > |R_{1, \downarrow}|$ and $|R_{1, \uparrow}| > |R_{1, \downarrow}|$, which leads to a contradiction.
At last, if both $R_1 \neq 0$ and $R_2 \neq 0$, then $\langle u_1 | \Theta u_1 \rangle = 0$ implies $R_1 + R_2 = R_{31} + R_{31}$ and $R_1 - R_2 = R_{31} - R_{31}$, which means that $R_1 = R_{31}$ and $R_1 = -R_{31}$. Again, since $R_1 \neq 0$ and $R_2 \neq 0$, we should have $|R_{1}| \gg |R_{31}|$ and $|R_{1}| \gg |R_{31}|$, which leads to a contradiction, in all the above three cases, other than $R_1 = R_2 = 0$, we always find $P(k) \neq 0$. Thus, $k_s = 0$, $k_z = \pm \pi/2$ is the only pair of zeros.

The $Z_2$ invariant of this two-band toy model can be determined by a much easier formula by Fu and Kane, provided the constant $a$ is zero. In this case, the model is also invariant under the spatial inversion, then the $Z_2$ invariant is the product of the eigenvalues of the spatial inversion operator at the four time-reversal-invariant momentum (TRIM) points. We assume that $s_i$ in our model describes pseudo-spins, and the spatial inversion will exchange the two sublattices. Under these assumptions, the inversion is given by the operator $P = \sigma_i \otimes I$. It is easy to verify that $H = PHP$. The eigenvalues of $P$ is $\text{sgn}(R_1)$ at the four TRIM points, which are one +1 and three −1 or vice versa. Therefore, the $Z_2$ invariant is −1, which implies a topological nontrivial QSH state.

4. Relation to second Chern number and singular points of wave function

In the previous section, the $Z_2$ invariant is directly constructed from the matrix element of the time reversal operator $\Theta$. But its geometric meaning is not very clear compared with the Chern number of the time reversal breaking Hamiltonian. As pointed out by B. Simon many years ago, the topological invariant of the time reversal invariant Hamiltonian system is the second Chern number [13]. The nonzero second Chern number corresponds to the nontrivial elements of $\pi_3(sp(2)) = \pi_3(S^3) = Z$. This result seems to contradict the $Z_2$ classification. Actually, the second Chern number only works for a Hamiltonian in 4D. If we apply it to lower dimensions, we can treat extra spatial coordinates as adiabatic changing parameters. Following similar arguments to Witten’s $SU(2)$ global anomaly [19], one can show that, for lower dimensional models, the second Chern number reduces to a $Z_2$ invariant and the topological nontrivial one corresponds to an odd second Chern number, which also corresponds to the nontrivial elements of $\pi_3(sp(2)) = \pi_3(S^3) = Z_2$.

In the more general 4D model, the geometric meaning of the topological invariant can be understood much more easily. In this case, the nonzero Chern number is also the topological obstruction which prevents us from defining the wave function and Berry phase globally on the base manifold. We can understand this in an exact parallel way as we did for the first Chern number of the QAH state. To this end, we consider the following model:

$$H = \sum_{i=1}^{5} R_i \Gamma_i$$

with $\Gamma_i = \sigma_i \otimes I$ for $i = 1, 2, 3$ and $\Gamma_4 = \sigma_2 \otimes I$, $\Gamma_5 = \sigma_5 \otimes I$. The connection with the model of equation (9), discussed above, can be obtained by taking

$$R = (\sin k_x, \sin k_y, \sin k_z, m$$

$$+ \cos k_x, + \cos k_y, + \cos k_z, + \cos k_z)$$

and then treating the momentum $k_{1,2}$ as adiabatic parameters.

The energy bands are $E = \pm R$, with double degeneracy. Here $R = \sqrt{\sum_{i=1}^{5} R_i^2}$. To be concrete, we only consider the lower two degenerate bands. The wave functions are given by

$$|\psi_1\rangle = \frac{1}{\sqrt{2R(R + R_2)}} (-R_1 + iR_3, -R_1 - iR_3, R_5 + R, 0)^T$$

$$|\psi_2\rangle = \frac{1}{\sqrt{2R(R + R_2)}} (-R_1 + iR_3, R_3 + iR_4, 0, R_5 + R)^T$$

For convenience, we perform the calculations in terms of differential forms. The non-Abelian Berry phase is $A_j = \langle \psi_i | d\psi_j \rangle$, which is a $su(2)$ Lie algebra valued one-form. Since $A_j$ is traceless, it can be expanded by Pauli matrices as $A = \sum_{a=1}^{3} A^a \sigma_a/2$, with the following components

$$A^1 = \frac{1}{R} \sum_{i=1}^{5} R_i R_1 - R_2 dR_i + R_3 dR_3 - R_3 dR_2$$

$$A^2 = \frac{1}{R} \sum_{i=1}^{5} R_i dR_1 - R_2 dR_3 + R_3 dR_2 - R_3 dR_4$$

$$A^3 = \frac{1}{R} \sum_{i=1}^{5} R_i dR_2 - R_2 dR_3 + R_3 dR_3 - R_3 dR_4$$

The Berry curvature is defined as $F = dA + A \wedge A$. Here $F$ is also traceless, thus $\text{Tr} F = 0$ and the first order Chern number $\int \text{Tr} F = 0$ as required by the time reversal invariance. Expanding $F$ by Pauli matrices as $F = \sum_{a=1}^{3} F^a \sigma_a/2$, we find the following results

$$F^1 = -\frac{1}{R} \sum_{i=1}^{5} R_i R_1 A^1 + \frac{1}{R} \sum_{i=1}^{5} R_i dR_1 \wedge dR_2$$

$$+ \frac{1}{R} \sum_{i=1}^{5} R_i \wedge dR_3$$

$$+ \frac{1}{R} \sum_{i=1}^{5} R_i \wedge dR_4$$

$$F^2 = -\frac{1}{R} \sum_{i=1}^{5} R_i R_1 A^2 + \frac{1}{R} \sum_{i=1}^{5} R_i dR_1 \wedge dR_2$$

$$+ \frac{1}{R} \sum_{i=1}^{5} R_i \wedge dR_3$$

$$+ \frac{1}{R} \sum_{i=1}^{5} R_i \wedge dR_4$$

$$F^3 = -\frac{1}{R} \sum_{i=1}^{5} R_i R_1 A^3 + \frac{1}{R} \sum_{i=1}^{5} R_i dR_1 \wedge dR_2$$

$$+ \frac{1}{R} \sum_{i=1}^{5} R_i \wedge dR_3$$

$$+ \frac{1}{R} \sum_{i=1}^{5} R_i \wedge dR_4$$

The second Chern number is related to the winding number of mapping from $T^4$ to $S^3$.

$$c_2 = \frac{1}{8\pi^2} \int \text{Tr} F^2 = \frac{1}{8\pi^2} \int \sum_{a=1}^{3} F^a dF^a$$

$$\Rightarrow c_2 = \frac{3}{8\pi^2} \int \frac{1}{R} \sum_{i=1}^{5} (-1)^{i-1} R_i dR_1 \cdots dR_{i-1} dR_{i+1} \cdots dR_5 = 1$$

\[4\]
To ease the notations, we omit the $\lambda$ from now on. The detailed derivation of the above results is in the appendix A.

One can see that $|\psi_{1,2}\rangle$ is ill-defined at the points satisfying $R_i=0$ for $i=1, \ldots, 4$ and $R_5 \ll 0$. To cover the whole manifold we can introduce another wave function with a different gauge choice.

$$|\psi_1\rangle = \frac{1}{\sqrt{2(R-R_5)}} (R-R_5, 0, -R_3-iR_4, -R_1-iR_2)$$

$$|\psi_2\rangle = \frac{1}{\sqrt{2(R-R_5)}} (0, R-R_5, -R_1+iR_4, R_3-iR_1)$$

$|\psi_{1,2}\rangle$ are ill defined at the points satisfying $R_i=0$ for $i=1, \ldots, 4$ and $R_5 \gg 0$. Other than these points, both of them are well defined, and are related to each other by a gauge transformation.

$$|\psi_1\rangle = g |\psi_2\rangle, \quad g = -i \begin{pmatrix} 0 & R_1 + i R_4 & R_1 + i R_4 \\ R_0 & -R_1 - i R_4 & -R_1 + i R_4 \\ -i R_1 + i R_4 & -i R_1 - i R_4 & R_1 - i R_4 \end{pmatrix}$$

Here $R_0 = (R_1^2 + R_2^2 + R_3^2 + R_4^2)^{1/2}$. It is easy to see that $g$ is unitary and det $g = 1$ thus belongs to $SU(2)$. Now the Berry phase and Berry curvature are transformed as $A^\theta = g^{-1} A g + g^{-1} \gamma g$ and $F^\theta = g^{-1} F g$. The second Chern number can also be understood from $g$. Let $|\psi\rangle$ and $|\psi\rangle$ be defined on two 4D discs $D_1$ and $D_2$. The boundary between $D_1$ and $D_2$ are 3D sphere $S^3$. We know $\text{Tr} F^\theta$ are closed and thus can be locally written as $\text{Tr} F^\theta = \omega_3$, where $\omega_3 = \text{Tr}(A F - A^2 / 3)$ is the Chern-Simons 3-form. $\omega_3$ is not gauge invariant and is transformed as $\omega_3^g = o - \text{Tr}(g^{-1} \gamma g) + d\omega_3$. Then the second Chern number is also given by

$$c_2 = \frac{1}{8\pi} \left( \int d\omega_3 + \int d\omega_3^g \right) = \frac{1}{8\pi} \left( \int d\omega_3 - \int d\omega_3^g \right)$$

$$= -\frac{1}{2\pi} \int S^3 \text{Tr}(g^{-1}\gamma g)^3$$

$$= -\frac{1}{2\pi} \int S^3 \sum_{j=1}^4 (-1)^{j-1} R_0 dR_1 \cdots dR_{j-1} dR_{j+1} \cdots dR_4 = -1$$

This explicitly shows that the Chern number is related to $\pi_3(S^3)$.

To show the relation with the instanton solution of non-Abelian gauge theory, we first map the northern half of $S^4$ to $\mathbb{R}^4$ by a stereographic projection, as follows

$$r_j = \frac{R_j}{R_5}, \quad \text{Inverse: } R_j = \frac{r_j}{\sqrt{R^2 + r^2}}, \quad R_5 = \frac{R}{\sqrt{R^2 + r^2}}$$

$$\quad (i = 1, \ldots, 4).$$

It maps the north pole of $S^4$ to the origin in $\mathbb{R}^4$ and maps the equator to the infinite boundary of $\mathbb{R}^4$. After this mapping, the Berry phase can be written as

$$A_\mu = -i \frac{r_\mu r^{-1} \partial_\mu g}{R^2 + r^2 + R \sqrt{R^2 + r^2}}, \quad g = \frac{1}{r} (r_\mu + ir_\sigma \gamma_\mu),$$

which does not satisfy the self-adjoint condition $F^\mu_\nu = \pm \frac{1}{2} \epsilon_{\mu\nu\lambda} F^\nu_\lambda$. Since it has the same Chern number as an instanton, one can always find a continuous coordinate transformation to connect these two solutions. Here we can slightly generalize the above stereographic projection as

$$R_i = f(r) r_i, \quad R_5 = \sqrt{R^2 - f^2(r)} r^2, \quad i = 1, \ldots, 4$$

The resulting Berry phase is

$$A_\mu = -i \frac{f^2(r) g^{-1} \partial_\mu g}{R^2 + R \sqrt{R^2 - f^2(r)} r^2}, \quad g = \frac{1}{r} (r_\mu + ir_\sigma \gamma_\mu).$$

Then it is easy to verify that, by taking $f(r) = \sqrt{r^2 + 2R^2}$, equation (33) will become the standard instanton solution $A_\mu = -i \frac{r^2}{R^2 + r^2} g^{-1} \partial_\mu g$. This is closely parallel to the fact that the $U(1)$ Berry phase of a time reversal-breaking two-band model is the same as a magnetic monopole solution.

5. Three-orbital copper-oxygen model with spin current order

We can apply the same method to understand the three-orbital copper-oxygen model given by the Hamiltonian $H = H_{KE} + H_{int}$ as discussed in section 2. The Hamiltonian can be written in matrix form as

$$H = \begin{pmatrix} 0 & i R_1 & -i R_2 + a \\ -i R_1 & 0 & i s_i R_3 \\ i R_2 + a & -i s_i R_3 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & i R_3 \\ 0 & -i R_3 & 0 \end{pmatrix}$$

with $R_1 = \sin \frac{k_x}{2}$, $R_2 = -\sin \frac{k_y}{2}$, and $R_3 = \cos \frac{k_x}{2} \cos \frac{k_y}{2}$. Note that $R_3$ is always positive for $-\pi \leq k_x, k_y \leq \pi$. $s_i$ is the $i$ component of spin. Here we also introduce a small positive constant $a$ in order to lift the degeneracy of the spin up and spin down bands. With the spin degree of freedom, the Hamiltonian is actually a six by six matrix:

$$H = \begin{pmatrix} 0 & -i R_1 & 0 \\ -i R_1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & i R_3 \\ 0 & -i R_3 & 0 \end{pmatrix}$$

The energy band can be solved from the following cubic equation

$$E^3 - (a^2 + R^2) E + 2a R_3 (s_i R_3) = 0$$

with $R = \sqrt{R_1^2 + R_2^2 + R_3^2}$. At general momentum, the last term of the above equation is different for spin up and spin down, so the degeneracy is lifted at these momenta. Now consider the four TRIM points $(0, 0)$, $(0, \pi)$, $(\pi, 0)$, and $(\pi, \pi)$. At $(0, 0)$, $R_1 = 0$, and at the other three points, $R_3 = 0$. The last term of equation (36) is always zero at TRIM points, thus the spin up and spin down bands degenerate at these points, as required.

As we already know from [6], the top band of the Hamiltonian equation (34) with $a = 0$ and $s_i = \pm 1$ has Chern number $\pm 1$ respectively. Since adding a constant will not change the Chern number, for nonzero $a$, the spin up and down of the top bands of equation (34) still have the Chern number $\pm 1$ respectively. As in the two-band case, we want
to show that the top band has nontrivial Chern parity by counting the number of zero pairs of the Pfaffian \( P(\mathbf{k}) \). Again the Pfaffian is simply \( P(\mathbf{k}) = \langle u_1(\mathbf{k}) | \Theta | u_1(\mathbf{k}) \rangle \). Suppose the three-bands are \( E_{1,2,3} \). It is easy to verify for small \( a \) that the three-bands are always separated by gaps. We will only consider the top band \( E_3 \). Since the Hamiltonian is traceless, \( E_1 + E_2 + E_3 = 0 \), thus we must have \( E_3 \gg 0 \).

There are many ways to write the eigenfunctions: we can write it in a particular gauge as

\[
|u_\pm(\mathbf{k})\rangle \propto \begin{cases} aE_3 - R_1(sR_3) - iE_3R_2 \\ i(E_3(sR_3) - aR_1) - R_1R_2 \\ E_3^2 - R_1^2 \end{cases}
\] (37)

The wavefunction \( |u_\pm\rangle \) is well defined if its three components are not equal to zero at the same time. As in the two-band example, the zeros usually occur at singular points of the wave function. Therefore, we first consider the special momentum point \( \mathbf{k}^* \) where \( |u_{kz=+1}\rangle \) is not well defined or its three components are all zero. From the real part of the 2nd component, we have \( R_1R_2 = 0 \). If we have \( R_1 = 0 \), then the 3rd component requires \( E_3 = 0 \), which is impossible. Thus, we must have \( R_2 = 0 \) or \( E_3 = 0 \). Suppose we consider the case that \( R_2 > 0 \) or \( k_z \gg 0 \); then we have \( E_3 = R_1 \). The imaginary part of the 2nd component gives us \( R_3 = a \). Thus we find out that \( \mathbf{k}^* = (2\cos^{-1}a, 0) \). Then equation (36) become

\[
E^3 - (2a^2 + R_1^2)E + 2a^2R_1 = 0
\]

and one can verify that \( E = E_1 \) indeed satisfies this equation. In summary, at \( \mathbf{k}^* \), we have \( R_2 = 0, R_3 = a \) and \( E_3 = R_1 \) and the Hamiltonian becomes

\[
H_{kz=1} = \begin{pmatrix} 0 & iR_1 & a \\ -iR_1 & 0 & ia \\ a & -ia & 0 \end{pmatrix}
\] (38)

The three eigenvalues are \( R_1 \) and \( \frac{1}{2}(-R_1 \pm \sqrt{R_1^2 + 8a^2}) \). Clearly, if \( R_1 \gg 0 \) and \( a \) is a small positive number, \( R_1 \) is the top band. \( \frac{1}{2}(-R_1 + \sqrt{R_1^2 + 8a^2}) \approx 0 \) is the middle band. \( \frac{1}{2}(-R_1 + \sqrt{R_1^2 + 8a^2}) \approx -R_1 \) is the lower band. So, this is consistent with our previous assumption that \( R_1 \) is the top band. The eigenstate corresponding to \( E_3 = R_1 \) is

\[
|u_\pm\rangle = (i, 1, 0)^T
\] (39)

Now we can also compute the top eigenvalue of \( H_{kz=-1} \) at \( \mathbf{k}^* \). At this point, we find

\[
H_{kz=-1} = \begin{pmatrix} 0 & iR_1 & a \\ -iR_1 & 0 & -ia \\ a & ia & 0 \end{pmatrix}
\] (40)

The three eigenvalues, from bottom to top, are \(-R_1\)

\[
\frac{1}{2}(R_1 - \sqrt{R_1^2 + 8a^2})
\]

and \( \frac{1}{2}(R_1 + \sqrt{R_1^2 + 8a^2}) \), respectively.

So the top band is \( E_3 = \frac{1}{2}(R_1 + \sqrt{R_1^2 + 8a^2}) \) and the corresponding eigenstate is

\[
|u_\pm\rangle \propto \begin{pmatrix} 2a^2 + R_1^2 + R_1\sqrt{R_1^2 + 8a^2} \\ -i(2a^2 + R_1^2 + R_1\sqrt{R_1^2 + 8a^2}) \\ a(3R_1 + \sqrt{R_1^2 + 8a^2}) \end{pmatrix}
\] (41)

Then we find \( \langle u_\pm | \Theta | u_\pm \rangle | \langle u_\pm | \rangle^* = 0 \). Thus \( \pm \mathbf{k}^* \) is pair of zero points of \( P(\mathbf{k}) \).

Now we show that this is the only pair of zeros of \( P(\mathbf{k}) \). Above, we only discussed the special momentum point \( \mathbf{k}^* \) on which the wave function equation (37) is not well defined. Other than these points, we can always use equation (37). Denote the top band of \( H_{kz=1} \) to be \( E_\rho \) and top band of \( H_{kz=-1} \) to be \( E_\nu \). It is easy to find that

\[
P(\mathbf{k}) = \langle u_\pm(\mathbf{k}) | \Theta | u_\pm(\mathbf{k}) \rangle \propto \langle u_\pm(\mathbf{k}) | (|u_\pm(\mathbf{k})\rangle)^* = A + iB
\]

\[
A = a^2(E_\rho E_\nu - R_1^2) - R_1^2(E_\rho^2 + E_\nu^2) + E_\rho E_\nu(E_\rho^2 + R_1^2) + R_1^2R_2
\]

\[
B = 2a(E_\rho E_\nu - R_1^2)R_2
\] (42)

Now we want to show \( A \) and \( B \) cannot be zero at the same time.

First, we consider the case \( R_2 > 0 \). If we assume \( B = 0 \), then this means \( E_\rho E_\nu = R_1^2 \). We know that \( E_\nu \) satisfy equations \( E_\nu^2 - (a^2 + R_1^2) \). Summing up these two equations, and making use of the fact that \( E_\rho \) are positive, we find the following identity

\[
E_\rho^2 + E_\nu^2 = E_\rho E_\nu + a^2 + R_1^2
\] (43)

Combine with \( E_\rho E_\nu = R_1^2 \), we find \( E_\rho^2 + E_\nu^2 = a^2 + R_1^2 + R_1^2 \). Now plug all the above results into the expression of \( A \), we find that \( A = -R_1^2(a^2 + R_1^2 + R_1^2) \). We know that both \( a^2 + R_1^2 + R_1^2 > 0 \) and \( R_1^2 = E_\nu E_\rho > 0 \), thus \( A \neq 0 \) in this case.

Second, we consider the case \( R_2 = 0 \). If we assume that \( A = 0 \), by making use of identity equation (43), we find that

\[
A = (E_\rho E_\nu)^3 + (a^2 - R_1^2 - R_1^2)(E_\rho E_\nu) - 2a^2R_1^2 = 0 \]

(44)

To find a contradiction, we need to derive another identity of \( E_\rho E_\nu \). Subtracting the two equations \( E_\rho E_\nu = (a^2 + R_1^2) \pm 2aR_1E_\nu \), we find that \( (E_\nu - E_\rho) = -2aR_1E_\nu \). Taking the square of this equation, and making use of equation (43), we find the desired identity

\[
-(E_\rho E_\nu)^3 + (a^2 + R_1^2)(E_\rho E_\nu)^2 - 2aR_1E_\nu^2 = 0
\] (45)

Multiplying equation (44) with \( E_\rho E_\nu \), and adding it to equation (45), we find \( (E_\rho E_\nu)^3 = 2R_1^2E_\rho + (E_\rho E_\nu)^2 \). Combining this result with equation (44), we find \( (a^2 - R_1^2)(E_\rho E_\nu) - 2aR_1E_\nu^2 = 0 \). Since we do not consider the special points which satisfy \( R_2 = 0 \) and \( R_3 = \pm a \), we find \( E_\rho E_\nu = 2R_1^2 \). By plugging this result back to equation (44), we find a contradiction. Therefore, in this case, we also have \( A \neq 0 \).

In summary, other than the special points, there are no more zeros of \( P(\mathbf{k}) \). Thus, the \( Z_2 \) invariance is \( -1 \), indicating the QSH state. Similar to the two-band model, the singular points of the eigenfunction, and their gauge dependence, can be explicitly demonstrated by connecting
the $Z_2$ invariant to the second Chern number. But the calculation will be much more complicated than in the two-band case.

6. Conclusion

We have discussed the possible QSH state in a three-band model motivated by a lattice of copper-oxygen planes of high-temperature superconductors. The calculation of the Chern parity, or $Z_2$ invariant, is through a detailed analysis of the singular points of the eigenfunctions. We show that the the zeros of the Pfaffians of the time reversal operator are coincident with the singular points of the eigenfunction. It is known through the dimensional reduction that the nontrivial Chern parity corresponds to the odd second Chern number. But the calculation, one can verify the following results.

\begin{equation}
F^1 = \frac{1}{R^2(R + R_5)} \left[ m_0 \wedge m_0 - m_2 \wedge m_3 \right] = - \frac{R^2 - R_5^2}{2} \frac{dm_1}{R^3}
\end{equation}

Collecting all the above results, we find

\begin{equation}
F^1 = \frac{1}{R^2(R + R_5)} \left[ m_0 \wedge m_0 - m_2 \wedge m_3 \right] = - \frac{R^2 - R_5^2}{2} \frac{dm_1}{R^3} \tag{A.8}
\end{equation}

From the definition of $m_i$ and their outer derivatives $dm_i = 2(dR_i \wedge dR_1 + dR_2 \wedge dR_3)$, it is easy to see that equation (A.9) agrees with equation (23). The other two components can be obtained by similar methods.

To compute the second Chern number, we introduce the volume form of n-sphere

\begin{equation}
\Omega_n = \sum_{i=1}^{n} (-1)^{i-1} R_i dR_i \cdots dR_{i+1} \cdots dR_n \tag{A.10}
\end{equation}

To ease the notation, we omit the $\wedge$ between $dR_i$. By direct calculation, one can verify the following results.

\begin{align}
&dm_1 \wedge dm_1 = -6i dR_1 \cdots dR_5 
\tag{A.11} \\
&dm_1 \wedge m_2 \wedge m_3 = -2(R^2 - R_5^2) dR_1 \cdots dR_4 
\tag{A.12} \\
&m_1 \wedge m_2 \wedge m_3 = -(R^2 - R_5^2) \Omega_4 
\tag{A.13} \\
&dm_1 \wedge m_1 = -2 \Omega_4 
\tag{A.14}
\end{align}

Then we have

\begin{align}
\frac{1}{2} F^2 \wedge F^2 &= \frac{R^2}{R^6} dR_1 \cdots dR_4 + \frac{R_5(R^2 - R_5^2)}{R^6(R + R_5)} dR_1 \cdots dR_4 \\
&+ \frac{(R^2 - R_5^2)}{R^6(R + R_5)} \Omega_4 \wedge dR_5 + \frac{R_5}{R^6} \Omega_4 \wedge dR_5 \\
&= \frac{1}{R^6} (\Omega_4 \wedge dR_5 + R_5 dR_1 \cdots dR_4) = \frac{1}{R^5} \Omega_5
\end{align}

Here $\frac{1}{R^5} \Omega_5$ is the volume form of 4 dimensional unit sphere.

\begin{align}
&\frac{1}{2} F^2 \wedge F^2 \text{ and } \frac{1}{2} F^3 \wedge F^3 \text{ will give the same result as above.} \\
&\text{Therefore we derived equation (26).}
\end{align}

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