Adiabatic Pumping of Chern-Simons Axion Coupling

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We study the adiabatic pumping of the Chern-Simons axion (CSA) coupling along a parametric loop characterized by a nonzero second Chern number $C^{(2)}$ from the viewpoint of the hybrid Wannier representation, in which the Wannier charge centers are visualized as sheets defined over a projected 2D Brillouin zone. We derive a new formula for the CSA coupling, expressing it as an integral involving Berry curvatures and potentials defined on the Wannier charge center sheets. We show that a loop characterized by a nonzero $C^{(2)}$ requires a series of sheet-touching events at which 2π quanta of Berry curvature are passed from sheet to sheet, in such a way that e^2/h units of CSA coupling are pumped by a lattice vector by the end of the cycle. We illustrate these behaviors via explicit calculations on a model tight-binding Hamiltonian and discuss their implications.

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The discovery of topological insulators and related classes of materials in recent years has generated interest in the Chern-Simons axion (CSA) coupling, which makes an isotropic contribution α^{CS} to the magnetoelectric response tensor of the material. This coupling, defined as $\alpha_{ij} = (\partial P_i/\partial B_j)_E = (\partial M_j/\partial E_i)_B$, where P (M) is the polarization (magnetization) and E (B) is the electric (magnetic) field, is conventionally expressed in terms of a dimensionless parameter θ defined via

$$\alpha_{ij}^{\mathrm{CS}} = \frac{\theta e^2}{2\pi h}\delta_{ij}, \tag{1}$$

where θ is determined by the band structure of the insulator via an integral over the Brillouin zone (BZ) of a Chern-Simons 3-form according to

$$\theta = -\frac{1}{4\pi}\int d^3k\epsilon^{ijk}\mathrm{Tr}\left[A_i\partial_j A_k - i\frac{2}{3}A_iA_jA_k\right]. \tag{2}$$

Here $A_i^{nm} = i\langle u_n|\partial_i|u_m\rangle$ is the Berry connection (or non-Abelian gauge field) in Cartesian direction i, where $u_n(\mathbf{k})$ is the periodic part of the Bloch function of the nth occupied band, and the trace is over occupied bands.

The ground-state properties of a band insulator are invariant under any gauge transformation, that is, any unitary transformation $U_{nn'}(\mathbf{k})$ that mixes only the occupied bands. It can be shown that an arbitrary gauge transformation either leaves the 3-form integral in Eq. (2) unchanged or else it shifts it by exactly 2π times an integer. Thus, θ is best regarded as a phase angle that is only well-defined modulo 2π. As a consequence, the presence of either time reversal (TR) or inversion (either of which flips the sign of θ) requires θ to be quantized to an integer multiple of π, with an odd (even) value corresponding to an odd (even) strong Z_2 topological index of a TR-invariant 3D insulator [1,2]. One way to understand the ambiguity of θ modulo 2π, which corresponds to an ambiguity of α^{CS} modulo e^2/h, is to realize that the magnetoelectric coupling is related to the surface anomalous Hall conductivity (AHC) by $\sigma = (\theta/2\pi + C)e^2/h$. Thus, the measurable magnetoelectric response can be changed by a quantum if a layer with nonzero Chern number is attached to the surface, changing the effective value of θ by 2π.

An interesting consequence of this 2π ambiguity is that, if an insulator is allowed to evolve adiabatically around a closed loop in the space of parameters determining the crystal Hamiltonian, with the gap remaining open, the fact that the system returns to the initial physical state means that θ must either return to its original value or change by $2\pi C^{(2)}$, where $C^{(2)}$ is an integer known as a "second Chern number." This possibility of "pumping θ by 2π" has been discussed and demonstrated for some theoretical models [1,2], but the characteristic behaviors of a system undergoing such an adiabatic loop have largely remained unexplored.

Recently, we showed that the hybrid Wannier representation can be a useful and insightful tool for computing topological indices and inspecting the topological properties of 3D insulators [3]. In this approach, the occupied-state wave functions are transformed into a maximally localized Wannier representation in one chosen direction, while remaining Bloch-like in the orthogonal directions. The resulting hybrid Wannier functions (HWFs) inherit the topological character of the insulator, and plots of their Wannier charge centers (WCCs) over the 2D BZ ("Wannier sheets") were shown to provide a useful means of visualizing the topological properties of insulators, allowing us to discriminate between normal, strong topological, weak topological, crystalline topological, and related states [3–6].

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With these motivations, we ask what happens if an adiabatic cycle that pumps θ by 2π is viewed from the point of view of the HWF representation. How do the WCC sheets evolve? Is there a characteristic behavior that signals the presence of a nontrivial cycle (i.e., a nonzero second Chern number)? Answering in the affirmative, we show that quanta e^2/h of Berry curvature are passed from one WCC sheet to the next in a series of isolated band-touching events, in such a way that one quantum of Berry curvature is pumped by an entire lattice vector by the close of the cycle. We illustrate this amusing and instructive result via numerical calculations on a 3D spinor tight-binding model and discuss its implications.

We begin with a brief review of the construction of the hybrid Wannier representation. We choose a special direction, here $\hat{z}$, along which the Wannier transformation is carried out, so that the HWFs are localized in z while remaining Bloch-like in the other two directions [7,8]. Explicitly,

$$|W_{ln}(k_x,k_y)\rangle = \frac{c}{2\pi}\int dk_z e^{ik_z(z-lc)}|u_{n,\mathbf{k}}\rangle, \tag{3}$$

where l is a layer index and c is the lattice constant along $\hat{z}$. In general, there is a $U(N)$ gauge freedom in choosing the N representatives of the occupied space, $|\tilde{u}_{n,\mathbf{k}}\rangle = \sum_m U_{nm}|u_{m,\mathbf{k}}\rangle$, but there is a unique gauge that minimizes the spread functional of the WFs along $\hat{z}$ [8]. These maximally localized HWFs and their WCCs $\bar{z}_n(k_x,k_y) = \langle W_{n0}|z|W_{n0}\rangle$ can be constructed using standard methods [8,9].

For a 2D insulator the WCCs can be plotted as curves $\bar{z}_n$ versus $k_\perp$ in a 1D projected BZ [4,10], while for a 3D insulator they can be visualized as sheets plotted over the 2D projected BZ. In previous work [3], we have shown that these WCC sheets allow one to see how electrons are adiabatically pumped along $\hat{z}$ as k_x and k_y are varied, thus discriminating between normal and Chern insulators when TR is broken, or between normal and Z_2-odd insulators in the TR-invariant (TRI) case [3].

It is also of interest to consider the behavior of the WCC sheets as the crystal Hamiltonian is carried adiabatically around a loop defined by some cyclic parameter α corresponding, e.g., to some combination of atomic displacements and/or external fields. A celebrated result of Thouless [11] is that this results in quantized adiabatic charge transport, i.e., the pumping of exactly one electron per unit cell by a lattice vector $\mathbf{R}$ during the cycle. Normally $\mathbf{R} = \mathbf{0}$, but, for example, if $\mathbf{R} = c\hat{z}$, this corresponds to the pumping of one electron by one period along z during the cycle (a first Chern number of $C = 1$), i.e., a change in electric polarization $\Delta P_z = -e/A_{\text{cell}}$ with A_{cell} the projected unit cell area.

Let us see how this evolution occurs from the viewpoint of the HWF representation. Intuitively, we expect each WCC sheet to drift along z with increasing α such that it replaces the one above it, and is replaced by the one below it, at the end of the cycle. We begin by defining Berry potentials "living on the sheets" representation as

$$A_{x,ln,l'm} = \langle W_{ln}|i\partial_x|W_{l'm}\rangle, \tag{4}$$

and similarly for A_y. These are functions of (k_x, k_y) and also matrices in the space of sheet labels ln (the nth sheet in cell l along z). The corresponding Berry potentials in the Bloch representation are then just

$$A_{x,nm}(\mathbf{k}) = \sum_l e^{ik_z lc}A_{x,0n,lm}(k_x,k_y), \tag{5}$$

$$A_{z,nm}(\mathbf{k}) = \bar{z}_n(k_x,k_y)\delta_{nm}. \tag{6}$$

Plugging into the Berry-phase formula for the electronic contribution $P_j = -e(2\pi)^{-3}\sum_n \int d^3k A_{jn}(\mathbf{k})$, we find

$$P_z = \frac{-e}{(2\pi)^2 c}\sum_n \int d^2k \bar{z}_n(k_x,k_y), \tag{7}$$

and similarly for P_x or P_y with $A_{j,0n,0n}$ replacing $\bar{z}_n$. For the case of a parametric loop that pumps electrons along z, the change $\Delta P_z = -e/A_{\text{cell}}$ would occur via the gradual migration of the $\bar{z}(k_x,k_y)$ along the $+\hat{z}$ direction, with a relabeling of sheets required at the end of the loop.

Now we again consider an adiabatic cycle in a 3D insulator, but this time one that results in the pumping of the CSA coupling, increasing θ by 2π times the second Chern number $C^{(2)}$ defined earlier. This corresponds to a pumping of Berry curvature, instead of electric charge, along z during the adiabatic cycle. For this purpose, we define a Berry curvature on the WCC sheets as $\Omega_{xy,ln,l'm}(k_x,k_y) = i\langle\partial_x W_{ln}|\partial_y W_{l'm}\rangle - i\langle\partial_y W_{ln}|\partial_x W_{l'm}\rangle$. The relation to the Berry curvature in the Bloch representation is similar to that for A in Eq. (5). The intrinsic AHC σ_{yx} of the crystal is just given by integrating the trace of Ω_{xy} in the Bloch representation over the 3D BZ, and this is easily shown to be equal to $(e^2/hc)\sum_n C_n$, where C_n is the Chern number of the nth sheet in the home unit cell, given by $C_n = (2\pi)^{-1}\int d^2k\Omega_{xy,0n,0n}$. We shall exclude quantum anomalous Hall insulators from our discussion here, so we can assume that $\sum_n C_n = 0$, but importantly the individual C_n can be nonzero.

We now address the central issue of this Letter, namely, how to represent the CSA coupling θ in the HWF representation. Starting from Eq. (2), this can be written as

$$\theta = \theta_{z\Omega} + \theta_{\Delta xy}, \tag{8}$$

where

$$\theta_{z\Omega} = -\frac{1}{2\pi}\int d^3k \mathrm{Tr}[A_z \Omega_{xy}], \quad (9)$$

$$\theta_{\Delta xy} = -\frac{1}{2\pi}\int d^3k \mathrm{Tr}[A_y \partial_z A_x - iA_z[A_x, A_y]]. \quad (10)$$

Performing the k_z integrations, these are expressed in the HWF representation as

$$\theta_{z\Omega} = -\frac{1}{c}\int d^2k \sum_n \bar{z}_n \Omega_{xy,0n,0n}, \quad (11)$$

$$\theta_{\Delta xy} = \frac{i}{c}\int d^2k \sum_{lmn} (\bar{z}_{lm} - \bar{z}_{0n}) A_{x,0n,lm} A_{y,lm,0n}, \quad (12)$$

where $\bar{z}_{lm} = lc + \bar{z}_m$. In deriving Eq. (12), we have used that

$$\frac{c}{2\pi}\int dk_z \mathrm{Tr}[A_y \partial_z A_x] = \sum_l \sum_{nm} (ilc) A_{x,0n,lm} A_{y,lm,0n}. \quad (13)$$

Equations. (8), (11), and (12) constitute a major result of the present work [12].

Of primary concern to us here is the "Berry curvature dipole" term $\theta_{z\Omega}$ in Eq. (11), which describes the extent to which concentrations of positive and negative Berry curvature on the WCC sheets, given by $\Omega_{xy,0n,0n}(k_x, k_y)$, are displaced from one another along the $\hat{z}$ direction as given by $\bar{z}_n(k_x, k_y)$. Note that $\theta_{z\Omega}$ is shifted by $-2\pi C_n$ if the choice of WCC sheets comprising the home unit cell is changed so as to shift some $\bar{z}_n$ by c. The $\theta_{z\Omega}$ term is therefore the one that has the 2π ambiguity, and we shall see that it is responsible for the pumping of CSA coupling. The second term $\theta_{\Delta xy}$, given by Eq. (12), is an intersheet contribution in which the z separation between sheets at (k_x, k_y) is coupled to the off-diagonal (intersheet) matrix elements of the Berry potentials. There is no 2π ambiguity associated with this term, and as we shall see, it typically remains small even when θ is not. We regard it as a correction term that is needed for quantitative accuracy but is not relevant to topological considerations.

We now illustrate the concepts introduced above in the context of a simple tight-binding model. Following Essin *et al.* [1], we start with the Fu-Kane-Mele (FKM) model [13], which is a four-band model of s orbitals on a diamond lattice with spin-orbit interaction,

$$H_{\mathrm{FKM}} = \sum_{\langle ij\rangle} t(\mathbf{e}_{ij}) c_i^\dagger c_j + i\lambda_{\mathrm{so}} \sum_{\langle\langle ij\rangle\rangle} c_i^\dagger \mathbf{s}\cdot(\mathbf{d}_{ij}^1 \times \mathbf{d}_{ij}^2) c_j. \quad (14)$$

The first term is a sum over first-neighbor hoppings, where $\mathbf{e}_{ij}$ is the bond vector, while the second term involves second-neighbor hops in which vectors $\mathbf{d}_{ij}^{1,2}$ describe the two first-neighbor bonds that make up the second-neighbor hop. We take the cubic lattice constant to be unity. In the original FKM model $t(\mathbf{e}_{ij}) = t_0$ independent of hopping direction, but following Ref. [1], we take $t(\mathbf{e}_{ij}) = t_0(3+\delta)$ for the bond along (111) and t_0 for the other three bonds. We set the first-neighbor and spin-dependent second-neighbor hoppings to $t_0 = 1$ and $\lambda_{\mathrm{so}} = 1$, respectively, and assume two bands are occupied.

The strong topological and trivial phases are separated from each other by a band touching at the Γ point when $\delta = 0$. Again following Essin *et al.* [1], we add a staggered Zeeman field h, and define an adiabatic loop parametrized by $\delta(\alpha) = m\cos(\alpha)$ and $h(\alpha) = m\sin(\alpha)$, where α runs from 0 to 2π, such that the system remains insulating on the loop and θ is pumped by 2π. The HWF representation is constructed with $\hat{z}$ along the (111) direction.

The WCC sheets derived from the two occupied bands in the FKM model are shown in Fig. 1, where one pair of sheets and one copy of their periodic images along $\hat{z}$ are shown for some points around the adiabatic loop [14]. The evolution of the Wannier sheet positions is plotted in Figs. 2(a) and 2(b) at the four TRI points, namely, at the BZ center Γ and at the three equivalent M points, e.g., (π, π).

The system has TR symmetry at $\alpha = 0$ and π, where the system is Z_2 even and Z_2 odd, respectively, and where the WCC sheets pair up at the four TRI points due to Kramers degeneracy [3]. In the normal phase at $\alpha = 0$, this results in a pair of sheets connected by Dirac points at all four TRI momenta, and each pair is well separated from its neighbors along $\hat{z}$. As α increases, the Dirac crossings are gapped and the sheets begin to separate. At the three M points, the separation between the pair remains quite small, and the same sheets touch again at $\alpha = \pi$, as is obvious from Fig. 2(a). At the Γ point, however, the sheets separate strongly and eventually reconnect with their neighbors from the next unit cell along $\hat{z}$ when $\alpha = \pi$. The swapping

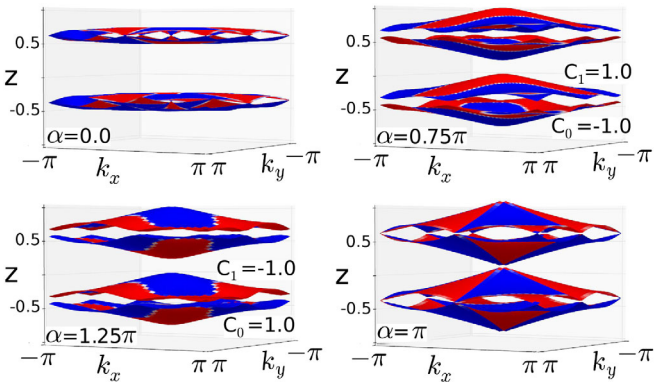

FIG. 1 (color online). The two WCC sheets of the half filled FKM model, and one set of periodic images, at four stages $\alpha = (0, 3\pi/4, \pi, 5\pi/4)$ along the parametric cycle (clockwise from upper left). Blue and red colors show positive and negative values of Berry curvature Ω_z on the sheets, respectively. The Chern numbers associated with the individual WCC sheets are shown for those cases where sheets do not touch.

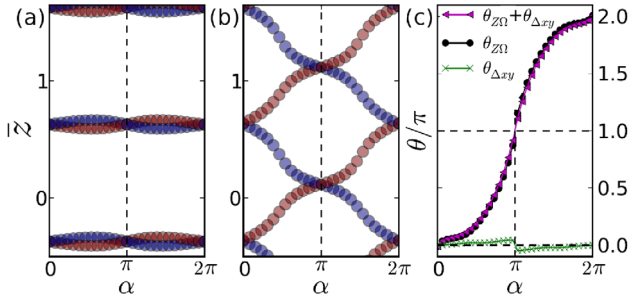

FIG. 2 (color online). WCCs at (a) M and (b) Γ of the 2D BZ for the FKM model as a function of the adiabatic loop parameter α. Blue and red colors indicate positive and negative values of Berry curvature, respectively. (c) CSA coupling $\theta(\alpha)$ and its contributions $\theta_{z\Omega}$ and $\theta_{\Delta xy}$ for the same adiabatic loop.

of partners at an odd number of the TRI points (here, only at Γ) is characteristic of the strong topological (Z_2-odd) phase at $\alpha = \pi$. Note, however, that the WCC sheets, taken together, have no net displacement along the $\hat{z}$ direction, so no charge is pumped.

To see what happens to the CSA coupling θ during this cycle, we inspect the Berry curvature Ω_{xy} on the sheets, represented by the color-scale shading in Figs. 1, 2(a), and 2(b). We see that the behavior near the M points is uninteresting; positive and negative Berry curvature contributions separate slightly at first, but they then reverse and recross, and never give a large contribution to $\theta_{z\Omega}$, as given by Eq. (11). Near Γ, however, the story is strikingly different. A negative (red) increment of Berry curvature is transported along $+\hat{z}$ while a positive (blue) contribution is carried along $-\hat{z}$ as α evolves from 0 to π. For small and positive α we expect that the total Berry curvature near Γ in the top and bottom sheets (at $\bar{z}_2$ and $\bar{z}_1$) should be $-\pi$ and π, respectively, characteristic of a weakly gapped Dirac point. Thus, the contribution to the Berry curvature dipole term $\theta_{z\Omega}$ from the vicinity of Γ, which is approximately $\pi(\bar{z}_2(0,0) - \bar{z}_1(0,0))/c$, grows gradually as α increases and the sheets get farther apart at Γ. As $\alpha \to \pi$, the separation between the sheets at Γ approaches a full lattice constant c and the contribution to $\theta_{z\Omega}$ approaches π.

This expectation is confirmed in Fig. 2(c), where we plot θ and its contributions $\theta_{z\Omega}$ and $\theta_{\Delta xy}$ versus α. The nontopological $\theta_{\Delta xy}$ term is almost negligible everywhere around the adiabatic loop, and is not discussed further. As α passes through π there is a Dirac touching at Γ between sheet 2 in the home cell and sheet 1 in the cell above, with a hand-off of -2π units of Berry curvature (or a Chern number of -1) from the former to the latter, with the concentration of Berry curvature near Γ in band 2 switching from $-\pi$ to π. A direct evaluation of Eq. (11) would show $\theta_{z\Omega}$ and θ dropping discontinuously by 2π as α crosses through π, but we make use of the gauge freedom to apply a 2π shift of θ to impose physical continuity when drawing the curves in Fig. 2(c).

Here we have illustrated the behavior of just one model system, and we have found that the pumping of θ by 2π is accomplished by a series of touching events between WCC sheets, such that one Chern number of Berry curvature is handed off to the neighboring sheet with each touching. But it is now clear in retrospect that any cycle that pumps θ by 2π must involve such a sequence of touching events, because if these events did not occur, the CSA coupling could not be passed along by a lattice vector during the cycle. Incidentally, this observation also explains why a nontrivial θ pumping cycle is impossible in a system with a single occupied band, since in this case the WCC sheets are always separated by $c\hat{z}$ and can never touch.

One can also consider the corresponding evolution of the Berry curvatures and Chern transfers for finite slabs, where the bulk of the slab undergoes the same cyclic evolution. If the surface Hamiltonian could be constantly readjusted so as to remain insulating, the net result at the end of the cycle would be to change the surface AHC by $\pm e^2/h$ at the bottom and top surfaces of the slab, respectively. In the more common case that the surface returns to its initial state at the end of the cycle, the AHC must return to itself too, so the slab is topologically required to have a metallic surface phase over some interval of α. During this α interval, the surface AHC changes continuously with changing filling in such a way as to contribute $\mp e^2/h$ by the time the surface band is completely filled or depleted, removing the extra Chern number pumped from the bulk. The existence of such surface states can be an experimental signature characterizing any adiabatic loop with a nonzero second Chern number.

In summary, we have demonstrated that the WCC sheets as defined in the HWF representation, which had previously been shown to be useful for identifying and visualizing the topological properties of nontrivial insulating phases, also provides an insightful characterization of a nontrivial parametric loop characterized by a second Chern number. By defining Berry connections and curvatures associated with the WCC sheets, we have derived a new formula for the CSA axion coupling θ as a decomposition into a topological Berry curvature dipole term and a nontopological correction term. In this kind of adiabatic cycle it is not the charge, but the sheet Berry curvature, that is pumped during the cycle. In our formulation the 2π ambiguity of θ is readily evident when some sheets have nonzero Chern numbers, in which case a different assignment of sheets to the home unit cell can shift θ by 2π, and the link to the surface anomalous Hall conductivity becomes more direct. We also speculate that Eqs. (11) and (12) may provide a more efficient practical means of computing θ than those used previously, since there is no need to establish a smooth gauge in the 3D Brillouin zone. In any case, we believe that our extended development of the HWF representation should prove broadly useful in

characterizing the adiabatic evolution of topological materials and their magnetoelectric properties.

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