

Geometric and nongeometric contributions to the surface anomalous Hall conductivity

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A magnetoelectric insulator exposed to a *dc* electric field develops an orbital magnetization, which in turn generates bound circulating currents at the surfaces. We consider the anomalous Hall part of this current response at an insulating surface of a slab. In contrast to the quantized anomalous Hall conductivity of a Chern insulator, which comes entirely from the *k*-space Berry curvature, we find that the surface anomalous Hall conductivity is not a purely geometric property of the ground-state wave functions, having in general a nongeometric part as well. That non-geometric part is the surface manifestation of an anisotropic bulk response of the crystal, the cross-gap contribution to the orbital magnetoelectric tensor. The geometric part of the surface anomalous Hall conductivity can change by multiples of e^2/h depending on the surface preparation, but is otherwise isotropic and fixed by the bulk. We calculate it unambiguously from an expression involving the metric-curvature tensor (the Berry curvature part is not enough) of the slab wave functions.

I. INTRODUCTION

Certain surface properties of crystals are strongly constrained by the bulk, and as a result they are very robust with respect to local perturbations. An example is the areal charge density σ_{surf} bound to an insulating surface of a polar insulator. For an unreconstructed defect-free surface with outward normal $\hat{n}$, it is given by [1]

$$\sigma_{\text{surf}} = \left(\mathbf{P} + \frac{e\mathbf{R}}{V_c} \right) \cdot \hat{n}, \quad (1)$$

where $\mathbf{P}$ is the bulk electric polarization, $\mathbf{R}$ is a lattice vector, and V_c is the volume of a unit cell. According to the Berry-phase theory [2], $\mathbf{P}$ is only defined modulo $e\mathbf{R}/V_c$, since it is possible to change its value by that amount by adjusting the phases of the Bloch wave functions. Equation (1) assumes that a definite choice of gauge has been made so that a unique value of $\mathbf{P}$ has been established. (Here the word “gauge” refers to the freedom to adjust the phases of the Bloch eigenstates or, more generally, to perform a unitary transformation at each $\mathbf{k}$ among the occupied Bloch states [3].) The second term in Eq. (1) amounts to an integer number of electrons per surface unit cell. Its presence is required because it is in principle possible to prepare the insulating surface in different ways such that the macroscopic charge per surface cell changes by a multiple of the elementary charge e . Thus, the quantized part of σ_{surf} depends on the details at the surface but the unquantized part does not (it is a bulk property).

In this work, we consider a similar situation that arises in insulating crystals that display the linear magnetoelectric (ME) effect, whereby an applied magnetic field $\mathbf{B}$ induces an electric polarization $\mathbf{P}$, and conversely an applied electric field $\mathcal{E}$ induces a magnetization $\mathbf{M}$ [4, 5].

The linear ME tensor is defined as

$$\alpha_{ab} = \left. \frac{\partial P_a}{\partial B_b} \right|_{\mathcal{E}=0} = \left. \frac{\partial M_b}{\partial \mathcal{E}_a} \right|_{B=0}. \quad (2)$$

The full ME response contains both frozen-ion and lattice-mediated contributions, and each can be further decomposed into spin and orbital parts. In the following, we focus exclusively on the frozen-ion orbital response.

The bulk magnetization induced by an electric field generates bound surface currents

$$\mathbf{K} = \mathbf{M} \times \hat{n}. \quad (3)$$

For an insulating surface this is the full current response, which can be described by a 2×3 surface conductivity tensor $\sigma_{ab}^{\text{surf}}$. The surface anomalous Hall conductivity (AHC) is then defined as the antisymmetric part of the 2×2 block that accounts for the surface current induced by an in-plane electric field. Writing that part in vector form as $\sigma_{\text{surf}}^{\text{AH}} \hat{n}$ where

$$\sigma_{\text{surf}}^{\text{AH}} = -\frac{1}{2} \epsilon_{cdb} \sigma_{cd}^{\text{surf}} n_b, \quad (4)$$

the surface anomalous Hall current density becomes

$$\mathbf{K}^{\text{AH}} = \sigma_{\text{surf}}^{\text{AH}} \hat{n} \times \mathcal{E}. \quad (5)$$

From Eqs. (2) and (3) we find

$$\sigma_{cd}^{\text{surf}} = \frac{\partial K_c}{\partial \mathcal{E}_d} = \frac{\partial}{\partial \mathcal{E}_d} \epsilon_{cea} M_e n_a = \epsilon_{cea} \alpha_{de} n_a, \quad (6)$$

which plugged into Eq. (4) leads to

$$\sigma_{\text{surf}}^{\text{AH}} = -\frac{1}{2} \text{Tr}(\alpha) + \frac{1}{2} \alpha_{ab} n_a n_b. \quad (7)$$

Note that the antisymmetric part of the ME tensor does not contribute to Eq. (7). Separating α_{ab} into an isotropic trace piece and a traceless part,

$$\alpha_{ab} = \alpha_{\text{iso}} \delta_{ab} + \tilde{\alpha}_{ab}, \quad (8)$$

we arrive at the relation

$$\sigma_{\text{surf}}^{\text{AH}} = -\alpha_{\text{iso}} + \frac{1}{2}\tilde{\alpha}_{ab}\hat{n}_a\hat{n}_b. \quad (9)$$

Whenever the symmetric anisotropic (quadrupole) part of the bulk ME tensor is nonzero, the surface AHC depends on the surface orientation via the second term.

A key observation is that α_{iso} , like $\mathbf{P}$, carries a quantum of indeterminacy: certain gauge transformations among the Bloch wave functions change its value by integer multiples of the quantum of conductance e^2/h [6, 7]. Because of this ambiguity, Eq. (9) needs to be sharpened; once a definite gauge choice has been made leading to a unique value of α_{iso} , Eq. (9) should be upgraded to

$$\sigma_{\text{surf}}^{\text{AH}} = -\alpha_{\text{iso}} + m\frac{e^2}{h} + \frac{1}{2}\tilde{\alpha}_{ab}\hat{n}_a\hat{n}_b. \quad (10)$$

The added term reflects the possibility of modifying the insulating surface in such a way that the surface AHC changes by a multiple of the quantum of conductance.¹ This can be done, in principle, by stitching a Chern insulating layer to the surface [7, 8] or otherwise changing the surface Hamiltonian, or by means of an adiabatic pumping cycle [10, 11]. As a result only the nonquantized part of the surface AHC is a bulk property, in close analogy with Eq. (1) for the surface charge. (One difference with respect to Eq. (1) is that since the quantum of conductance in Eq. (10) is unit-cell-independent, its value does not get reduced in the presence of surface reconstruction.)

We are now ready to formulate the main question behind the present work. Suppose we have a ME insulator (it should break both inversion and time reversal symmetry [4]), and we consider a specific insulating surface with orientation $\hat{\mathbf{n}}$. How can we calculate the surface AHC, not just up to a quantum, but exactly? Since we are given a definite surface Hamiltonian, there should be a definite answer without any quantum of ambiguity.

We shall answer this question by first calculating the local conductivity from its definition as the linear current-density response to a homogeneous electric field,

$$\sigma_{ab}(\mathbf{r}) = \left. \frac{\partial j_a(\mathbf{r})}{\partial \mathcal{E}_b} \right|_{\mathcal{E}=0}, \quad (11)$$

and then obtaining the surface AHC of a slab as an integral of its antisymmetric part. The integral spans a surface unit cell in the in-plane directions, and in the surface-normal direction it extends from the bulklike interior region of the slab up the surface. As a numerical

check of the resulting expression for $\sigma_{\text{surf}}^{\text{AH}}$, we have evaluated it for tight-binding models, finding consistent results, via Eq. (10), with the bulk ME tensor calculated as in Refs. 12 and 13.

The manuscript is organized as follows. The local AHC is discussed in Sec. II, where we first derive a quantum-mechanical expression from linear response, and then identify a geometric contribution. Those expressions are used in Sec. III to calculate the surface AHC of a slab, which we again separate into geometric and nongeometric parts. In Sec. IV the resulting formalism is used to study numerically the surface AHC of two different tight-binding (TB) models. We conclude with a Summary, and in the Appendix we review the relation between surface AHC and the phenomenology of axion electrodynamics.

II. LOCAL ANOMALOUS HALL CONDUCTIVITY

A. Linear-response calculation

Consider a bounded electron system at zero temperature described a single-particle Hamiltonian $\hat{H}$. The current-density operator reads

$$\hat{\mathbf{j}}(\mathbf{r}) = -\frac{e}{2}[\hat{\mathbf{n}}(\mathbf{r})\hat{\mathbf{v}} + \hat{\mathbf{v}}\hat{\mathbf{n}}(\mathbf{r})], \quad (12)$$

where $\hat{\mathbf{n}}(\mathbf{r}) = |\mathbf{r}\rangle\langle\mathbf{r}|$, $\hat{\mathbf{v}} = (1/i\hbar)[\hat{\mathbf{r}}, \hat{H}]$ is the velocity operator, and $e > 0$ is the elementary charge. The current density at a point $\mathbf{r}$ is given by

$$\mathbf{j}(\mathbf{r}) = \text{Tr} [\hat{P}\hat{\mathbf{j}}(\mathbf{r})] = -e \text{Re} \langle \mathbf{r} | \hat{\mathbf{v}} \hat{P} | \mathbf{r} \rangle, \quad (13)$$

where $\hat{P}$ denotes the projection operator onto the occupied states. To evaluate the local conductivity (11) we let $\hat{H} = \hat{H}_0 + e\mathcal{E} \cdot \hat{\mathbf{r}}$, and note that since $[\hat{r}_a, \hat{r}_b] = 0$ we have $\hat{\mathbf{v}} = (1/i\hbar)[\mathbf{r}, \hat{H}_0]$, so that Eq. (13) depends on $\mathcal{E}$ through $\hat{P}$ only.² We immediately find $\sigma_{ab}(\mathbf{r}) = (-e)\text{Re} \langle \mathbf{r} | \hat{v}_a \partial_{\mathcal{E}_b} \hat{P} | \mathbf{r} \rangle$, where $(\partial \hat{P} / \partial \mathcal{E})_{\mathcal{E}=0}$ has been written as $\partial_{\mathcal{E}} \hat{P}$. Expressing the local AHC in vector form as done in Eq. (4) for the surface AHC,

$$\sigma_c^{\text{AH}}(\mathbf{r}) = -\frac{1}{2}\varepsilon_{abc}\sigma_{ab}(\mathbf{r}), \quad (14)$$

we obtain

$$\mathbf{j}^{\text{AH}}(\mathbf{r}) = \boldsymbol{\sigma}^{\text{AH}}(\mathbf{r}) \times \boldsymbol{\mathcal{E}} \quad (15)$$

for the AH current density, with the local AHC given by

$$\boldsymbol{\sigma}^{\text{AH}}(\mathbf{r}) = \frac{e}{2} \text{Re} \langle \mathbf{r} | \hat{\mathbf{v}} \times \partial_{\mathcal{E}} \hat{P} | \mathbf{r} \rangle. \quad (16)$$

¹ There are two scenarios compatible with Eq. (10). If the integer m is the same for all crystal facets, the entire surface is insulating and the term me^2/h gives an isotropic contribution to the surface AHC [8]. Otherwise the contribution me^2/h is anisotropic, and there are chiral conducting channels along the lines of intersection between adjacent facets with different m values [9].

² We are ignoring local-field corrections, which introduce a dependence of $\hat{H}_0$ on $\mathcal{E}$ through the self-consistent charge density. Such terms are not difficult to derive, but they are absent from our non-self-consistent TB calculations.

The operator $\partial_{\mathbf{E}}\hat{P}$ can be evaluated by expanding the ground-state projector $\hat{P}_0 = \hat{P}(\mathbf{E} = 0)$ as $\sum_v |v\rangle\langle v|$, where $|v\rangle$ denotes an occupied energy eigenstate. From first-order perturbation theory we get

$$\partial_{\mathbf{E}}\hat{P} = -e \sum_{v,c} \left(|c\rangle \frac{\langle c|\hat{\mathbf{r}}|v\rangle}{E_{cv}} \langle v| + |v\rangle \frac{\langle v|\hat{\mathbf{r}}|c\rangle}{E_{cv}} \langle c| \right), \quad (17)$$

where $|c\rangle$ is an empty eigenstate and $E_{cv} = E_c - E_v$.

Although Eq. (17) contains matrix elements of the non-periodic position operator $\hat{\mathbf{r}}$, they remain well-defined under periodic boundary conditions thanks to the identity $\langle v|\hat{\mathbf{r}}|c\rangle = i\hbar\langle v|\hat{\mathbf{v}}|c\rangle/E_{cv}$, valid for off-diagonal matrix elements. Equation (16) is therefore a suitable starting point for the calculation of the surface AHC of a slab to be carried out in Sec. III.

B. Geometric (Chern-Simons) contribution

Consider a bounded sample whose microscopic AHC is given by $\sigma^{\text{AH}}(\mathbf{r})$ at every point in space. The sample as a whole has an isotropic ME response given by

$$\mathbf{a}_{\text{iso}} = \frac{1}{3} \sum_a \frac{\partial m_a}{\partial \mathcal{E}_a}, \quad (18)$$

where $\mathbf{m}$ is the orbital moment

$$\mathbf{m} = \frac{1}{2} \int \mathbf{r} \times \mathbf{j}(\mathbf{r}) d^3r. \quad (19)$$

If the sample has a macroscopic volume V and is globally insulating (both in the interior region and in the entire surface region), then the extensive coefficient $\mathbf{a}_{\text{iso}}$ is related to the bulk coefficient α_{iso} by [8]

$$\frac{\mathbf{a}_{\text{iso}}}{V} = \alpha_{\text{iso}} - \frac{me^2}{h}, \quad (20)$$

where the value of m depends on the choice of branch for α_{iso} . (Note that the right-hand-side is equal to minus the first two terms in Eq. (10) for the surface AHC. As discussed in Appendix A, those terms are described by the phenomenology of axion electrodynamics [6, 14].) Plugging Eq. (19) into Eq. (18) and then comparing with Eq. (14) for σ^{AH} , we find

$$\mathbf{a}_{\text{iso}} = -\frac{1}{3} \int \mathbf{r} \cdot \sigma^{\text{AH}}(\mathbf{r}) d^3r. \quad (21)$$

This relation will help us identify a geometric contribution to the local AHC, but first we need some results from the microscopic theory of the orbital ME response.

The quantum-mechanical expression for the bulk ME tensor α_{ab} comprises an isotropic geometric term known as the Chern-Simons (CS) term, and a nongeometric term known as the Kubo or cross-gap (cg) term that has both

isotropic and anisotropic parts [12, 13]. The relation between those two terms and the decomposition in Eq. (8) can be summarized as follows,

$$\alpha_{ab} = \underbrace{(\alpha_{\text{CS}} + \alpha_{\text{iso}}^{\text{cg}})}_{\alpha_{\text{iso}}} \delta_{ab} + \tilde{\alpha}_{ab}. \quad (22)$$

The expressions for α_{CS} and α_{ab}^{cg} are given in Refs. 12 and 13. α_{CS} takes the form of a Brillouin zone (BZ) integral of the Chern-Simons three-form of the valence states, which is only well-defined modulo e^2/h [6, 7]. α_{ab}^{cg} is given by a more conventional-looking linear-response expression, and carries no quantum of ambiguity. Besides the unperturbed cell-periodic valence states $|u_{\mathbf{k}v}\rangle$ and their first $\mathbf{k}$ -derivatives (the quantities entering α_{CS}), the expression for α_{ab}^{cg} involves $|\partial_{\mathbf{E}}u_{\mathbf{k}v}\rangle$ given by Eq. (33) below, and some additional velocity matrix elements.

For a (globally insulating) bounded sample, the ME tensor $\mathbf{a}_{ab} = (\partial m_b / \partial \mathcal{E}_a)_{\mathbf{B}=0}$ can also be decomposed in the manner of Eq. (22). In this case the isotropic CS contribution carries no quantum of ambiguity, and takes the form [12]

$$\begin{aligned} \mathbf{a}_{\text{CS}} &= -\frac{2\pi e^2}{3h} \varepsilon_{abc} \text{Im Tr} \left[\hat{P}_0 \hat{r}_a \hat{P}_0 \hat{r}_b \hat{P}_0 \hat{r}_c \right] \\ &= \frac{2\pi e^2}{3h} \varepsilon_{abc} \int r_c \text{Im} \langle \mathbf{r} | \hat{P}_0 \hat{r}_a \hat{Q}_0 \hat{r}_b \hat{P}_0 | \mathbf{r} \rangle d^3r, \end{aligned} \quad (23)$$

where $\hat{Q}_0 = \hat{1} - \hat{P}_0$. Comparing with Eq. (21), we are led to identify a CS contribution to the local AHC given by

$$\sigma_{\text{CS}}^{\text{AH}}(\mathbf{r}) = \frac{e^2}{h} \mathbf{C}(\mathbf{r}), \quad (24a)$$

$$\mathbf{C}(\mathbf{r}) = -2\pi \text{Im} \langle \mathbf{r} | \hat{P}_0 \hat{\mathbf{r}} \hat{Q}_0 \times \hat{Q}_0 \hat{\mathbf{r}} \hat{P}_0 | \mathbf{r} \rangle. \quad (24b)$$

The quantity $\mathbf{C}(\mathbf{r})$ has units of inverse length in three dimensions. Its integral over a bounded sample vanishes identically [15], but $\mathbf{C}(\mathbf{r})$ can be locally nonzero in systems that break time-reversal symmetry [16].

In view of Eq. (24), we decompose the net local AHC of Eq. (16) as

$$\sigma^{\text{AH}}(\mathbf{r}) = \sigma_{\text{CS}}^{\text{AH}}(\mathbf{r}) + \overbrace{\sigma^{\text{AH}}(\mathbf{r}) - \sigma_{\text{CS}}^{\text{AH}}(\mathbf{r})}^{\sigma_{\text{cg}}^{\text{AH}}(\mathbf{r})}. \quad (25)$$

The second term, denoted the cross-gap term by analogy with the “upper” decomposition of α_{ab} in Eq. (22), was overlooked in a recent study of the local AHC [17], where only the CS term was considered.

Equations (16), (24), and (25) are the main results of this section, and in the next section we will use them to calculate and analyze the AHC of an insulating surface.

III. SURFACE ANOMALOUS HALL CONDUCTIVITY

A. Evaluation in a slab geometry

Consider a thick insulating slab with the outward normal $\hat{\mathbf{n}} = \hat{\mathbf{z}}$ of the top surface pointing along a bulk reciprocal-lattice vector $\mathbf{b}_3$. We assume a defect-free surface, and introduce a z -resolved AHC for the slab by averaging the z component of the local AHC (16) over a surface unit cell at fixed z ,

$$\sigma_{\text{slab}}^{\text{AH}}(z) = \frac{1}{A_c} \int_{A_c} \sigma_z^{\text{AH}}(x, y, z) dx dy. \quad (26)$$

The macroscopic AHC of the entire slab is obtained by integrating over all z ,

$$\sigma_{\text{slab}}^{\text{AH}} = \int_{-\infty}^{+\infty} \sigma_{\text{slab}}^{\text{AH}}(z) dz, \quad (27)$$

and because the slab is insulating the result is necessarily quantized in units of e^2/h [18],

$$\sigma_{\text{slab}}^{\text{AH}} = \frac{e^2}{h} C_{\text{slab}}. \quad (28)$$

The integer Chern number C_{slab} is defined in Eq. (36) below, and systems with $C_{\text{slab}} \neq 0$ are known as quantum anomalous Hall insulators (or Chern insulators).

To ensure that the surfaces can be made insulating and that they have well-defined AHCs, the three bulk Chern indices C_x , C_y , and C_z must vanish. The surface AHC can then be calculated as follows. First we filter out the atomic-scale oscillations in $\sigma_{\text{slab}}^{\text{AH}}(z)$ by performing a “sliding-window average” over one vertical lattice constant $c = 2\pi/|\mathbf{b}_3|$,

$$\bar{\sigma}_{\text{slab}}^{\text{AH}}(z) = \frac{1}{c} \int_{z-c/2}^{z+c/2} \sigma_{\text{slab}}^{\text{AH}}(z') dz'. \quad (29)$$

Because $C_z = 0$, there can be no macroscopic AH current flowing in-plane in the bulklike interior region of the

slab. Equation (29) must therefore give a vanishing result when z lies deep below the surface, and the result can only become nonzero near the surfaces. The AHC of the top surface is obtained by integrating from the middle of the slab at $z = 0$ (or from any other bulklike point) up to the vacuum region above the slab,³

$$\sigma_{\text{surf}}^{\text{AH}} = \int_0^{+\infty} \bar{\sigma}_{\text{slab}}^{\text{AH}}(z) dz, \quad (30)$$

and at the bottom surface the AHC is $C_{\text{slab}}e^2/h - \sigma_{\text{surf}}^{\text{AH}}$.

B. Total surface anomalous Hall conductivity

To evaluate the net AHC at a given surface, we need an expression for the z -resolved slab AHC defined by Eq. (26). We begin by expanding the projection operator $\hat{P}$ in terms of the valence eigenstates of the slab, which are Bloch-like along x and y ,

$$\begin{aligned} \hat{P} &= \frac{1}{N} \sum_{\mathbf{k}v} |\psi_{\mathbf{k}v}\rangle \langle \psi_{\mathbf{k}v}| \\ &= e^{i\mathbf{k}\cdot\hat{\mathbf{r}}} \left(\frac{1}{N} \sum_{\mathbf{k}v} |u_{\mathbf{k}v}\rangle \langle u_{\mathbf{k}v}| \right) e^{-i\mathbf{k}\cdot\hat{\mathbf{r}}}, \end{aligned} \quad (31)$$

where the summation in $\mathbf{k} = (k_x, k_y)$ is over a uniform mesh of N points covering the surface Brillouin zone (SBZ). The linear change in $\hat{P}$ induced by an in-plane electric field is given by (compare with Eq. (17) for bounded samples)

$$\partial_{\boldsymbol{\varepsilon}} \hat{P} = \frac{1}{N} \sum_{\mathbf{k}v} e^{i\mathbf{k}\cdot\hat{\mathbf{r}}} \left(|\tilde{\partial}_{\boldsymbol{\varepsilon}} u_{\mathbf{k}v}\rangle \langle u_{\mathbf{k}v}| + |u_{\mathbf{k}v}\rangle \langle \tilde{\partial}_{\boldsymbol{\varepsilon}} u_{\mathbf{k}v}| \right) e^{-i\mathbf{k}\cdot\hat{\mathbf{r}}}, \quad (32)$$

where

$$|\tilde{\partial}_{\boldsymbol{\varepsilon}} u_{\mathbf{k}v}\rangle = ie \sum_c |u_{\mathbf{k}c}\rangle \frac{\hbar \mathbf{v}_{\mathbf{k}cv}}{E_{\mathbf{k}cv}^2} \quad (33)$$

is the projection of $|\partial_{\boldsymbol{\varepsilon}} u_{\mathbf{k}v}\rangle$ onto the conduction bands, and $\mathbf{v}_{\mathbf{k}cv} = \langle u_{\mathbf{k}c} | \hat{\mathbf{v}}_{\mathbf{k}} | u_{\mathbf{k}v} \rangle$ with $\hat{\mathbf{v}}_{\mathbf{k}} = e^{-i\mathbf{k}\cdot\hat{\mathbf{r}}} \hat{\mathbf{v}} e^{i\mathbf{k}\cdot\hat{\mathbf{r}}}$. Inserting Eq. (32) in Eq. (16) for $\sigma^{\text{AH}}(\mathbf{r})$, plugging the result in Eq. (26), and letting $N \rightarrow \infty$, we obtain

$$\sigma_{\text{slab}}^{\text{AH}}(z) = \frac{e}{4\pi\hbar} \int_{\text{SBZ}} d^2k \int_{A_c} dx dy \sum_v \text{Re} \left[\langle \mathbf{r} | \hbar \hat{\mathbf{v}}_{\mathbf{k}} \times \left(|\tilde{\partial}_{\boldsymbol{\varepsilon}} u_{\mathbf{k}v}\rangle \langle u_{\mathbf{k}v}| \mathbf{r} + |u_{\mathbf{k}v}\rangle \langle \tilde{\partial}_{\boldsymbol{\varepsilon}} u_{\mathbf{k}v}| \mathbf{r} \right) \right]_z. \quad (34)$$

As a first application of the above expression, let us integrate it over all z to obtain the macroscopic AHC (27)

³ The same strategy can be used to calculate the macroscopic surface charge density σ_{surf} from the volume density $\rho(\mathbf{r})$: see Eq. (43) in Ref. 1.

of the entire slab. The result is

$$\sigma_{\text{slab}}^{\text{AH}} = -\frac{e^2}{2\pi h} \int d^2k \operatorname{Im} \sum_{vc} \frac{\hbar^2 v_{vc}^x v_{cv}^y}{E_{cv}^2} - (x \leftrightarrow y), \quad (35)$$

where the subscript $\mathbf{k}$ has been dropped for brevity. The energy denominator can be removed using the identity $v_{vc} = -iE_{cv}\mathbf{A}_{cv}$, where $\mathbf{A}_{nm} = \langle u_n | \partial_{\mathbf{k}} u_m \rangle$ is the Berry connection matrix. Since $\operatorname{Im} \sum_{vv'} A_{vv'}^x A_{v'v}^y = 0$, the sum over conduction bands c can be replaced by a sum over all bands n (the term $n = v$ vanishes), and comparing with the Berry curvature $\Omega_v^{xy} = -2\operatorname{Im} \sum_{n \neq v} A_{vn}^x A_{nv}^y$ we recover Eq. (28) for the slab AHC, with

$$C_{\text{slab}} = \frac{1}{2\pi} \int_{\text{SBZ}} d^2k \sum_v \Omega_v^{xy} \quad (36)$$

the Chern number of the slab [18].

The surface AHC of a slab is calculated in a similar manner, by first inserting Eq. (34) in Eq. (29), and then inserting the latter in Eq. (30).

C. Geometric (Chern-Simons) contribution

To find the geometric part of the surface AHC, we repeat the steps in the previous subsection but replacing the full local AHC (16) with the CS contribution (24). Inserting Eq. (31) for $\hat{P}_0$ in Eq. (24b), we get

$$C_z(\mathbf{r}) = -\frac{4\pi}{N^2} \operatorname{Im} \sum_{\mathbf{k}\mathbf{k}'} \sum_{vv'} \psi_{\mathbf{k}v}^*(\mathbf{r}) \psi_{\mathbf{k}'v'}(\mathbf{r}) \langle \psi_{\mathbf{k}v} | \hat{x} \hat{Q}_0 \hat{y} | \psi_{\mathbf{k}v} \rangle. \quad (37)$$

Now write $\hat{Q}_0$ as $(1/N) \sum_{\mathbf{k}c} |\psi_{\mathbf{k}c}\rangle \langle \psi_{\mathbf{k}c}|$ and use [19]

$$\langle \psi_{\mathbf{k}v} | \hat{r}_j | \psi_{\mathbf{k}'c} \rangle = iN \langle u_{\mathbf{k}v} | \partial_{k_j} u_{\mathbf{k}c} \rangle \delta_{\mathbf{k}\mathbf{k}'} \quad (38)$$

to obtain

$$C_z(\mathbf{r}) = -\frac{4\pi}{N} \operatorname{Im} \sum_{\mathbf{k}} u_{\mathbf{k}v}^*(\mathbf{r}) u_{\mathbf{k}v'}(\mathbf{r}) \mathcal{F}_{\mathbf{k}v'v}^{xy}, \quad (39)$$

where we have introduced the metric-curvature tensor for the valence states of the slab,

$$\mathcal{F}_{\mathbf{k}v'v}^{xy} = \sum_c \langle \partial_{k_x} u_{\mathbf{k}v'} | u_{\mathbf{k}c} \rangle \langle u_{\mathbf{k}c} | \partial_{k_y} u_{\mathbf{k}v} \rangle, \quad (40)$$

whose real and imaginary parts give the quantum metric and the non-Abelian Berry-curvature matrix, respectively [3]. Inserting Eq. (39) in Eq. (24a) for $\sigma_{\text{CS}}^{\text{AH}}(\mathbf{r})$ and plugging the result in Eq. (26) yields

$$\sigma_{\text{slab,CS}}^{\text{AH}}(z) = -\frac{e^2}{\pi h} \int_{\text{SBZ}} d^2k \operatorname{Im} \sum_{vv'} \mathcal{O}_{vv'}(z) \mathcal{F}_{v'v}^{xy}, \quad (41)$$

with

$$\mathcal{O}_{vv'}(z) = \int_{A_c} u_v^*(x, y, z) u_{v'}(x, y, z) dx dy \quad (42)$$

the overlap integral between valence states over a surface unit cell at fixed z .

Integration of Eq. (41) over all z yields the CS contribution to the slab AHC. Actually this is the total slab AHC, since using the identities $\int \mathcal{O}_{vv'}(z) dz = \delta_{vv'}$ and $-2 \sum_v \operatorname{Im} \mathcal{F}_{vv}^{xy} = \sum_v \Omega_v^{xy}$ and then comparing with Eq. (36), we find⁴

$$\sigma_{\text{slab,CS}}^{\text{AH}} = \frac{e^2}{h} C_{\text{slab}}, \quad (43)$$

which is the same as Eq. (28) for the total AHC of the slab, obtained earlier by integrating Eq. (34) over all z . We conclude that the difference

$$\sigma_{\text{slab,cg}}^{\text{AH}}(z) = \sigma_{\text{slab}}^{\text{AH}}(z) - \sigma_{\text{slab,CS}}^{\text{AH}}(z) \quad (44)$$

between Eqs. (34) and (41) must integrate to zero across the entire slab,

$$\int_{-\infty}^{+\infty} \sigma_{\text{slab,cg}}^{\text{AH}}(z) dz = 0. \quad (45)$$

Following the notation in Eq. (25) for the local AHC, we refer to that difference as the cross-gap (or nongeometric) contribution to the z -resolved slab AHC.

Turning now to the surface AHC, we note that Eq. (44) does not have to integrate to zero across one half of the slab, so that a nongeometric contribution is generally present in the surface AHC. We also note that since $\int_0^\infty \mathcal{O}_{vv'}(z) dz$, in contrast to $\int_{-\infty}^{+\infty} \mathcal{O}_{vv'}(z) dz$, can have an imaginary part, the quantum metric contributes to the geometric part of the surface AHC along with the Berry curvature. These two properties distinguish the surface AHC from the intrinsic bulk AHC, which is governed by the Berry curvature alone.

Finally, suppose that a Chern-insulator layer is deposited on the top surface without closing the energy gap. This will change the surface AHC by $C_{\text{layer}} e^2/h$, and it is clear from the preceeding analysis that the added amount will go into the CS term, which therefore contains the quantized part me^2/h of Eq. (10) for the surface AHC.

This concludes the formalism part of the paper. To review, the surface AHC is calculated from Eqs. (29) and (30), where we insert either Eq. (34) to obtain the grand total, or Eq. (41) to obtain the CS contribution. The difference between the two defines the cross-gap contribution to the surface AHC.

IV. NUMERICAL RESULTS

In the following, we present the results of our numerical calculations of the surface AHC for two different TB

⁴ Defining $C(x, y)$ as the integral over all z of $C_z(x, y, z)$ given by Eq. (24b), Eq. (43) becomes $C_{\text{slab}} = (1/A_c) \int_{A_c} C(x, y) dx dy$. The dimensionless quantity $C(x, y)$ is local in two dimensions, and it has been named the “local Chern marker” [16].

models. The results are compared, via Eq. (10), with the bulk ME tensor calculated as in Ref. 12. First, let us briefly describe how to implement in TB the expressions for the surface AHC obtained in the previous section.

A. Tight-binding formulation of the surface anomalous Hall conductivity

In the TB context the integration over z in Eq. (30) for the surface AHC gets replaced by a summation over a layer index l , and Eq. (29) becomes a coarse-grained layer-resolved AHC. For models with two layers per cell, such as the ones considered below, it reads

$$\bar{\sigma}_{\text{slab}}^{\text{AH}}(l + 1/2) = \frac{1}{2} [\sigma_{\text{slab}}^{\text{AH}}(l) + \sigma_{\text{slab}}^{\text{AH}}(l + 1)], \quad (46)$$

where $\sigma_{\text{slab}}^{\text{AH}}(l)$ is obtained from Eq. (34) by replacing $|\mathbf{r}\rangle$ with $|i\rangle$ representing a TB basis orbital $\phi_i(\mathbf{r}) = \langle \mathbf{r} | i \rangle$. In the calculations reported below we make the diagonal approximation $\langle i | \hat{\mathbf{r}} | j \rangle = \tau_i \delta_{ij}$ for the position operator in the TB basis, and the velocity operator $\hat{\mathbf{v}} = (1/i\hbar)[\hat{\mathbf{r}}, \hat{H}]$ is evaluated accordingly [20].

As for the CS contribution to the surface AHC, Eq. (40) for the metric-curvature tensor remains unchanged while $\mathcal{O}_{vv'}(z)$ in Eq. (41) gets replaced by $\mathcal{O}_{vv'}(l) = \sum_{i \in l} u_v^*(i) u_{v'}(i)$, where the summation runs over the orbitals within one surface unit cell in layer l .

B. Anisotropic cubic-lattice model

As our first test case, we consider a model of a ME insulator with no symmetry. This provides the most challenging case for the theory, since all nine components of the ME tensor are nonzero and different from one another. The resulting surface AHC depends on the surface orientation, and it has both CS and cross-gap contributions.

We choose the TB model described in Appendix A of Ref. 12. This is a spinless model defined on a cubic lattice, with one orbital per site and eight sites per cell, where inversion and time-reversal symmetry are broken by assigning random on-site energies and complex first-neighbor hoppings of fixed magnitude. We take the model parameters listed in Table A.1 of Ref. 12, and choose the two lowest bands to be the valence bands. As in that work, all parameters are kept fixed except for one hopping phase φ which is scanned from 0 to 2π , and the results are plotted as a function of this phase φ .

This model is intended as a model for a conventional ME insulator, in which the isotropic response α_{iso}/V of an insulating crystallite cut from the bulk crystal is very small relative to the quantum e^2/h . That response is most naturally described by choosing $\alpha_{\text{iso}} \in [-e^2/2h, e^2/2h]$ and $m = 0$ in Eq. (20), so that Eq. (10) for the surface AHC reduces to Eq. (9). (In the next subsection, we will consider a model with the opposite

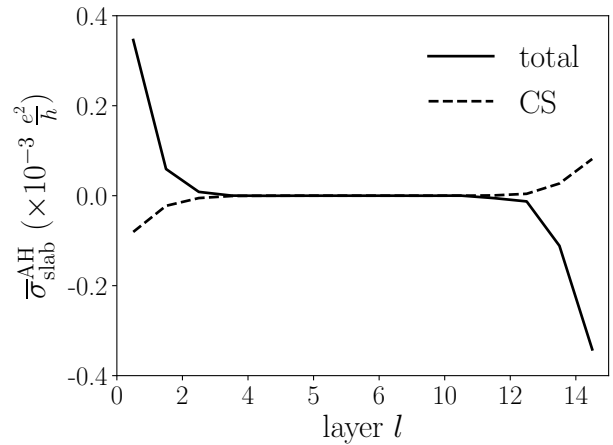


FIG. 1. Coarse-grained layer-resolved AHC [Eq. (46)] for a sixteen-atom-thick slab of the cubic-lattice model with $\varphi = \pi$.

characteristics, i.e., with a large isotropic ME response of the order of e^2/h .)

We calculate the surface AHC for a slab with a thickness of sixteen atomic layers (eight lattice constants) along z . The layer-resolved AHC displays strong oscillations from one layer to the next, which we filter out using Eq. (46). The resulting smooth curve is plotted as the solid line in Fig. 1 for $\varphi = \pi$, and the dashed line shows the CS contribution. Both quantities are nonzero in the surface regions only, quickly dropping to almost zero within four subsurface layers, and they have opposite signs on the two surfaces, as expected since $C_{\text{slab}} = 0$. On a given surface, the CS part of the AHC has the opposite sign compared to the total. This implies that the surface AHC is dominated by the cross-gap contribution, as tends to be the case in ordinary ME insulators [8].

The net AHC of the top surface is obtained by summing Eq. (46) over the layers in the upper half of the slab. The result is plotted versus φ as the solid line in the top panel of Fig. 2, where the CS contribution is again shown as a dashed line. For comparison, we plot as filled (total) and empty (CS) circles the quantity appearing on the right-hand-side of Eq. (9), with the bulk ME tensor calculated under periodic boundary conditions as described in Ref. 12. The excellent numerical agreement between the independently-calculated left- and right-hand sides of Eq. (9) validates our expressions for the surface AHC.

In the lower panel of Fig. 2 we show results for a slab cut along x . The total surface AHC is different from that on the upper panel, as generally expected from Eq. (9) for an anisotropic model. The CS part is however the same in both panels, confirming that the (nonquantized) CS surface AHC does not depend on the surface orientation.

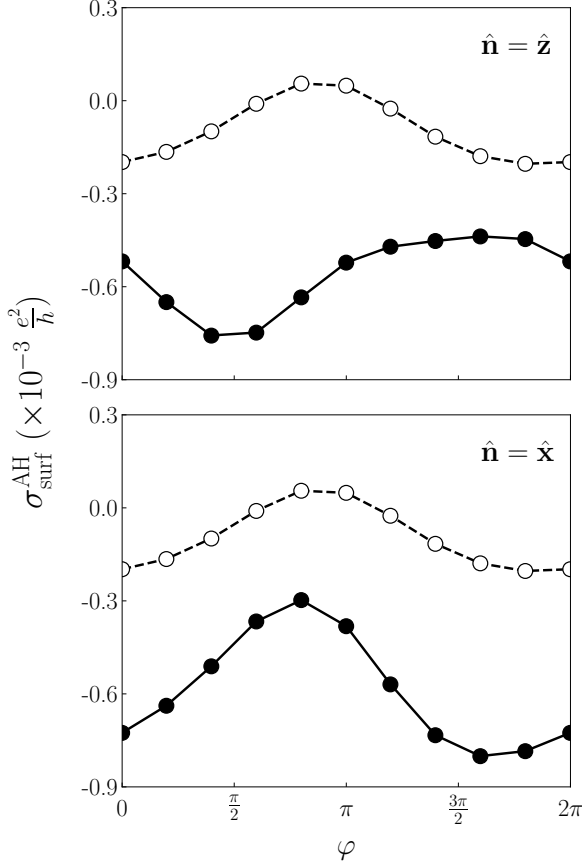


FIG. 2. AHC of the top surface (upper panel) and of the right surface (lower panel) of sixteen-layer slabs of the cubic-lattice model cut along z and x respectively, as a function of the cyclic parameter φ . The solid (dashed) lines denote the total (CS) surface AHC. Circles represent the quantity appearing on the right-hand-side of Eq. (9), with filled and empty circles denoting the total and the CS piece, respectively.

C. Layered Haldane model

We now turn to a model for which α_{iso} , when chosen in the range $[-e^2/2h, e^2/2h]$, is not always small compared to the quantum e^2/h , so that the choice of branch becomes ambiguous. We choose the TB model introduced in Ref. 11. This is a layered model on a hexagonal lattice, with four orbitals per cell. It can be obtained by stacking Haldane-model [21] layers with alternating parameters, and then coupling them via interlayer hopping terms. The model acts as a quantum pump of axion ME coupling: a slow periodic variation in its parameters can gradually change the isotropic ME coupling by e^2/h over one cycle. This pumping behavior of the model was demonstrated in Ref. 11, and here we consider the implications for the surface AHC.

We begin by noting that the cross-gap contribution to the ME tensor vanishes identically for this model. The reason can be found in Ref. 13, where a set of conditions

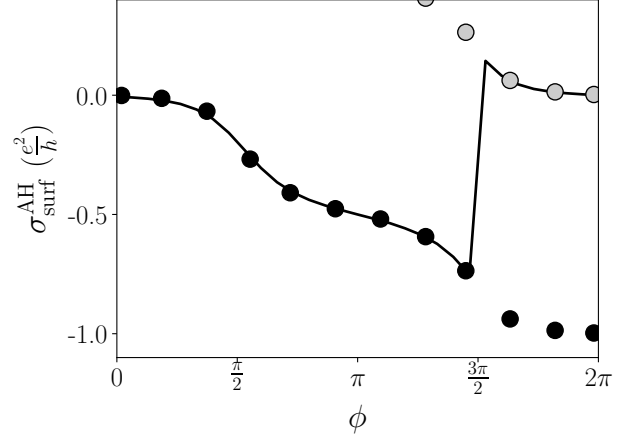


FIG. 3. Cyclic evolution of the Hamiltonian of a ten-layer slab of the layered Haldane model, during which the isotropic ME coupling α_{CS} of the bulk crystal changes by e^2/h . The AHC of the top surface is plotted as a solid line, and the black and grey circles denote two different branches of $-\alpha_{\text{CS}}$. For a given choice of branch, Eq. (47) is satisfied throughout out the cycle with the value of m increasing by one at $\phi_c = 3\pi/2$.

were derived under which α_{ab}^{cg} vanishes in certain four-band models having some kind of particle-hole symmetry. Those conditions hold for several models proposed in the literature, including the present one. Since $\alpha_{ab}^{\text{cg}} = 0$, Eq. (22) reduces to $\alpha_{ab} = \alpha_{\text{CS}}\delta_{ab}$ and Eq. (10) becomes

$$\sigma_{\text{surf}}^{\text{AH}} = -\alpha_{\text{CS}} + m \frac{e^2}{h}. \quad (47)$$

We construct a slab containing ten hexagonal layers stacked along z , and monitor the evolution of the surface AHC during one pumping cycle. The cycle is parametrized by an angle ϕ that modulates the model parameters according to Eqs. (57c) and (61) in Ref. 11. As in Sec. III.D of that work, the entire slab, including the surfaces, returns to its initial state at the end of the cycle, so that the slab Hamiltonian is itself cyclic,

$$\hat{H}_{\text{slab}}(\phi = 2\pi) = \hat{H}_{\text{slab}}(\phi = 0). \quad (48)$$

The quantities $\sigma_{\text{surf}}^{\text{AH}}(\phi)$ and $-\alpha_{\text{CS}}(\phi)$ are plotted in Fig. 3 as solid lines and filled circles, respectively; $-\alpha_{\text{CS}}$ is a multivalued bulk quantity, and two different branches are shown as black and grey circles. Equation (47) assumes that a specific branch has been selected, and we choose the one represented by the black circles. With that choice, Eq. (47) is satisfied with $m = 0$ for $0 < \phi < 3\pi/2$ and with $m = 1$ for $3\pi/2 < \phi < 2\pi$.

The actual value of m at each ϕ depends on the choice of bulk gauge, but we stress that that it would not have been possible to satisfy Eq. (47) keeping m fixed for all ϕ . Equation (48) implies

$$\sigma_{\text{surf}}^{\text{AH}}(\phi = 2\pi) = \sigma_{\text{surf}}^{\text{AH}}(\phi = 0), \quad (49)$$

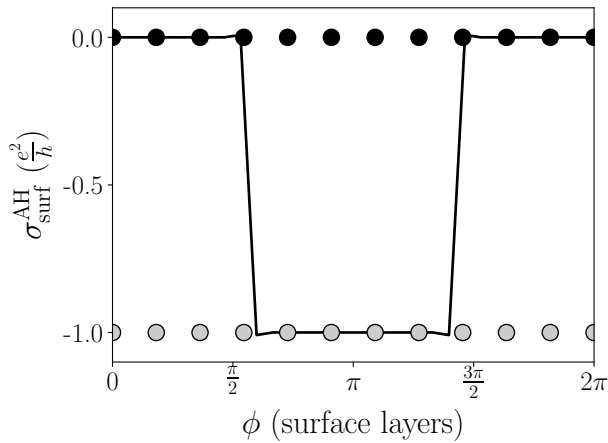


FIG. 4. The same quantities as in Fig. 3, but now for a cyclic evolution of the Hamiltonian of the surface layers only, keeping the Hamiltonian of the rest of the slab fixed.

and the only way this can be reconciled with the pumping behavior in the bulk region,

$$\alpha_{\text{CS}}(\phi = 2\pi) = \alpha_{\text{CS}}(\phi = 0) + \frac{e^2}{h}, \quad (50)$$

is if the integer m in Eq. (47) increases by one during the cycle. This change in the quantized part of the surface AHC is caused by a topological phase transition at the surface: the energy gap of the surface bands closes at $\phi_c = 3\pi/2$, forming a Weyl point in (k_x, k_y, ϕ) -space that transfers a quantum of Berry-curvature flux between the valence and conduction bands as ϕ crosses ϕ_c [11].

As mentioned in the Introduction, it is also possible to change the quantized part of the surface AHC by modifying the surface Hamiltonian only. This is illustrated in Fig. 4, where we held the Hamiltonian of all subsurface layers fixed at $\phi = 0$, but modulated the onsite energy of the top and bottom layers by ϕ according to Eq. (57c) in Ref. 11. Now the bulk ME coupling α_{CS} is held at zero for all ϕ , as indicated by the black circles. The surface AHC vanishes during half of the cycle leading to $m = 0$ in Eq. (47), and it becomes $-e^2/h$ during the other half where $m = -1$. At the critical points $\phi_c = \pi/2$ and $3\pi/2$, the surface states become gapless.

V. SUMMARY

In this work we have derived practical expressions for calculating the surface AHC of an insulating slab, including the quantized part that depends on the surface preparation. That quantized part resides in a geometric term that involves both the Berry curvature and the quantum metric of the slab wave functions.

We also found an additional contribution, of a nongeometric nature, to the surface AHC. Like the nonquantized part of the geometric term, this “cross-gap” contribution

is only apparently a surface property, but is in fact fully determined by the cross-gap contribution to the bulk ME tensor [12, 13]. Because it does not contribute to the bulk AHC [or to the net AHC of a slab, see Eq. (45)], this nongeometric term was missed in previous works [7, 17] where the spatially-resolved AHC was formulated using a local version of the Berry-curvature formula for the bulk AHC.

As a numerical check we have carried out simulations on TB models, confirming that the phenomenological relation in Eq. (10) between the surface AHC and the bulk ME tensor is satisfied by our expressions. The simulations on the layered Haldane model illustrate different ways of inducing topological phase transitions at the surfaces that change the surface AHC by quantized amounts.

An alternative strategy, based on “hybrid Wannier functions,” for determining the quantized part of the surface AHC was proposed in Ref. 11. We find the present approach to be simpler to implement and use, because it only involves gauge-invariant quantities derived from the induced current density at linear order in $\mathcal{E}$. Moreover, it is formulated directly in terms of the energy eigenstates, without having to transform to a gauge where the hybrid Wannier functions are maximally-localized. The present formulation is also more complete as it provides the full surface AHC (not just the geometric part), which we calculate from its fundamental definition in Eq. (30).

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Appendix A: Surface anomalous Hall conductivity and axion electrodynamics

In the phenomenology of axion electrodynamics [6, 14], the isotropic ME response α_{iso} of the medium is promoted to a macroscopic field $\alpha_{\text{iso}}(\mathbf{r}, t)$, where $\mathbf{r}$ is a coarse-grained variable that ignores microscopic variations occurring on the atomic scale. One can then show that only the spatial and temporal *gradients* of the axion field enter Maxwell’s equations [14]. In particular, in spatially inhomogeneous regions such as surfaces and interfaces there is a contribution $\nabla \alpha_{\text{iso}}(\mathbf{r}) \times \mathcal{E}$ to the local current density. According to Eq. (15) $\nabla \alpha_{\text{iso}}(\mathbf{r})$ amounts to a local AHC, which we will refer to as the axion piece $\sigma_{\text{axion}}^{\text{AH}}(\mathbf{r})$.

In a defect-free surface region of a slab the axion field only depends on surface-normal coordinate z , and the z -resolved axion AHC of the slab becomes

$$\bar{\sigma}_{\text{slab, axion}}^{\text{AH}}(z) = \frac{d}{dz} \alpha_{\text{iso}}(z). \quad (\text{A1})$$

Plugging this in Eq. (30) and then setting $\alpha_{\text{iso}}(z) = 0$ above the slab we find

$$\sigma_{\text{surf,axion}}^{\text{AH}} = -\alpha_{\text{iso}}(z = 0), \quad (\text{A2})$$

where $\alpha_{\text{iso}}(z = 0)$ denotes the constant value of the axion field in the bulklike region far below the surface. When viewed as a purely bulk quantity, $\alpha_{\text{iso}}(z = 0)$ is only defined modulo e^2/h . But when it is calculated by in-

tegrating $d\alpha_{\text{iso}}(z)/dz$ across a specific surface, a unique value is obtained [9]. We write that unique value as

$$\sigma_{\text{surf,axion}}^{\text{AH}} = -\alpha_{\text{iso}} + m \frac{e^2}{h}, \quad (\text{A3})$$

where the integer m depends on the details at the surface and on the branch choice for the bulk α_{iso} . In conclusion, the axion surface AHC comprises the first two terms in Eq. (10) for the full surface AHC.

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- [1] D. Vanderbilt and R. D. King-Smith, “Electric polarization as a bulk quantity and its relation to surface charge,” *Phys. Rev. B* **48**, 4442 (1993).
 - [2] R. D. King-Smith and David Vanderbilt, “Theory of polarization of crystalline solids,” *Phys. Rev. B* **47**, 1651 (1993).
 - [3] N. Marzari and D. Vanderbilt, “Maximally localized generalized Wannier functions for composite energy bands,” *Phys. Rev. B* **56**, 12847 (1997).
 - [4] L. D. Landau and E. M. Lifshitz, *Electrodynamics of Continuous Media*, 2nd ed. (Pergamon Press, Oxford, 1984).
 - [5] M. Fiebig, “Revival of the magnetoelectric effect,” *J. Phys. D: Appl. Phys.* **38**, R123 (2005).
 - [6] X.-L. Qi, T. L. Hughes, and S.-C. Zhang, “Topological field theory of time-reversal invariant insulators,” *Phys. Rev. B* **78**, 195424 (2008).
 - [7] A. M. Essin, J. E. Moore, and D. Vanderbilt, “Magnetoelectric Polarizability and Axion Electrodynamics in Crystalline Insulators,” *Phys. Rev. Lett.* **102**, 146805 (2009).
 - [8] S. Coh, D. Vanderbilt, A. Malashevich, and I. Souza, “Chern-Simons orbital magnetoelectric coupling in generic insulators,” *Phys. Rev. B* **83**, 085108 (2011).
 - [9] M. Sitté, A. Rosch, E. Altman, and L. Fritz, “Topological Insulators in Magnetic Fields: Quantum Hall Effect and Edge Channels with a Nonquantized θ Term,” *Phys. Rev. Lett.* **108**, 126807 (2012).
 - [10] M. Taherinejad and D. Vanderbilt, “Adiabatic Pumping of Chern-Simons Axion Coupling,” *Phys. Rev. Lett.* **114**, 096401 (2015).
 - [11] T. Olsen, M. Taherinejad, D. Vanderbilt, and I. Souza, “Surface theorem for the Chern-Simons axion coupling,” *Phys. Rev. B* **95**, 075137 (2017).
 - [12] A. Malashevich, I. Souza, S. Coh, and D. Vanderbilt, “Theory of orbital magnetoelectric response,” *New J. Phys.* **12**, 053032 (2010).
 - [13] A. M. Essin, A. M. Turner, J. E. Moore, and D. Vanderbilt, “Orbital magnetoelectric coupling in band insulators,” *Phys. Rev. B* **81**, 205104 (2010).
 - [14] F. Wilczek, “Two applications of axion electrodynamics,” *Phys. Rev. Lett.* **58**, 1799 (1987).
 - [15] I. Souza and D. Vanderbilt, “Dichroic f -sum rule and the orbital magnetization of crystals,” *Phys. Rev. B* **77**, 054438 (2008).
 - [16] R. Bianco and R. Resta, “Mapping topological order in coordinate space,” *Phys. Rev. B* **84**, 241106 (2011).
 - [17] A. Marrazzo and R. Resta, “Locality of the anomalous Hall conductivity,” *Phys. Rev. B* **95**, 121114 (2017).
 - [18] D. Xiao, M.-C. Chang, and Q. Niu, “Berry phase effects on electronic properties,” *Rev. Mod. Phys.* **82**, 1959 (2010).
 - [19] E. I. Blount, “Formalisms of Band Theory,” *Solid State Phys.* **13**, 305 (1962).
 - [20] T. B. Boykin, “Current density and continuity in discretized models,” *Eur. Phys. J.* **31**, 1077 (2010).
 - [21] F. D. M. Haldane, “Model for a quantum Hall effect without Landau levels: Condensed-matter realization of the “parity anomaly”,” *Phys. Rev. Lett.* **61**, 2015 (1988).