Magnetoelectric polarizability and axion electrodynamics in crystalline insulators

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Spin-orbit coupling can lead in two- and three-dimensional solids to time-reversal-invariant insulating phases that are "topological" in the same sense as the integer quantum Hall effect and similarly have protected edge or surface states. The three-dimensional topological insulator is known to have unusual magnetoelectric properties referred to as "axion electrodynamics": it supports an electromagnetic coupling $\Delta\mathcal{L}_{EM} = (\theta e^2/2\pi h)\mathbf{E}\cdot\mathbf{B}$ with $\theta = \pi$, giving a half-integer surface Hall conductivity $\sigma_{xy} = (n+1/2)e^2/h$. An approach to θ in any three-dimensional crystal is developed based on the Berry-phase theory of polarization: $\theta e^2/2\pi h$ is the bulk orbital magnetoelectric polarizability (the polarization induced by an applied magnetic field). We compute the orbital magnetoelectric polarizability for a simple model and show that it predicts the fractional part of surface σ_{xy}, computed using a slab geometry. Although θ is not quantized once time-reversal and inversion symmetries are broken, it remains a bulk quantity for the same reasons as ordinary polarization.

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The behavior of electric and magnetic fields can be strongly modified inside an insulating solid. Changes to the dielectric constant or magnetic permeability could be regarded as just numerical renormalizations of vacuum properties, but the solid environment can also yield entirely new behavior. For example, it has been known for two decades that three-dimensional (3D) insulators can generate an electromagnetic coupling of the form ($c = 1$)

$$\Delta\mathcal{L}_{EM} = \frac{\theta e^2}{2\pi h}\mathbf{E}\cdot\mathbf{B} = \frac{\theta e^2}{16\pi h}\epsilon^{\alpha\beta\gamma\delta}F_{\alpha\beta}F_{\gamma\delta}. \qquad (1)$$

This coupling was labeled "axion electrodynamics" [1] since a Lagrangian density of this form can describe the interaction of a dynamical "axion field" $\theta(\boldsymbol{x}, t)$ with the electromagnetic field. It plays no role in vacuum electrodynamics since the parameter θ couples to a total derivative, $\epsilon^{\alpha\beta\gamma\delta}F_{\alpha\beta}F_{\gamma\delta} = 2\epsilon^{\alpha\beta\gamma\delta}\partial_\alpha(A_\beta F_{\gamma\delta})$, and so does not modify the classical equations of motion if θ is constant.

This theory is invariant under $\theta \to \theta + 2\pi$, and the time-reversal operator T maps $\theta \to -\theta$ (since $\mathbf{E} \to \mathbf{E}$ and $\mathbf{B} \to -\mathbf{B}$), so T invariance is consistent with $\theta = \pi$ as well as $\theta = 0$. [1] Thus θ is a "topological invariant" of T-invariant insulators, that is, a property stable under continuous changes as long as the material remains insulating and T-symmetric. The prototypical invariant of this type is the TKNN integer C that gives the quantum Hall conductance, $\sigma_{xy} = Ce^2/h$. [2]

T-invariant band insulators turn out to have topological invariants beyond those of the TKNN type. In 2D there is a $\mathbb{Z}_2$ invariant [3] that distinguishes "ordinary" from "$\mathbb{Z}_2$-odd" insulators, with "quantum spin Hall" states [4, 5] providing examples of the latter. In 3D there is a similar invariant [6–8] that can be computed either from the 2D invariant on certain planes [6] or, with additional symmetry, from a certain index at the eight time-reversal-invariant momenta [8]. The resulting "strong topological insulator" in 3D has Dirac surface modes that have recently been observed in photoemission on $Bi_{0.9}Sb_{0.1}$ [9]. The $\theta = \pi$ value in Eq. (1) is related to these surface Dirac modes [1, 10–13]: the fact that each gapless 2D Dirac mode, under a weak applied field, becomes a gapped Hall insulator with $|\sigma_{xy}| = e^2/2h$ is the microscopic origin of the θ coupling.

Insulators that instead have broken time-reversal T and also inversion P—so-called "magnetoelectric" (or "multiferroic") materials—have been the topic of intense experimental and theoretical investigations in recent years [14, 15]. In general the first-order magnetoelectric coupling α is a tensor giving a contribution of the form $\alpha_{ij}E_iB_j$, as indeed expected for magnetoelectric couplings arising from lattice displacements and Zeeman interactions. Here we discuss only the frozen-lattice coupling via the orbital magnetization, which we denote as the orbital magnetoelectic polarizability (OMP). Remarkably the OMP is indeed only a *scalar* as in Eq. (1) and generates "axion electrodynamics."

In the present letter, we provide a simple derivation of this result via an expression for the OMP as an integral of the Chern-Simons 3-form over the Brillouin zone. In particular, defining the Berry connection $\mathcal{A}_j^{\mu\nu} = i\langle u_\mu|\partial_j|u_\nu\rangle$ where $|u_\nu\rangle$ is the cell-periodic Bloch function of occupied band ν and $\partial_j = \partial/\partial k_j$, we obtain

$$\theta = \frac{1}{2\pi}\int_{\mathrm{BZ}} d^3k\ \epsilon_{ijk}\,\mathrm{Tr}[\mathcal{A}_i\partial_j\mathcal{A}_k - i\frac{2}{3}\mathcal{A}_i\mathcal{A}_j\mathcal{A}_k] \qquad (2)$$

where the trace is over occupied bands. This is essentially Eq. (78) of recent work by Qi, Hughes, and Zhang [13] that, among other results, importantly made the connection between 3D $\mathbb{Z}_2$ topological insulators and axion electrodynamics with $\theta = \pi$. Our derivation shows that this integral describes the orbital magnetoelectric polarizability (rather than a polarization [13]) and follows directly from an extension [16] of the Berry-phase theory of polarization [17] to the case of slow spatial variations of the Hamiltonian. The OMP angle θ is a bulk property in exactly the same sense as electric polarization [17, 18]. We show that Eq. (2) is amenable to direct calculation using established band-structure methods and discuss its symmetry properties. Explicit numerical calculations on model crystals are presented in order to validate the theory and to illustrate how a non-zero θ corresponds to a "fractionalization" of the quantum Hall effect (QHE) at the surfaces of magnetoelectric insulators [1, 12, 13].

From Eq. (1) it follows that

$$\theta \frac{e^2}{2\pi h} = \frac{\partial M}{\partial E} = \frac{\partial}{\partial E}\frac{\partial}{\partial B}\langle H\rangle = \frac{\partial P}{\partial B} \tag{3}$$

evaluated at $E = B = 0$, where $\langle H\rangle$ is the ground-state energy and we have used the commutativity of partial derivatives. Thus the OMP can be approached from several points of view. (i) It can be regarded as describing the *electric* polarization arising from the application of a small *magnetic* field. (ii) It can be regarded as describing the orbital *magnetization* arising from the application of a small *electric* field. (iii) It also gives the (dissipationless) *surface Hall conductivity* at the surface of the crystal, provided that the surface is insulating. Note that (iii) follows from (ii): for a surface with unit normal $\hat{\mathbf{n}}$ and electric field along $\mathbf{E}$, the resulting surface current $\mathbf{K} = \mathbf{M}\times\hat{\mathbf{n}}$ is proportional to $\mathbf{E}\times\hat{\mathbf{n}}$. Since θ is only well-defined modulo 2π, one sees that the surface conductivity of an insulating surface is determined, modulo the quantum e^2/h, by the bulk bandstructure alone. There is an elegant analogy here to the case of electric polarization, where the surface charge of an insulating surface is determined, modulo the quantum e/S, by the bulk bandstructure alone (S is the surface cell area).

The above discussion suggests several possible approaches to the derivation of a bulk formula for the OMP θ. One would be to follow (ii) and compute the orbital magnetization [19, 20] in an applied electrical field. We choose to focus here on (i) instead, working via dP/dB. Our derivation starts from the semiclassical wavepacket analysis of Xiao *et al.* [16], who analyzed how a slow spatial variation of the local Hamiltonian in an insulator may generate an additional polarization $\mathbf{P}^{(\mathrm{in})}$ associated with the inhomogeneity, beyond the spatially integrated periodic-crystal Berry-phase polarization. For the case of an orthorhombic 3D crystal with M occupied bands in which the slow spatial variation occurs along the y direction in a supercell of length l_y, they obtain

$$\langle \Delta P_x^{(\mathrm{in})}\rangle = \frac{e}{4}\int_0^1 d\lambda \int_{\mathrm{BZ}} \frac{d^3k}{(2\pi)^3}\int_0^{l_y}\frac{dy}{l_y}\,\epsilon_{ijkl}\,\mathrm{Tr}\left[\mathcal{F}_{ij}\mathcal{F}_{kl}\right] \tag{4}$$

for the change in the supercell-averaged inhomogeneously induced polarization that occurs as a global parameter λ evolves adiabatically from 0 to 1. Here indices $ijkl$ run over (k_x, k_y, y, λ), $\mathcal{F}_{ij} = \partial_i\mathcal{A}_j - \partial_j\mathcal{A}_i - i[\mathcal{A}_i,\mathcal{A}_j]$ is the Berry field-strength tensor ($\mathcal{A}_\lambda = i\langle u|\partial_\lambda|u\rangle$), and the trace and commutator refer to band indices.

Because $\mathcal{F}$ is gauge-covariant, the integrand in Eq. (4) is explicitly gauge-invariant. In fact it is just the non-Abelian second Chern class [21], so that Eq. (4) is path-invariant modulo a quantum $e/a_z l_y$, where a_z is the lattice constant in the z direction. Moreover, the λ integral can be performed to obtain an expression in terms of the non-Abelian Chern-Simons 3-form [21]. Thus,

$$\langle P_x^{(\mathrm{in})}\rangle = e\int_{\mathrm{BZ}}\frac{d^3k}{(2\pi)^3}\int_0^{l_y}\frac{dy}{l_y}\,\epsilon_{ijk}\mathrm{Tr}[\mathcal{A}_i\partial_j\mathcal{A}_k - \frac{2i}{3}\mathcal{A}_i\mathcal{A}_j\mathcal{A}_k] \tag{5}$$

where ijk now run only over (k_x, k_y, y). The integrand is not gauge-invariant, and while it is not obvious that the integral is gauge-invariant, the Chern-Simons theory implies that it is, modulo the quantum $e/a_z l_y$.

We now apply this result to study the polarization induced by a magnetic field, which may be regarded as arising from a spatial inhomogeneity in the electromagnetic vector potential $\mathbf{A}(\mathbf{r})$. In particular, we compute $\langle P_x^{(\mathrm{in})}\rangle$ for the case of $\mathbf{A} = By\hat{\mathbf{z}}$ with $B = h/ea_z l_y$, i.e., a B-field along $\hat{x}$ with one flux quantum threading the supercell. This has the effect of taking $k_z \to k_z + eBy/\hbar$, and this is the only way y will enter into the Hamiltonian, so that $|\partial_y u\rangle = (Be/\hbar)|\partial_{k_z} u\rangle$ and

$$\langle P_x^{(\mathrm{in})}\rangle = \frac{Be^2}{\hbar}\int_{\mathrm{BZ}}\frac{d^3k}{(2\pi)^3}\,\epsilon_{ijk}\,\mathrm{Tr}[\mathcal{A}_i\partial_j\mathcal{A}_k - i\frac{2}{3}\mathcal{A}_i\mathcal{A}_j\mathcal{A}_k] \tag{6}$$

where ijk now run over (k_x, k_y, k_z). Using Eq. (3) we easily arrive at Eq. (2) as one of our main results.

Before proceeding, we briefly discuss the symmetry properties of the OMP. Clearly the combination $\mathbf{E}\cdot\mathbf{B}$ in Eq. (1) is odd under T and also odd under inversion P (although it is even under the combination PT [27]). It is also odd under any improper rotation, such as a simple mirror reflection. This implies that $\theta = -\theta$ if the crystal has *any* of the above symmetries. This would force an ordinary coupling to vanish, but since θ is only well-defined modulo 2π, it actually only forces $\theta = 0$ or π. Thus, one can obtain an insulator with quantized $\theta = \pi$ not only for T-invariant systems (regardless of whether they obey inversion symmetry), but also for inversion- and mirror-symmetric crystals regardless of T symmetry [12]. When none of these symmetries is present, one generically has a non-zero (and non-π) value of θ, but restricted to the surprisingly simple scalar form of Eq. (1).

In the remainder of this Letter, we validate and illustrate the above theory via numerical calculations on a tight-binding Hamiltonian that generates non-zero values of θ. We start with the model of Fu, Kane, and Mele [8] for a 3D topological insulator on the diamond lattice, and add a staggered Zeeman term to break T:

$$H = \sum_{\langle ij \rangle} t_{ij} c_i^\dagger c_j + i \frac{4\lambda_{SO}}{a^2} \sum_{\langle\langle ij \rangle\rangle} c_i^\dagger \boldsymbol{\sigma} \cdot (\boldsymbol{d}_{ij}^1 \times \boldsymbol{d}_{ij}^2) c_j + \boldsymbol{h} \cdot \left(\sum_{i \in A} c_i^\dagger \boldsymbol{\sigma} c_i - \sum_{i \in B} c_i^\dagger \boldsymbol{\sigma} c_i \right). \quad (7)$$

In the first term, the nearest-neighbor hopping amplitude depends on the bond direction; we take $t_{[111]} = 3t + m\cos\beta$, $t_{[\bar{1}11]} = t_{[1\bar{1}1]} = t_{[11\bar{1}]} = t$. The second term describes spin-dependent hopping between pairs of second neighbors $\langle\langle ij \rangle\rangle$, where $\boldsymbol{d}_{ij}^1$ and $\boldsymbol{d}_{ij}^2$ are the connecting first-neighbor legs and $\boldsymbol{\sigma}$ are the Pauli spin matrices. The linear size of the face-centered cubic (fcc) conventional cell is a. The last term is the new ingredient and describes a staggered Zeeman field with opposite signs on the two fcc sublattices A and B.

At half filling, with $0 < m < 2t$ and λ_{SO} sufficiently large, the original model has a direct band gap of $2m$ at $\beta = \pi$. We take $|\boldsymbol{h}| = m \sin\beta$ and choose $\boldsymbol{h}$ in the [111] direction; varying the single parameter β keeps the gap constant and interpolates between the ordinary ($\beta = 0$) and the topological ($\beta = \pi$) insulator.

We have calculated θ using four different methods and found that they agree (Figure 1). Using established methods [22], we can obtain θ from Eq. (2), as shown for $\beta = \pi/4$ and $\beta = \pi/2$ (filled squares). This computation requires finding a smooth gauge for $\mathcal{A}$, which is equivalent to finding localized Wannier functions.

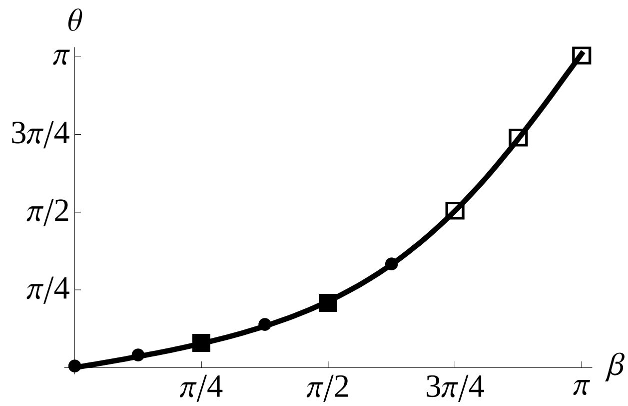

FIG. 1: The magnetoelectric polarizability θ (in units of $e^2/2\pi h$). The curve is obtained from the second Chern integral, Eq. (9). The filled squares are computed by the Chern-Simons form, Eq. (2). The open squares are the slopes of P *vs.* B, Eq. (8). The remaining points are obtained by layer-resolved σ_{xy} calculations using Eq. (11).

Since a tight-binding model is not computationally demanding, we have also calculated the polarization resulting from one flux quantum in a large supercell, using [17]

$$P_i = e \int_{BZ} \frac{d^3k}{(2\pi)^3} \mathrm{Tr}\, \mathcal{A}_i \,. \quad (8)$$

Plotting the values for a number of supercell sizes against the corresponding B allows us to approximate dP/dB, shown as open squares in Figure 1. Further, we have calculated the orbital magnetization response in a slab geometry, as we describe shortly. We have also exploited the simple nature of the tight-binding model to compute $\theta(\beta)$ from the formula [13, 16] (see also Eq. (4))

$$\theta(\beta) = \frac{1}{16\pi} \int_0^\beta d\beta' \int d^3\mathbf{k}\, \epsilon_{ijkl} \mathrm{Tr}[\mathcal{F}_{ij}(\mathbf{k}, \beta') \mathcal{F}_{kl}(\mathbf{k}, \beta')], \quad (9)$$

plotted as the curve in Figure 1. The sign of θ is fixed here by the choice of a particular path in Hamiltonian space from the initial $\theta = 0$ value at $\beta = 0$.

We now discuss the surface Hall conductivity, possibly the most accessible experimental realization of θ. Its fractional part in units of e^2/h is determined purely by bulk properties. Consider a material with coupling θ in a slab geometry that is finite in the $\hat{\mathbf{z}}$ direction and surrounded by $\theta = 0$ vacuum. This leads [1] to surface Hall conductivity $(\theta + 2\pi r)e^2/(2\pi h)$ at the top surface and $(-\theta - 2\pi s)e^2/(2\pi h)$ at the bottom surface, for some surface-dependent integers r and s, consistent with the total Hall conductivity of the slab being an integer multiple of e^2/h. In a finite geometry, if the total Hall conductance $(r - s)e^2/h$ is nonzero, there must be conducting 1D edge channels at the boundaries between surfaces.

The 3D topological insulator has $\theta = \pi$ so that each surface should have half-integer Hall conductance. The spatial contributions to the Hall conductance in the slab geometry can be resolved as follows. The unit cell is a supercell containing some number N of original unit cells in the $\hat{\mathbf{z}}$ direction, with translational invariance remaining in the $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ directions. The TKNN integer is [2, 23]

$$C = \frac{1}{2\pi} \int d^2k \sum_\nu \mathcal{F}_{xy}^{\nu\nu} = \frac{i}{2\pi} \int d^2k \sum_\nu \epsilon_{ij} \langle \partial_i u_\nu | \partial_j u_\nu \rangle = \frac{i}{2\pi} \int d^2k\, \mathrm{Tr}\left[\mathcal{P} \epsilon_{ij} \partial_i \mathcal{P} \partial_j \mathcal{P} \right]. \quad (10)$$

Here ν runs over occupied bands, $|u_\nu\rangle$ are the Bloch wavefunctions, i and j take the values k_x and k_y, and $\mathcal{P} = \sum_\nu |u_\nu\rangle\langle u_\nu|$ is the projection operator onto the occupied subspace, which is manifestly gauge-invariant. To know how different $\hat{\mathbf{z}}$ layers contribute to the TKNN number, we define a real-space projection $\tilde{\mathcal{P}}_n$ onto layer n within the slab supercell, and compute

$$C(n) = \frac{i}{2\pi} \int d^2k\, \mathrm{Tr}\left[\mathcal{P} \epsilon_{ij} (\partial_i \mathcal{P}) \tilde{\mathcal{P}}_n (\partial_j \mathcal{P}) \right]. \quad (11)$$

The results, presented in Fig. 2, confirm that the surface layers have half-integer Hall conductance when $\beta = \pi$ in (7) and that the sign on each surface is switched by local T-breaking perturbations. This suggests a possible experiment on the 3D topological insulator: applying a weak uniform magnetic field in almost any direction to a

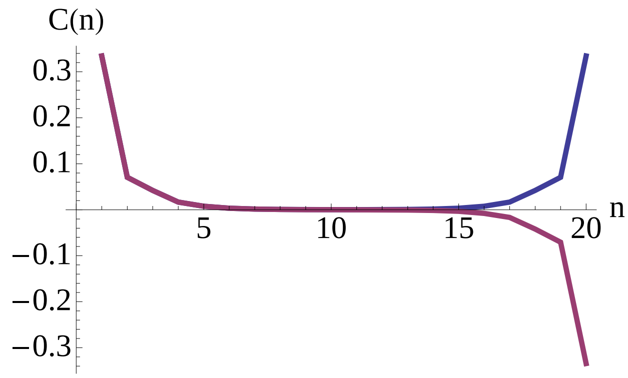

FIG. 2: (Color online) The layer-resolved Hall conductivity (in units of e^2/h) at $\beta = \pi$ in a slab of twenty layers, with $m = t/2$ and $\lambda_{SO} = t/4$, terminated in $(\bar{1}11)$ planes. Since there are gapless surface states at $\beta = \pi$, a surface term was added to Eq. (7) that breaks T locally and gaps the surface states. Switching the sign of this perturbation at one surface (the two curves) switches the current direction at that surface, causing a transition between integer quantum Hall states.

crystal or film leads to an integer quantum Hall state with the sign depending on the field direction, $\sigma_{xy} = \pm e^2/h$. The state with $r - s = 0$ does not occur because the magnetic field acts oppositely at the two surfaces.

The ambiguity in the surface conductance (the integer r above) indicates that there may be one or more integer quantum-Hall layers at each surface. It is the same as the ambiguity of specifying the bulk property θ, discussed in connection with Eq. (5). This ambiguity also appears in the supercell polarization in small field: Eq. (8) only gives the polarization (and hence differences in polarization) modulo the "quantum of polarization" [17] which, for the case of the flux-threaded supercell of Eq. (6), is $\Delta P_x = e/a_z l_y$. Since the magnetic field is $B_x = h/ea_z l_y$,

$$\Delta \frac{P_x}{B_x} = \frac{e^2}{h} = 2\pi \frac{e^2}{2\pi h}. \quad (12)$$

Therefore, θ has an associated ambiguity of 2π, in agreement with the predictions of axion electrodynamics.

Finally, using Eq. (2) we have calculated θ for a Hamiltonian that breaks PT (as well as P and T) by adding a weak, uniform (*i.e.*, not staggered) Zeeman coupling. For some values of β this lifts all degeneracies, allowing separation of the intraband and interband contributions to θ. A single band can have nonzero θ as long as there are more than two bands in total [24]. Because interband contributions are nonzero in general, θ is a property of the whole occupied spectrum and not a sum of individual band contributions, unlike the polarization.

The weak-field-driven integer quantum Hall transition in a film of 3D topological insulator is one experimental signature that $\theta = \pi$. For general θ, optical conductivity measurement of a single surface's Hall conductivity may be feasible. A more exotic signature is that a magnetic monopole acquires electrical charge in a θ-vacuum [25]. Recently "spin ice" materials such as the pyrochlore magnet $Dy_2Ti_2O_7$ have been argued to support monopole excitations [26]; if the background material has nonzero θ, such monopoles carry fractional electrical charge $\theta e/2\pi$.

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