

# Effect of the boundary on thermodynamic quantities such as magnetization

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In this paper, we investigate in general how thermodynamic quantities such as the polarization, magnetization, and the magnetoelectric tensor are affected by the boundaries. We show that when the calculation with periodic boundary conditions does not involve a Berry's phase, the quantity in question is determined unambiguously by the bulk, even in the presence of gapless surface states. When the calculation involves a Berry's phase, the bulk can only determine the quantity up to some quantized value, given that (i) there are no gapless surface states, (ii) the surfaces do not break the symmetries preserved by the bulk, and (iii) the system is kept at charge neutrality. If any of the above conditions is violated, the quantity is then determined entirely by the details at the boundary. Due to the strong dependence on the boundary, this kind of thermodynamic quantity, such as the isotropic magnetoelectric coefficient, cannot be measured in the bulk without careful control at the boundary. One thus cannot distinguish between a topological insulator and a trivial insulator in three dimensions by any local measurement in the bulk.

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## I. INTRODUCTION

Recently, there has been resurging interest in understanding the general orbital magnetoelectric (ME) response.<sup>1-4</sup> This is due to the fact that the isotropic magnetoelectric effect, or the so-called  $\theta$  term,  $\mathcal{L}_\theta = (\theta e^2/2\pi h) \mathbf{E} \cdot \mathbf{B}$  with  $\theta = \pi$ , is suggested to describe the time-reversal-invariant (TRI) topological band insulator (TBI) in three spatial dimensions (3d).<sup>5</sup> Usually, the signature of the 3d TBI is the existence of an odd number of Dirac cones on the boundary surfaces, when the time-reversal symmetry (TRS) is preserved.<sup>6</sup> When the surface states are gapped out by breaking the TRS locally on the boundaries, a half-integer quantum Hall effect will take place and give rise to a quantized bulk magnetoelectric response.<sup>5</sup> Later, people discover that this isotropic response is only a part of the more general anisotropic orbital ME tensor defined in the bulk:<sup>2</sup>

$$\alpha_{ij} = \alpha_\theta \delta_{ij} + \alpha_{3dij}; \quad (1)$$

we define  $\alpha_\theta = \frac{1}{3} \text{Tr} \alpha_{ij}$ , and  $\alpha_{3d}$  is therefore traceless.  $\alpha_{ij}$  describes either the orbital magnetopolarizability (OMP) or the orbital electric susceptibility (OES):

$$\alpha_{ij} = dP_i/dB_j = dM_j/dE_i; \quad (2)$$

OMP and OES are equal via a Maxwell relation.

One peculiarity of the ME tensor is that  $\alpha_\theta$  is only determined up to integer multiples of  $e^2/h$  by the bulk band structure.<sup>2,3</sup> The specific value of  $\alpha_\theta$  depends on the details at the boundary. From the polarization perspective, if we attach an integer quantum Hall (IQH) layer with filling  $\nu = \pm 1$  respectively on the top and bottom surfaces of a cylinder, the OMP, i.e.,  $dP/dB$ , along the axis of the cylinder will change by  $e^2/h$  due to the density locking to the magnetic field of the top and the bottom IQH layer. From the magnetization perspective, if we attach an IQH layer with filling  $\nu = 1$  on the side surfaces of the cylinder, the OES,  $dM/dE$ , will also change by  $e^2/h$  due to the extra Hall current flowing on the surface in response to the electric field. Either way, the ME effect is only determined up to an integer multiple of  $e^2/h$ . In the bulk, this ambiguity corresponds well to the fact that  $\theta$  as a coefficient in front of  $(\mathbf{E} \cdot \mathbf{B})$  is an angle only defined up to

integer multiple of  $2\pi$  because  $\int \mathbf{E} \cdot \mathbf{B} d^3x dt$  is quantized.  $\alpha$  is odd under TRS, but this ambiguity makes it possible for  $\alpha_\theta$  not to vanish with TRS preserved, as  $\alpha_\theta = \pm e^2/2h$  differ from each other by  $e^2/h$ .  $\alpha_\theta = 0$  and  $\alpha_\theta = e^2/2h$  then describe two different insulating states of matter under TRS.

However, the above properties raise some questions. From the polarization perspective this ambiguity from the bulk is not so surprising since the zero-field polarization is already ambiguous with periodic boundary conditions.<sup>7,8</sup> From the magnetization perspective, however, this ambiguity is a bit more puzzling because one commonly regards magnetization as a bulk property.<sup>9,10</sup> In particular, with periodic boundary conditions there seems to be no reason to expect any ambiguity in the magnetization, whereas the ambiguity in the polarization is easily understood.

Before answering this rather specific question, we note that there is an even more general one: to what extent are thermodynamic quantities such as polarization, magnetization, and ME response determined by the bulk? Unlike the conventional thermodynamic quantities, which are entirely independent of the boundary, we have already seen that boundary sometimes plays a role. How can we tell when a thermodynamic variable will depend on the boundary and when it will not?

In the following, we will discuss case by case the ground-state polarization, orbital magnetization, and the magnetoelectric tensor. We will argue that some of them depends on the boundary and others do not, and verify our claim with numerical simulations. By matching the observations with our previous calculation done with periodic boundary conditions, we can then directly tell from the calculation with periodic boundary conditions how different thermodynamic quantities depend on boundaries.

## II. GROUND-STATE POLARIZATION

The ground-state polarization is given by the following formula with periodic boundary conditions:<sup>7</sup>

$$P = -ie \int_{BZ} \frac{d^d k}{2\pi^d} \sum_{\alpha(k) \in occ} \langle \alpha(k) | \frac{\partial}{\partial k} | \alpha(k) \rangle. \quad (3)$$

In one spatial dimension (1d), the polarization is defined modulo  $e$  with periodic boundary conditions:  $P = P_0 + ne$ , with  $n$  being an integer. This corresponds to the observation that with periodic boundary conditions we can move every electron to the next unit cell and return to the original state, while the two states should, by definition, have polarization that differ by  $e$ . With two ends, the polarization will take one specific value, depending on the number of charges we put at the two ends.

However, if there are zero modes at the two ends, the polarization is then ambiguous, as theoretically we can consider the superposition of states of different occupancy of the zero modes. The bulk value of the polarization thus depends entirely on the boundary.

In 3d it is a bit more interesting. For simplicity let us assume the system sits on a cubic lattice of size  $a$ . Now the bulk formula has an ambiguity of  $e/a^2$ , which also corresponds well to the fact that we can move every electron to the next unit cell and return to the same state. However, with boundary surfaces the situation becomes quite different. Consider a capacitor setup. We are allowed to put any number of charges on each of the opposing surfaces, resulting in a change of the polarization in units of  $e/A$  ( $A$  is the total surface area). In the thermodynamic limit, we can put any finite density of charges on the surface, and the polarization in the bulk can take any value. Our bulk formula is thus no longer valid. To accommodate the charge on the surface, however, the system needs to either be in a metallic state near the boundary or to break the lattice translation symmetry in the two in-plane directions. If neither condition is satisfied, then we can only add an integer number of electrons per unit cell, and the bulk formula is recovered, with the remaining ambiguity determined by the surface.

How can the bulk formula become invalid? We note that the ground-state polarization can be understood as a Berry's phase when one adiabatically turns on the electric field. First, in order for the Berry's phase to make any sense, the system has to be gapped. This is the reason why a metallic surface can render the bulk formula invalid. Second, if we break the lattice translation symmetry in the two directions perpendicular to the electric field, we can no longer integrate over the momentum in those directions but should instead sum over a large number of subbands labeled by the remaining momentum along the direction of the electric field. The polarization will have an ambiguity of  $e/A$  in this case. This is different from the conventional thermodynamic quantity, which requires symmetry breaking in the bulk to change its value. The Berry's phase is thus a rather fragile thermodynamic quantity.

### III. GROUND-STATE ORBITAL MAGNETIZATION

It is not immediately obvious that the orbital magnetization is independent of the boundary. In the bulk the operator  $\hat{M} \propto (\mathbf{r} \times \mathbf{v})$  is ill defined, with periodic boundary conditions, and seems to be growing as one goes near the boundary. Indeed, when one numerically computes  $\langle \hat{M} \rangle$  summing over the local orbitals, there is a finite contribution from the boundary orbitals, which renders the total orbital magnetization different from the "local" bulk contribution.<sup>10</sup> Nevertheless, it has been shown<sup>10</sup> that the boundary contribution is, in fact, independent

of the details at the boundary via the use of local Wannier functions in an insulator with zero Chern number.

However, in a Chern insulator, a local Wannier function cannot be found<sup>11,12</sup> because the Bloch functions cannot be periodic and smoothly defined over the Brillouin zone. To see that even in this case the orbital magnetization is still independent of the boundaries, we can consider the following setup.

Suppose we have an insulator with a nonvanishing Chern number in two dimensions. Let us imagine putting an auxiliary layer of insulator on top, with an opposite Chern number, without any interaction with the original one. The new insulator as a whole has then a total Chern number of zero. We can therefore make a local Wannier orbital with a linear combination of orbitals from the two layers.<sup>13</sup> The argument then carries through for the insulator as a whole, and the total orbital magnetization should be independent of the boundary. Now since there is no interaction between the two layers, the total magnetization is just the sum of the magnetizations of the original insulator and the auxiliary insulator. We now consider a particular boundary condition where the two insulators couple to independent boundary terms that also do not interact with each other. Let us only vary the boundary terms that couple to the original insulator. The total magnetization cannot change and neither can the contribution from the auxiliary insulator. We thus have to conclude that even for a Chern insulator, the orbital magnetization is independent of the boundaries.

From this abstract point of view, the generalization to Chern insulators seems rather trivial. However, the presence of gapless chiral edge states may cause one to worry. Suppose we can gate the material to supply a constant chemical potential; what will happen if we turn up the electric potential on the edge? Will the edge current decrease because fewer edge states are occupied, or will it stay the same as required for the bulk magnetization not to change?

We do a straightforward numerical simulation to resolve this paradox. We choose the Hamiltonian to be

$$H = \sum_n c_n^\dagger (\tau_z - i\tau_x) c_{n+\hat{x}} + c_n^\dagger (\tau_z - i\tau_y) c_{n+\hat{y}} + mc_n^\dagger \tau_z c_n + \text{H.c.}, \quad (4)$$

where  $\tau$  are the Pauli matrices. At half filling with  $m = 1.5$ , the band carries a Chern number  $C_1 = 1$ . If we set the chemical potential  $\mu = 0$ , the ground state has no magnetization. If  $\mu$  is away from zero, there will be a ground-state magnetization. We put the Hamiltonian on a  $10 \times 10$  lattice and take open boundary conditions in both directions. The current on the vertical links is plotted in Fig. 1. We relate the current to the magnetization by  $I^b = \epsilon^{ab} \partial_a M$  and take the magnetization at the middle to represent the bulk magnetization. We see that while shifting the overall chemical potential creates circulating currents, altering the electric potential locally at the edge does not change the bulk magnetization. If we look closer in the latter case, while the current right at the edge is changed, there is a counterpropagating current near the edge, which keeps the total current localized near one edge constant. The counterpropagating current is just the integer quantum Hall response to the electric potential gradient. This bulk quantum

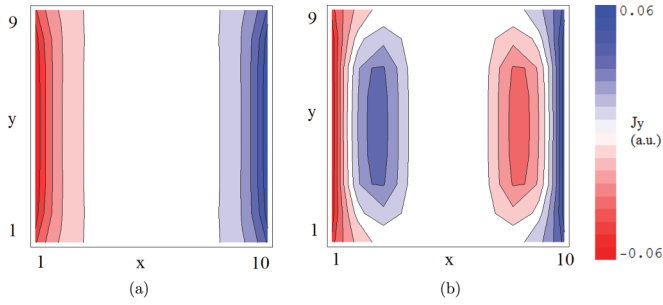


FIG. 1. (Color online) Color-coded plots for the current on the vertical links of the lattice. The current is measured in arbitrary units. Currents flowing upwards are plotted in blue, while current flowing downwards are plotted in red. The currents on the horizontal links are not plotted. (a)  $\mu = 0.5$ . As expected, some edge states are occupied, and we have circulating currents. (Only vertical currents are shown.) This gives rise to a bulk magnetization. (b) If we set  $\mu = 0$  but locally apply an electric potential  $V = -0.5$  to the first two rows at the boundary, the edge states are again occupied (the red and blues near the edge.) However, in the region next to those regions, counterpropagating currents arise. The bulk magnetization remains zero (barring some finite-size effect).

Hall current exactly compensates for the current carried by the now-unoccupied edge states and leaves the bulk magnetization insensitive to the change of the local potential near the edge.

A very similar puzzle arises in the  $S_z$ -conserved spin Hall insulator. On the edge there are counterpropagating TR-paired edge states. When we apply a uniform Zeeman field  $H_z$ , there will be a net circulating current from the edge states. We can therefore deduce a bulk orbital magnetization response to the Zeeman field. We call this the orbital-Zeeman susceptibility. However, one can locally break the  $S_z$  conservation together with the TR symmetry near the edge to gap out the edge states. In this case, will there still be a bulk magnetization response to the Zeeman field?

We take the previous model for spin-up electrons and pair it with its time reversal. We applied a uniform Zeeman field  $\delta H_z = 0.2 \sum_n c_n^\dagger S_z c_n$ . The numerical result is shown in Fig. 2. Here we can see that even though the edge states are gapped out by the local perturbations, the total current flowing near the edge remains the same. The local perturbation transfers the current from the states at the Fermi level to the occupied bands. In the end, while local properties can affect the gapless states and gap them out, the total current near the edge in the vicinity is unaffected.

We therefore conclude that the orbital magnetization, as well as the orbital-Zeeman susceptibility, is independent of the boundary for an insulator. While the circulating current may be carried by the edge states, the total amount is entirely insensitive to the local boundary conditions. One can understand this from a calculation with periodic boundary conditions: the magnetization is calculated as an energy density in a magnetic field. The total energy, unlike the Berry's phase, is a truly extensive property, so that the boundary contribution is irrelevant in the thermodynamic limit. The energy density in the bulk is thus entirely independent of the boundaries far enough away, whether there are gapless states or not.

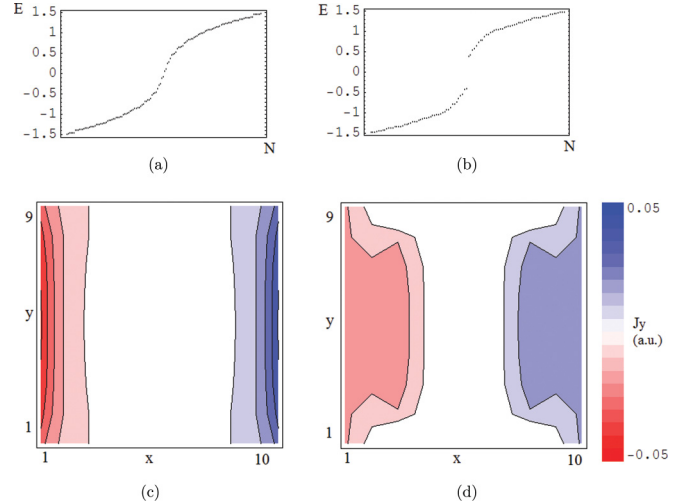


FIG. 2. (Color online) (a) and (b) Plots of the spectrum in ascending order. In (a), the symmetry is preserved on the edge. The edge states live inside the gap. In (b), by applying a time-reversal and  $S_z$  symmetry-breaking term near the boundary  $\delta H = \sum_{n \in \text{edge}} c_n^\dagger S_x c_n$ , we gap out the edge states. (c) and (d) Color-coded plots for the current on the vertical links, without and with the symmetry breaking term  $\delta H$ . While the current distributes slightly differently with or without the symmetry breaking term at the edges, the contributions to the bulk magnetization are identical.

#### IV. MAGNETOELECTRIC EFFECT

After the discussion of the polarization and the magnetization and seeing that they are thermodynamic quantities with very different behaviors, it is thus natural to ask the same question about the ME tensor and to ask how the Maxwell relation can be maintained. Before going into the details of the boundary dependence, however, let us first show that the anisotropic part  $\alpha_{3d}$  is independent of the boundaries.

In terms of electronic Green's functions and with periodic boundary conditions, we have derived the ME tensor from the OMP perspective as a Berry's phase in a magnetic field:<sup>14</sup>

$$\begin{aligned} \alpha_{ij} &= (\alpha_{wzw} + \alpha_{3d})_{ij}, \\ \alpha_{wzwijs} &= -\frac{\pi i}{6} \epsilon_{abcd} \text{Tr}^S(\mathbf{g} \partial_a \mathbf{g}^{-1} \mathbf{g} \partial_b \mathbf{g}^{-1} \mathbf{g} \partial_c \mathbf{g}^{-1} \mathbf{g} \partial_d \mathbf{g}^{-1} \mathbf{g}) \delta_{ij}; \\ \alpha_{3dij} &= -\frac{i}{6} \epsilon_{abj} \text{Tr}(g \partial_i g^{-1} g \partial_a g^{-1} g \partial_b g^{-1} g - \text{H.c.}). \end{aligned} \quad (5)$$

The traces include the frequency and momentum integral divided by factors of  $(2\pi)$ ;  $\text{Tr}^S$  denotes the integral and trace in one extra dimension in momentum space, with the original Brillouin zone and a trivial test system as the boundary. While the entire ME tensor is derived as a Berry's phase,  $\alpha_{3d}$  does not depend on the Green's function extended to the extra dimension. Without considering boundaries directly, we can show that  $\alpha_{3d}$  is independent of the boundaries by showing it extends smoothly to finite frequency and momentum.

At finite frequency and momentum, the ME response is understood as a term in the effective action which is proportional to  $E^i(q, \omega) B^j(-q, -\omega)$ . Unlike the uniform ME response, however, this term can no longer be understood as OMP or OES due to the fact that, unlike uniform

electromagnetic fields, the electric and magnetic fields at finite frequency and momentum are related by Faraday's law. The term nevertheless affects properties of the propagating electromagnetic waves. For our purposes, it suffices to show that the effective Lagrangian is continuous from  $q = 0$  to  $q \rightarrow 0$ . At any  $q \neq 0$ , we can calculate the effective Lagrangian with the conventional diagrammatic method. Calculated in the Appendix, the bubble diagram gives

$$S_{\text{ME}} = - \int \frac{d^4 q}{(2\pi)^4} B^\ell(q) E^k(-q) \alpha_{3d k \ell} + O(q). \quad (6)$$

Comparing with Eq. (5), we see that  $\alpha_{3d}$  is continuous, whereas  $\alpha_{\text{wzw}}$  is entirely absent at finite momentum. One might worry that we have missed  $\alpha_{\text{wzw}}$  in momentum space due to the fact that it is a total derivative in real space, which Fourier transforms to zero and cannot be seen in momentum space. However, one can evaluate the diagram in real space, and it is still absent. Fundamentally, this is due to the fact that the conventional perturbation theory is perturbative in orders of the gauge field, which breaks down with uniform field strength. Nevertheless, combining the two calculations, we can still say that  $\alpha_{3d}$  is a bulk property and is independent of the boundaries.  $\alpha_{\text{wzw}}$ , on the other hand, is similar to the polarization: it does depend on the boundary, but when there is no boundary, it presents itself as a Berry's phase. We note that one benefit of using the Green's function is that the separation of the local terms and boundary terms matches exactly how the expression depends on the extra dimension. That is, as long as the term can be expressed in terms of the Green's functions without being extended to one extra dimension, that term is locally measurable. This is not the case if we use the density matrices, either to calculate the same Berry's phase<sup>15</sup> or to calculate a current response to a pumping procedure.<sup>2</sup> In both calculations the ME tensor naturally separates into two terms, with the first term independent of the energy gap:

$$\alpha = \alpha_{\text{cs}} + \alpha_{\text{G}}; \quad (7)$$

$\alpha_{\text{cs}}$  is isotropic, but  $\alpha_{\text{G}}$  is not traceless. While  $\alpha_{\text{G}}$  can be uniquely determined by the bulk band structure and is independent of the boundaries, its trace is actually not measurable in the bulk.

Let us now focus on the isotropic part  $\alpha_{\text{wzw}}$ . In terms of polarization in a magnetic field, the ambiguity is no surprise. However, how does the ambiguity of the orbital magnetization in an electric field come about?

One origin of the ambiguity is from the fact that the perturbation of a uniform electric field grows with distance. It therefore naturally depends on the boundary, when there is one. When we consider periodic boundary conditions, however, it becomes less clear.

In order to study the OES with periodic boundary conditions, we first have to properly define the magnetization with periodic boundary conditions. Without the current at the boundary, one sensible definition of the magnetization is from the relation  $B = H + M$ . That is, in the absence of applied current (which generates  $H$ ), the magnetization simply equals the measured magnetic field. Note that with periodic boundary conditions and a finite volume, the magnetic field is quantized because the total magnetic flux through the sample is quantized in units of  $h/e$ . In this case we take the perspective

that the magnetic field will take the closest quantized value to the magnetization while the magnetization itself is still continuous.

In our previous work,<sup>15</sup> we have shown that in a magnetic field, the  $\theta$  term, which characterizes the isotropic part of the OMP, changes the quantization condition of the global electric flux. The ground state of the system thus carries an electric flux of  $-(\theta e^2/2\pi h)\Phi_B + ne$ , where  $n$  is some integer that minimizes the flux. Using  $0 = D = E + P$ , the  $\theta$  term thus gives an isotropic orbital magnetopolarization response  $\frac{\partial P}{\partial B} = \frac{\theta e^2}{2\pi h}$ . However, this result is valid only when  $(\Phi_B \theta e/2\pi h) < 1$ . In the thermodynamic limit this condition is always violated, and instead  $\frac{\partial P}{\partial B} = 0$ .

Similarly, to see whether the same term contributes to the OES of the system, we would like to investigate whether there is a uniform magnetic field when we constrain the path integral to a given average electric field in the same direction. However, the electric field and the magnetic field behave in intrinsically different ways when we formulate our theory assuming the existence of electric charges and the absence of magnetic monopoles: the quantization of the electric flux can change in the presence of the magnetic field, while the quantization of the magnetic flux is fixed at  $(h/e)$ . When we apply an electric flux, we can always imagine that the system is a coherent state composed of states with integer electric fluxes. The background magnetic field therefore does not have to be different from zero. Therefore, even at finite size, the  $\theta$  term does not give rise to the OES. The Maxwell relation between the isotropic OMP and the OES is thus violated. They are only equal in the thermodynamic limit, where the  $\theta$  term gives no contribution for either quantity. In other words, the isotropic OES is better thought of as a bulk-induced surface response, which vanishes when there are no boundary surfaces.

Now let us consider geometry with boundaries in some detail. From the result of Ref. 3, we know that with open boundary conditions in all directions, the OES has an ambiguity only determined by specific surface boundary conditions. We have also seen in the Introduction that in a cylinder geometry the ambiguity of the OES can come from the quantized Hall current on the side surfaces.

What if there are no side surfaces? Suppose we take periodic boundary conditions only in two directions to get rid of the side surfaces. Does the OES still have the same ambiguity? One naively would expect the situation to be similar to the case with periodic boundary conditions due to the absence of the possible circulating Hall currents. However, a more careful argument shows this is not the case. In fact, the system will spontaneously generate a magnetic field, which will then generate surface charge density  $\sigma = \pm(\nu + \theta/2\pi)e^2 B/h$  via the OMP response, to lower the electric energy. Minimizing the total energy as a function of  $B$ , we then get  $B = M = (\nu + \theta/2\pi)e^2 E/h$ . While at finite size the total magnetic flux is quantized in units of  $h/e$  in this setup, in the thermodynamic limit, the magnetic field will converge to the expected value, in contrast to the situations with periodic boundary conditions where it stays at zero. We have numerically confirmed this result by calculating the magnetization in the electric field using the momentum space formula for the magnetization derived in Ref. 10, as shown in Fig. 3.



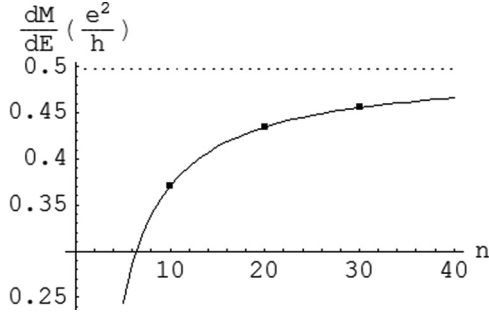


FIG. 3. The calculated OES vs  $n$ , the number of layers in the  $z$  direction, with the model described by Eq. (73) in Ref. 5 with  $\theta = 0$ ,  $m = c = 1$ . We take  $\theta = 0.5\pi$  at the top and bottom layers to gap out the edge states. (If we take  $\theta = \pm 0.5\pi$  on the two surfaces, respectively, the whole system will be a Chern insulator and can no longer be kept at charge neutrality without closing the gap in a magnetic field.) We put on an electric field such that the potential difference between the top and the bottom layers is 0.2. The squares show the calculated values. The solid curve is a fit by assuming a fixed width  $w$  of the surface charges when there is a magnetic field, such that  $\frac{dM}{dE} \propto (1 - \frac{w}{n})$ . The fit gives  $\frac{dM}{dE} = 0.50 \frac{e^2}{h}$  in the thermodynamic limit and  $w = 2.54$ . The OES changes sign as expected when we change to  $\theta = -0.5\pi$  on the boundary.

Before summing up, let us consider how gapless surface states can alter the ME response. Evidently, if we attach a fractional quantum Hall state to the side of the cylinder, the OES is going to change by a fraction of  $e^2/h$ .<sup>16</sup> In general the fraction is quite arbitrary, so in this case the bulk value of the isotropic OES is not valid. This corresponds to the fact that the fractional quantum Hall state has ground-state degeneracy. In general, we will therefore expect that any gapless surface state will destroy the bulk description of the isotropic ME response.

To sum up, the anisotropic part of the ME tensor  $\alpha_{3d}$  is independent of the boundaries. The isotropic part  $\alpha_{wz}$  depends partially on the boundary. While  $\alpha_{3d}$  is a truly local quantity,  $\alpha_{wz}$  only lives at  $q = 0$ . Adding the fact that both isotropic OES and OMP responses vanish with periodic boundary conditions in the thermodynamic limit, it is better to think of  $\alpha_{wz}$  as a quantized surface effect induced by the bulk.

## V. CONCLUSION

We have thus gone through polarization, magnetization, and magnetoelectric responses and have seen their dependence on the boundary. A bulk calculation done with periodic boundary conditions contains enough information to predict how the quantity in question depends on the boundary, however. In particular, using our formalism described in Ref. 14, any quantity that does not involve an extension of the Green's function to one extra dimension, such as the magnetization in zero electric field, is independent of the boundary. On the other hand, quantities that require an extension to extra dimensions, such as the polarization and the trace of the magnetoelectric tensor, will depend on the boundary. The bulk can determine their value up to some quantized amount only when (i) there are no gapless surface states, (ii) surfaces break no symmetry that is required to determine the bulk value with periodic boundary conditions, and (iii) the system is kept at charge neutrality. If any of the conditions are violated, the surface contribution will dominate and render the results obtained with periodic boundary conditions invalid. Thermodynamic quantities of this kind cannot be measured in the bulk without careful control at the boundary. Specifically, one cannot perform a local measurement to distinguish the topological insulator in 3d from a trivial insulator because (i) the coefficient of the  $\theta$  term will depend on the boundary and (ii) it is absent at finite  $q$ .

## ACKNOWLEDGMENTS

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## APPENDIX: ME EFFECT AT FINITE MOMENTUM

In the main text we have argued heuristically that the trace of the ME tensor comes entirely from the surface and therefore does not contribute at finite momentum. The locally measurable ME tensor is therefore traceless in the  $q \rightarrow 0$  limit. We can directly calculate the ME tensor at finite  $q$ : Fourier transforming and expanding the hopping Hamiltonian up to second order of  $A^\mu$ , we have

$$\Delta H = \sum_{k,q} c_{k+q/2}^\dagger \partial_u H(k) c_{k-q/2} A^\mu(-q) + \frac{1}{2} \sum_{k,q,q'} c_{k+(q+q')/2}^\dagger \partial_u \partial_v H(k) c_{k-(q+q')/2} A^\mu(-q) A^\nu(-q'); \quad (\text{A1})$$

$H_k \equiv \sum_{d_i} t_{d_i} \exp(ikd_i)$  is a matrix. Integrating out the electrons, the effective action at quadratic order of  $A_\mu$  reads

$$S_{\text{eff}} = \int \frac{d^4 q}{(2\pi)^4} \frac{i}{2} A^\mu(q) A^\nu(-q) \text{Tr} \left[ \partial_\mu \partial_\nu g^{-1}(k) g(k) + \partial_\mu g^{-1}(k) g \left( k + \frac{q}{2} \right) \partial_\nu g^{-1}(k) g \left( k - \frac{q}{2} \right) \right]; \quad (\text{A2})$$

similarly, the trace includes the integral of energy and momentum divided by  $2\pi$ . The first term in the trace is from the second term in Eq. (A1), usually called the paramagnetic current, and does not have  $q$  dependence. To compare with Eq. (5), we Taylor expand the second term to second order in  $q$  to get the behavior in the  $q \rightarrow 0$  limit (from here on, we drop the dependence on  $k$  to avoid clutter):

$$S_{\text{eff}} \sim \int \frac{d^4 q}{(2\pi)^4} - \frac{i}{4} q^\lambda q^\sigma A^\mu(q) A^\nu(-q) \text{Tr} \left( \partial_\mu g^{-1} \partial_\lambda g \partial_\nu g^{-1} \partial_\sigma g - \frac{1}{2} \partial_\mu g^{-1} \partial_\lambda \partial_\sigma g \partial_\nu g^{-1} g - \frac{1}{2} \partial_\mu g^{-1} g \partial_\nu g^{-1} \partial_\lambda \partial_\sigma g \right) + O(q^3). \quad (\text{A3})$$

To further simplify the expression, let us now take the Coulomb gauge. In the Coulomb gauge, we have to take either  $\lambda$  or  $\sigma$  to be in the time direction to have the expression contribute to the ME tensor. Since  $\partial_i \partial_\omega g^{-1} = 0$ , we can integrate by part the time derivative. Using  $\partial_\omega g = -g^2$  and renaming the indices  $i, j, k$ , now running through only the spatial directions, we get

$$S_{\text{ME}} \sim \int \frac{d^4 q}{(2\pi)^4} \frac{i}{2} \omega q^i A^j(q) A^k(-q) \text{Tr}(g \partial_j g^{-1} \partial_i g \partial_k g^{-1} g). \quad (\text{A4})$$

Now we need to massage the expression a little bit. Let us use  $(ijk)$  as shorthand notation for the expression  $\text{Tr}(g \partial_i g^{-1} \partial_j g \partial_k g^{-1} g)$ . Integrating by parts,<sup>14</sup> we have the following relation:

$$(ijk) + (jki) + (kij) = 0. \quad (\text{A5})$$

We therefore have

$$(jik) = \frac{2}{3}[2(jik) - (ikj) - (kji)]. \quad (\text{A6})$$

In the trace in Eq. (A4), only the part symmetric under the exchange of indices  $j$  and  $k$  would contribute, as we can change variables from  $q$  to  $-q$ , effectively exchanging  $A^j(q)$  and  $A^k(-q)$ . Therefore, in the expression above, we can exchange  $j$  and  $k$  freely. We therefore have

$$\begin{aligned} S_{\text{ME}} &\sim \int \frac{d^4 q}{(2\pi)^4} \frac{i}{6} \omega q^i A^j(q) A^k(-q) \\ &\quad \times [(jik) + (kij) - (ijk) - (kji)] \\ &= \int \frac{d^4 q}{(2\pi)^4} \frac{i}{6} \omega q^i A^j(q) A^k(-q) \epsilon_{ij\ell} \epsilon_{abl} [(kab) + (bak)]. \\ &= \int \frac{d^4 q}{(2\pi)^4} \frac{i}{6} B^\ell(q) E^k(-q) \epsilon_{abl} [(kab) + (bak)] \\ &\equiv - \int \frac{d^4 q}{(2\pi)^4} B^\ell(q) E^k(-q) \alpha_{k\ell}(q \rightarrow 0). \end{aligned} \quad (\text{A7})$$

$\alpha_{k\ell}(q \rightarrow 0) = -\frac{i}{6} \epsilon_{abl} [(kab) + (bak)]$  is traceless, as the two terms cancel each other with antisymmetrization.

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