

Axion electrodynamics in topological insulators

Ulysses Zhan*

University of California, Santa Barbara

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Topological insulators exhibit effects that can be effectively described by adding a so-called θ term in the action in addition to that of the usual electromagnetic action, which is called the axion electrodynamics. This article talks about the some properties of the axion electrodynamics, such as how the axion field is restricted by symmetries, and how it is related to the Berry phase. We also give two different ways of deriving the axion term, Fujikawa's method and the dimensional reduction method.

I. Introduction

Metals and insulators are conventionally distinguished by the existence of a band gap at the Fermi level in the latter. Relatively novel is the phase called the topological insulator, where band gaps exist in the bulk while there are gapless edge states [1]. It has unusual response to applied electromagnetic fields which can be encoded by an so-called θ term or axion term in the bulk of the form [2]

$$\mathcal{L}_{\text{axion}} := \theta \frac{e^2}{4\pi^2 \hbar c} \mathbf{B} \cdot \mathbf{E} \quad (1)$$

(using Gaussian units, $4\pi\epsilon_0 = 1$). If the system has time-reversal symmetry or spatial inversion symmetry, then θ is 0 (ordinary insulator) or $\pi \pmod{2\pi}$ (topological insulator); it is otherwise spacetime-dependent in general. The axion term was introduced in high-energy physics to resolve CP nonviolation problem in quantum chromodynamics [3] decades before it was introduced in the field of solid-state physics.

This article talks about the some properties of the axion electrodynamics and the reason of its existence in topological insulators. Section II gives an overview of what the axion electrodynamics is. Section III gives an phenomenological explanation of how the axion electrodynamics can come from Berry phase effects. Section IV explains why θ is defined modulo 2π . Section V explains why θ can only be 0 or π due to symmetries. Section VI and Section VII give two different ways of deriving the axion term.

II. Axion electrodynamics

The Lagrangian of axion electrodynamics is given by (omitting the terms for matter, etc.) [4]

$$\mathcal{L} := -\frac{1}{16\pi} F^{\mu\nu} F_{\mu\nu} + \frac{\alpha\theta}{\pi} \frac{1}{16\pi} \tilde{F}^{\mu\nu} F_{\mu\nu} - A_\mu J^\mu, \quad (2)$$

where $F_{\mu\nu} := \partial_\mu A_\nu - \partial_\nu A_\mu$ is the field strength tensor of the 4-potential A_μ , and $\tilde{F}^{\mu\nu} := \frac{1}{2}\epsilon^{\mu\nu\rho\sigma} F_{\rho\sigma}$ is its dual,

and J^μ is the current sourcing the 4-potential. The term involving θ is the axion term, which is the same as Equation 1 in the units $c = \hbar = 1$. The Euler-Lagrange equation for A_μ gives the Maxwell equations in the presence of the axion term, which in the 3D form read

$$\begin{cases} \nabla \cdot \mathbf{E} = 4\pi\rho - \frac{\alpha}{\pi} \mathbf{B} \cdot \nabla\theta, \\ \nabla \cdot \mathbf{B} = 0, \\ \nabla \times \mathbf{E} + \dot{\mathbf{B}} = 0, \\ \nabla \times \mathbf{B} - \dot{\mathbf{E}} = 4\pi\mathbf{J} + \frac{\alpha}{\pi} (\mathbf{B}\dot{\theta} - \mathbf{E} \times \nabla\theta). \end{cases} \quad (3)$$

If we define the electric displacement and the magnetic field as

$$\mathbf{D} := \mathbf{E} + \frac{\alpha\theta}{\pi} \mathbf{B}, \quad \mathbf{H} := \mathbf{B} - \frac{\alpha\theta}{\pi} \mathbf{E},$$

then we can recover the usual macroscopic Maxwell equations. This implies that the effect of the axion term may be realized by a linear magnetoelectric effect, which in general has the form [5]

$$\begin{cases} 4\pi\mathbf{P} = \boldsymbol{\chi}^e \mathbf{E} + \boldsymbol{\eta} \mathbf{H}, \\ 4\pi\mathbf{M} = \boldsymbol{\chi}^m \mathbf{H} + \boldsymbol{\eta} \mathbf{E}, \end{cases} \quad (4)$$

where \mathbf{P} and \mathbf{M} are electric polarization and magnetization, and $\boldsymbol{\chi}^e$ and $\boldsymbol{\chi}^m$ are the usual electric and magnetic susceptibilities, and $\boldsymbol{\eta}$ is called the magnetoelectric susceptibility. The two $\boldsymbol{\eta}$'s appearing for both electric polarization and magnetization must be equal because $\partial\mathbf{P}/\partial\mathbf{H} = \partial\mathbf{M}/\partial\mathbf{E}$ is a Maxwell relation. The susceptibilities are written in boldface because they are 3×3 matrices in general, but we will only consider the case where they are proportional to the identity matrix. To recover the axion term, η needs to equal $\alpha\theta/\pi$. The value of $\alpha = 7.3 \times 10^{-3}$ is larger than the magnetoelectric susceptibility of typical magnetoelectric materials by one or two orders of magnitude. For example, the magnetoelectric susceptibility for Cr_2O_3 , the first discovered magnetoelectric material, is 4.3×10^{-4} [6].

Notice that the axion term

$$\frac{\alpha\theta}{\pi} \frac{1}{16\pi} \tilde{F}^{\mu\nu} F_{\mu\nu} = \frac{\alpha\theta}{\pi} \frac{1}{16\pi} \partial_\mu (\tilde{F}^{\mu\nu} A_\nu)$$

is a total derivative if θ is a constant. One can also see this by noting that Equation 3 only involves the derivatives of θ . This means that the bulk of the topological

* youqiu@ucsb.edu

insulator cannot be told apart from an ordinary insulator, and the only difference is the behavior at the boundary.

III. Hall effect caused by Berry curvature

In this section, we will see a mechanism that can give rise to a magnetoelectric effect looking like Equation 4. This mechanism involves a Hall conductivity due to the Berry curvature, which is the intrinsic source of the anomalous Hall effect [7]. A detailed derivation of the Hall conductivity can be found in [8], and a review article [9]. The following is a brief derivation.

Suppose a time varying Hamiltonian $H(t)$ has instantaneous eigenstates $|u_n(t)\rangle$ (choosing phase such that $\langle u_n | \partial u_n / \partial t = 0$) with eigenvalues $\epsilon_n(t)$ (no degeneracy), then a wavefunction initially at $|\psi(0)\rangle = |u_n\rangle$ evolves as

$$|\psi\rangle = \left(|u_n\rangle - i \sum_{m \neq n} \frac{|u_m\rangle \langle u_m | \frac{\partial u_n}{\partial t} \rangle}{\epsilon_n - \epsilon_m} \right) e^{-i \int_0^t \epsilon_n dt}.$$

We can regard the instantaneous eigenstates as the bands of an electron in a periodic potential, which in turn can be expressed as periodic wavefunctions that are eigenstates of a wavevector-dependent Hamiltonian $H(\mathbf{k})$ (the Bloch Hamiltonian). Then, the expectation value of the velocity operator $\mathbf{v} = \partial H / \partial \mathbf{k}$ in the n th band can then be written as

$$\mathbf{v}_n = \frac{\partial \epsilon_n}{\partial \mathbf{k}} - i \sum_{m \neq n} \left(\frac{\langle u_n | \frac{\partial H}{\partial \mathbf{k}} | u_m \rangle \langle u_m | \frac{\partial u_n}{\partial t} \rangle}{\epsilon_n - \epsilon_m} - \text{c.c.} \right).$$

One can easily prove that

$$\langle u_n | \frac{\partial H}{\partial \mathbf{k}} | u_m \rangle = (\epsilon_n - \epsilon_m) \left\langle \frac{\partial u_n}{\partial \mathbf{k}} \middle| u_m \right\rangle,$$

so the velocity operator can be written as

$$\mathbf{v}_n = \frac{\partial \epsilon_n}{\partial \mathbf{k}} - i \left(\left\langle \frac{\partial u_n}{\partial \mathbf{k}} \middle| \frac{\partial u_n}{\partial t} \right\rangle - \text{c.c.} \right).$$

In the presence of a constant electric field \mathbf{E} , we can describe it as a time-varying vector potential $\mathbf{A} = -\mathbf{E}t$, which makes the Hamiltonian $H(\mathbf{k}) \rightarrow H(\mathbf{k} + e\mathbf{A})$ time-dependent. This then leads to $\mathbf{v}_n = \partial \epsilon_n / \partial \mathbf{k} + e\mathbf{b}_n \mathbf{E}$, where \mathbf{b}_n is the Berry curvature of the n th band, defined in terms of the Berry connection \mathbf{a}_n as

$$b_{ij} := \frac{\partial a_j}{\partial k_i} - \frac{\partial a_i}{\partial k_j}, \quad \mathbf{a}_n := i \left\langle u_n \middle| \frac{\partial u_n}{\partial \mathbf{k}} \right\rangle.$$

These velocities contribute to the current density $\mathbf{j} = \sigma \mathbf{E}$, where, at zero temperature in the presence of a band gap,

$$\sigma := e^2 \sum_{\text{filled } n} \int_{\text{BZ}} \frac{d^d k}{(2\pi)^d} \mathbf{b}_n. \quad (5)$$

Because σ is antisymmetric, \mathbf{j} is always perpendicular to \mathbf{E} .

The topological significance to this result is that, in 2D (in which case b is just a number), the integral $\frac{1}{2\pi} \int_{\text{BZ}} d^2 k b$ is necessarily an integer, which is a topological invariant called the (first) Chern number [10]. This means that the Hall conductance is quantized to be an integer multiple of $e^2/2\pi = \alpha/2\pi$. If the 2D surface is the surface of a 3D bulk material, then under external electric field \mathbf{E} , the Hall current is the surface current density $4\pi \mathbf{K} = n\alpha \mathbf{E} \times \hat{\mathbf{n}}$, where $n \in \mathbb{Z}$, and $\hat{\mathbf{n}}$ is the normal to the surface, and \mathbf{K} is the surface current density. This surface current density can be thought of as the magnetization current due to the magnetization $4\pi \mathbf{M} = n\alpha \mathbf{E}$, which gives the magnetoelectric susceptibility $\eta = n\alpha$. This recovers the axion electrodynamics with $\theta = n\pi$, which is 0 or π modulo 2π . This hints that surface states of an insulator may give rise to the axion electrodynamics phenomenologically.

IV. Quantization of the axion action

For the case where θ is a constant, although $\mathcal{L}_{\text{axion}}$ is a total derivative, its integral over the spacetime

$$S_{\text{axion}} := \int d^4 x \mathcal{L}_{\text{axion}}$$

is not necessarily zero even if the spacetime does not have a boundary. One can immediately see this by considering a torus spacetime (T^4) with uniform \mathbf{B} and \mathbf{E} pointing in the x^3 direction.

However, it can be shown that S_{axion} is actually quantized to be an integer multiple of θ . The following justification is a simplified version of [2]. The first point to make is that if the a spacetime coordinate, say x^2 , is periodic with period L , then A_2 is only defined modulo $2\pi/eL$. To see this, consider the gauge transformation $\Psi \rightarrow e^{2\pi i n x^2/L} \Psi$ (allowed if $n \in \mathbb{Z}$), which makes $A_2 \rightarrow A_2 + 2\pi n/eL$. Now, suppose that the spacetime is T^4 with size L^4 and that both \mathbf{B} and \mathbf{E} are uniform fields in the x^3 direction. Then, we can rewrite S_{axion} as

$$S_{\text{axion}} = \theta \frac{e^2}{4\pi^2} \int_{T^2} dx^0 dx^3 E \int_{T^2} dx^1 dx^2 B.$$

We have $B = \partial_1 A_2 - \partial_2 A_1$, so we can choose the gauge $A_1 = 0$ and $A_2 = Bx^1$. We know that x^1 is defined modulo L , and A_2 is defined modulo $2\pi/eL$. so B must be an integer multiple of $2\pi/eL^2$ to have consistent periodicity. The integral involving B is then $\int_{T^2} dx^1 dx^2 B = 2\pi n/e$, where $n \in \mathbb{Z}$. Similarly, we can deduce that the integral involving E is also of the form $2\pi m/e$ for some $m \in \mathbb{Z}$. Therefore, $S_{\text{axion}} = N\theta$, where $N := mn \in \mathbb{Z}$.

A more mathematically sophisticated way of saying this is that the second Chern number

$$N := \frac{1}{4\pi^2} \int_M F \wedge F$$

of the $U(1)$ bundle over the manifold M must be an integer [10].

The consequence of $S_{\text{axion}} = N\theta$ is that θ is only defined modulo 2π because $e^{iS_{\text{axion}}}$ is invariant under $\theta \rightarrow \theta + 2\pi$.

V. Quantization imposed by symmetries

For generic values of θ , the time reversal symmetry and spatial inversion symmetry are broken. Because \mathbf{E} is even and \mathbf{B} is odd under time reversal, $\mathbf{E} \cdot \mathbf{B}$ is odd under time reversal. Therefore, time reversal symmetry requires θ be equivalent to $-\theta$, which means θ is either 0 or π modulo 2π . Similarly, because \mathbf{E} is odd and \mathbf{B} is even under spatial inversion, $\mathbf{E} \cdot \mathbf{B}$ is also odd under spatial inversion. Therefore, spatial inversion symmetry also requires θ to be equal to 0 or π modulo 2π . If one of the two symmetries are broken, then θ can possibly take other values [11].

Besides these two symmetries, there may be other symmetries that make quantize θ to be 0 or π . Following [12], we will see that the symmetry of the combination of time reversal Θ and half lattice translation $T_{1/2}$ can also impose this quantization. Denote the momentum coordinates $k_i := \mathbf{k} \cdot \mathbf{a}_i$, where $\mathbf{a}_{1,2,3}$ are the lattice translation vectors. Then, the half lattice translation is explicitly defined as

$$T_{1/2}(\mathbf{k}) := e^{ik_3/2} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix},$$

where 1 in the matrix is the identity operator on half the unit cell. One can check that $T_{1/2}(\mathbf{k})^2 = e^{ik_3}$ is the usual lattice translation. The combination $S_{\mathbf{k}} := \Theta T_{1/2}(\mathbf{k})$ is antiunitary like Θ , but $S^2 = -e^{ik_3}$ instead of -1 . Now, consider the case where the Hamiltonian has the S symmetry: $S_{\mathbf{k}} H(\mathbf{k}) S_{\mathbf{k}}^{-1} = H(-\mathbf{k})$, where $H(\mathbf{k})$ is the Bloch Hamiltonian. On the $k_3 = 0$ plane, $S_{\mathbf{k}}^2 = -1$, which gives rise to a \mathbb{Z}_2 invariant, similar to how the time reversal symmetry gives rise to the standard \mathbb{Z}_2 invariant in the context of quantum spin Hall effect [13]. The S symmetry quantizes θ because $T_{1/2}$ does not affect θ (it adds a total derivative to the integrand in the Chern-Simons integral definition of θ , which is introduced in Section VII as Equation 8).

VI. Fujikawa's method

In this section, we will use Fujikawa's method to derive the axion term starting from the action of the form

$$S_{\text{TI}} := \int dt d^3r \bar{\psi} (i\gamma^\mu (\partial_\mu - ieA_\mu) - m_0) \psi,$$

where ψ is a Dirac spinor, and γ^μ are the gamma matrices. This action can be derived [14] from the effective

Hamiltonian

$$H_{\text{TI}}(\mathbf{k}) := v_F \mathbf{k} \cdot \boldsymbol{\alpha} + m_0 \alpha_4,$$

with minimal coupling $\mathbf{k} \rightarrow \mathbf{k} + e\mathbf{A}$, where the α matrices satisfy the Clifford algebra $\{\alpha_\mu, \alpha_\nu\} = 2\delta_{\mu\nu}$.

Following [15], first use Wick rotation $t \rightarrow -i\tau$, $A_0 \rightarrow iA_0$, $\gamma^j \rightarrow i\gamma_j$ to change the action to an integral in the Euclidean spacetime

$$S_{\text{TI}}^{\text{E}} := -iS_{\text{TI}} = \int d\tau d^3r \bar{\psi} (\gamma_\mu (\partial_\mu - ieA_\mu) + m_0) \psi$$

(superscript indices are not distinguished from subscript indices in Euclidean metric). Then, consider a local chiral transformation $\psi(x) \rightarrow e^{i\theta(x)\gamma_5} \psi(x)$. The functional measure $\mathcal{D}\bar{\psi} \mathcal{D}\psi$ (which is defined as the volume measure in the space of expansion coefficients of $\bar{\psi}$ and ψ in terms of plane wave solutions) in the path integral picks up a Jacobian factor $\exp(-2i \int d^4x \theta \mathcal{A})$, where the chiral anomaly \mathcal{A} is defined as

$$\mathcal{A}(x) = -\frac{\alpha}{2\pi} \frac{1}{16\pi} \tilde{F}^{\mu\nu} F_{\mu\nu}$$

(Fujikawa worked with general gauge groups and took the trace of the expression above; it is unnecessary for our case with $U(1)$). One can see that the Jacobian factor is just the exponential of the axion action, so the axion term is thus recovered.

VII. Dimensional reduction

Another way of deriving the axion term is through the method called dimensional reduction. In short, we can consider a $(4+1)$ -dimensional topological insulator and use it to develop an effective theory for $(3+1)$ -dimensional topological insulators. This method was reviewed by [16].

First, consider a simpler case where the topological effect of quantized pumping of $(1+1)$ -dimensional insulators are related to the first Chern number of a $(2+1)$ -dimensional model [17]. Rewrite Equation 5 in the 2D case as (summing over bands is suppressed to simplify notation)

$$\sigma = \frac{e}{2\pi} \oint dk_y G, \quad G(k_y) := \frac{e}{2\pi} \oint dk_x \left(\frac{\partial a_x}{\partial k_y} - \frac{\partial a_y}{\partial k_x} \right).$$

The result in Section III is basically that the first Chern number $n := \oint d\phi G(\phi)/e \in \mathbb{Z}$ (renaming k_y to ϕ) and that

$$j^\mu = -\frac{ne^2}{2\pi} \epsilon^{\mu\nu\tau} \partial_\nu A_\tau \quad (6)$$

(this comes from $\mathbf{j} = \boldsymbol{\sigma}\mathbf{E}$ and the continuity equation). This current can be described effectively by the action

$$S_{2\text{D}} := \frac{ne^2}{4\pi} \int dt d^2x \epsilon^{\mu\nu\tau} A_\mu \partial_\nu A_\tau,$$

in the sense that $j^\mu = -\delta S_{2D}/\delta A_\mu$. An action of this form is called the 3-dimensional abelian Chern–Simons action [18].

We can write $G(\phi) = \partial P(\phi)/\partial\phi$, where

$$P(\phi) := \frac{e}{2\pi} \oint dk_x a_x(k_x, \phi). \quad (7)$$

The quantization of n then translates to the quantization of $\Delta P := P(2\pi) - P(0)$, which is the winding number of P . Suppose the electric field is in the y direction, and then we can understand P as the charge polarization of the 1D system (in the x direction) because the current $j_x = e\partial P/\partial t$ (by noting that σ is the conductance and that $\phi = k_y$ is time-dependent by minimal coupling). From the continuity equation, we obtain

$$\frac{\partial \rho}{\partial t} = -\frac{\partial J_x}{\partial x} = -e \frac{\partial^2 P}{\partial x \partial t} \implies \rho = -e \frac{\partial P}{\partial x}.$$

We can then write

$$j^\mu = -e\epsilon^{\mu\nu} \frac{\partial P(\phi(x, t))}{\partial x^\nu},$$

where $\mu, \nu = 0, 1$ are spacetime indices in the 1D system. We now understand ϕ as a spacetime-dependent field in the 1D system. The current can effectively be described by the action

$$S_{1D} := e \int dt dx P(\phi) \epsilon^{\mu\nu} \partial_\mu A_\nu,$$

in the sense that $j^\mu = -\delta S_{1D}/\delta A_\mu$.

To work out the expression for $P(\phi)$, consider that the coordinate y of the 2D system is cyclic with period L_y so that the 2D system actually lives on a cylinder, and then think of the electric field E_y as being created by a increasing magnetic flux $\Phi(t) = E_y L_y t$ through the cylinder. During a time period $0 \leq t \leq 2\pi/eL_y E_y$, the magnetic flux goes from zero to one full flux quantum, which makes ϕ advance by a cycle of 2π . At the same time, P also advances linearly in time by ne because the charge is pumped at constant rate due to the constant current in the constant electric field. Therefore, P is linear in ϕ with slope $ne/2\pi$. Therefore, if we define $\theta := n\phi$, we have $P = e\theta/2\pi$, and thus recovering the axion action

$$S_{1D} = \frac{e^2}{2\pi} \int dt dx \theta \epsilon^{\mu\nu} \partial_\mu A_\nu.$$

We also get an expression of θ from Equation 7:

$$\theta = \oint dk_x a_x(k_x).$$

This is the integral of the Chern–Simons 1-form for the abelian gauge field a_x .

The process of getting S_{1D} from S_{2D} is the dimensional reduction, which can be applied to the $(4+1)$ -dimensional topological insulator to get S_{3D} from S_{4D} . The difference is that instead of the first Chern number, the quantization is given by the second Chern number. This time, we cannot rely on Equation 5 because it is not a topological invariant in 4D. One can work out that the effective action this time is the 5-dimensional abelian Chern–Simons action

$$S_{4D} = \frac{Ne^2}{24\pi^2} \int dt d^4x \epsilon^{\mu\nu\rho\sigma\tau} A_\mu \partial_\nu A_\rho \partial_\sigma A_\tau,$$

where N can be obtained by calculating Feynman diagrams, which turns out to be the second Chern number of the nonabelian Berry phase gauge field:

$$N = \frac{1}{32\pi^2} \int d^4k \epsilon^{ijkl} \text{Tr} b^{ij} b^{kl},$$

$$b^{ij} := \frac{\partial a^j}{\partial k^i} - \frac{\partial a^i}{\partial k^j} - i[a^i, a^j], \quad a_{mn}^i := i \left\langle u_m \left| \frac{\partial u_n}{\partial k^i} \right. \right\rangle.$$

The dimensional reduction then gives the axion action for the 3D system with θ expressed as the integral of the Chern–Simons 3-form of gauge field $a^{i=1,2,3}$ over the 3D Brillouin zone:

$$\theta = -\frac{1}{4\pi} \int d^3k \epsilon^{ijk} \text{Tr} \left(a^i \frac{\partial a^k}{\partial k^j} - \frac{2}{3} i a^i a^j a^k \right). \quad (8)$$

The method of dimensional reduction can be generalized to higher dimensions [18]. A $(2n+1)$ -dimensional topological insulator has the effective action in the form of an abelian Chern–Simons action in $2n+1$ dimensions, and the dimensional reduction gives an axion action in $2n$ dimensions where θ can be expressed as the integral of the Chern–Simons $(2n-1)$ -form of the Berry gauge field over the $(2n-1)$ -dimensional Brillouin zone.

VIII. Further readings

Axion electrodynamics in topological insulators is a rich subject where people have found many interesting results, many of which are not covered in this short article. Some notable ones are half-quantized conductance [19], quantized optical response [20], and tunable Casimir–Lifshitz repulsion [21].

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