Lecture notes on topological insulators

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Contents

I. ELECTROMAGNETIC RESPONSE OF SURFACE STATE

A. Magneto-electric coupling

Consider a cylindrical bar of topological insulator as shown in Fig. 1. Assuming that the Dirac point of the SS is *gapped by a TRS-breaking perturbation*, and *the chemical potential is inside the gap*, so that the SS has half-integer Hall conductance. If one applies an electric field along the z-axis of the cylinder, then on the surface there would be a circulating Hall current $j_H = (e^2/2h)E$. According to one of Ampere's theorem (Zangwill, 2013), the magnetic field produced by such a surface current is equivalent to that of an effective magnetization along the z-axis (in Gaussian units),

$$M = \frac{1}{c} j_H = \frac{e^2}{2hc} E. \tag{1.1}$$

Notice that M is proportional to E, instead of B. This is an example of **magneto-electric coupling**.

The thermodynamic potential for magneto-electric coupling is $U = -\chi_{ij} E_i B_j$ (see Sec. 51 of Landau and Lifshitz, 1984). This gives

$$P_i = -\frac{\partial U}{\partial E_i} = \chi_{ij} B_j, \tag{1.2}$$

$$M_j = -\frac{\partial U}{\partial B_j} = \chi_{ij} E_i. \tag{1.3}$$

Further differentiation gives

$$\chi_{ij} = \frac{\partial M_j}{\partial E_i} = \frac{\partial P_i}{\partial B_j}, \tag{1.4}$$

in which χ_{ij} is *not* required to be symmetric. Following Eq. (1.1), one has

$$P = \frac{e^2}{2hc} B. \tag{1.5}$$

For a heuristic explanation of the polarization induced by a magnetic field, see related discussion in Nomura, 2013.

Such a magneto-electric coupling can be obtained by adding a term $\mathcal{L}_\theta$ to the Lagrangian density of electromagnetic field (Qi *et al.*, 2009),

$$\mathcal{L}_{EM} = \frac{1}{8\pi}(E^2 - B^2) + \mathcal{L}_\theta - \rho\phi + \frac{1}{c}\mathbf{j}\cdot\mathbf{A}, \tag{1.6}$$

where

$$\mathcal{L}_\theta = \frac{e^2}{2hc}\mathbf{E}\cdot\mathbf{B} = \alpha\frac{\theta}{4\pi^2}\mathbf{E}\cdot\mathbf{B}, \tag{1.7}$$

$\alpha = e^2/\hbar c$ is the fine structure constant, and the **axion angle** $\theta = \pi$. The coupling strength $e^2/2h$ has its origin in the half-integer Hall effect.

We now introduce the 4-vector notation. Recall that

$$x^\mu = (ct, \mathbf{x}), \tag{1.8}$$

$$\partial^\mu = \left(\frac{\partial}{c\partial t}, -\frac{\partial}{\partial \mathbf{x}}\right), \tag{1.9}$$

$$j^\mu = (c\rho, \mathbf{j}), \tag{1.10}$$

$$A^\mu = (\phi, \mathbf{A}). \tag{1.11}$$

The electromagnetic field tensor is (see Chaps 11, 12 of Jackson, 1999),

$$F^{\mu\nu} \equiv \partial^\mu A^\nu - \partial^\nu A^\mu \tag{1.12}$$

$$= \begin{pmatrix} 0 & -E^1 & -E^2 & -E^3 \\ E^1 & 0 & -B^3 & B^2 \\ E^2 & B^3 & 0 & -B^1 \\ E^3 & -B^2 & B^1 & 0 \end{pmatrix}, \tag{1.13}$$

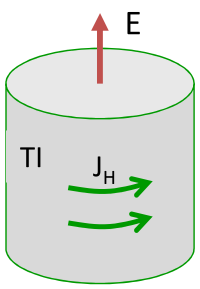

FIG. 1 A cylindrical topological insulator in an uniform electric field has a circulating surface Hall current.

with a dual tensor,

$$\tilde{F}^{\mu\nu} \equiv \frac{1}{2}\epsilon^{\mu\nu\delta\sigma}F_{\delta\sigma} \tag{1.14}$$

$$= \begin{pmatrix} 0 & -B^1 & -B^2 & -B^3 \\ B^1 & 0 & E^3 & -E^2 \\ B^2 & -E^3 & 0 & E^1 \\ B^3 & E^2 & -E^1 & 0 \end{pmatrix}. \tag{1.15}$$

It follows that,

$$F^{\mu\nu}F_{\mu\nu} = -2(E^2 - B^2), \tag{1.16}$$

$$\frac{1}{2}\epsilon^{\mu\nu\delta\sigma}F_{\mu\nu}F_{\delta\sigma} = -4\mathbf{E}\cdot\mathbf{B}. \tag{1.17}$$

Therefore,

$$\mathcal{L}_{EM} = -\frac{1}{16\pi}F^{\mu\nu}F_{\mu\nu} + \mathcal{L}_\theta - \frac{1}{c}j^\mu A_\mu, \tag{1.18}$$

and the axion term is

$$\mathcal{L}_\theta = -\alpha\frac{\theta}{16\pi^2}\frac{1}{2}\epsilon^{\mu\nu\delta\sigma}F_{\mu\nu}F_{\delta\sigma} \tag{1.19}$$

$$= -\alpha\frac{\theta}{16\pi^2}\epsilon^{\mu\nu\delta\sigma}\partial_\mu(A_\nu F_{\delta\sigma}), \tag{1.20}$$

which is a total derivative *if* the axion angle is uniform throughout the whole space.

Using the Euler-Lagrange equation of motion,

$$\frac{\partial\mathcal{L}_{EM}}{\partial A_\nu} - \partial_\mu\frac{\partial\mathcal{L}_{EM}}{\partial(\partial_\mu A_\nu)} = 0, \tag{1.21}$$

we have,

$$\partial_\mu\left(F^{\mu\nu} + \alpha\frac{\theta}{\pi}\tilde{F}^{\mu\nu}\right) = \frac{4\pi}{c}j^\nu. \tag{1.22}$$

Also, from Eq. (1.12), we have

$$\partial_\mu F_{\nu\lambda} + \partial_\nu F_{\lambda\mu} + \partial_\lambda F_{\mu\nu} = 0. \tag{1.23}$$

These two are Maxwell equations in relativistic covariant form.

B. Axion electrodynamics

When written in $\mathbf{E}, \mathbf{B}$ fields, the Maxwell equations are,

$$\nabla\cdot\left(\mathbf{E} + \alpha\frac{\theta}{\pi}\mathbf{B}\right) = 4\pi\rho, \tag{1.24}$$

$$\nabla\times\left(\mathbf{B} - \alpha\frac{\theta}{\pi}\mathbf{E}\right) = \frac{4\pi}{c}\mathbf{j} + \frac{1}{c}\frac{\partial}{\partial t}\left(\mathbf{E} + \alpha\frac{\theta}{\pi}\mathbf{B}\right), \tag{1.25}$$

$$\nabla\cdot\mathbf{B} = 0, \tag{1.26}$$

$$\nabla\times\mathbf{E} = -\frac{1}{c}\frac{\partial}{\partial t}\mathbf{B}. \tag{1.27}$$

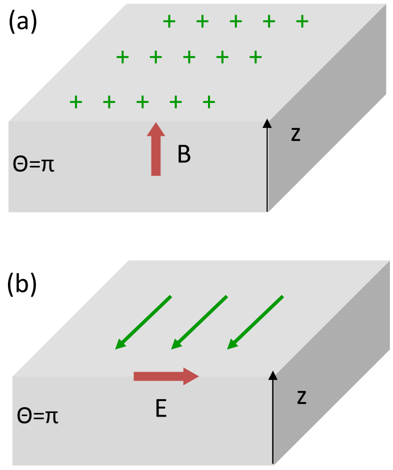

FIG. 2 (a) A magnetic field induces electric charges on the surface of a TI. (b) An electric field induces a Hall current on the surface of a TI.

One can move the axion terms to the right hand side of the equations, such that

$$\nabla\cdot\mathbf{E} = 4\pi(\rho + \rho_\theta), \tag{1.28}$$

$$\nabla\times\mathbf{B} = \frac{4\pi}{c}(\mathbf{j} + \mathbf{j}_\theta) + \frac{1}{c}\frac{\partial\mathbf{E}}{\partial t}, \tag{1.29}$$

$$\text{where}\quad \rho_\theta = -\frac{\alpha}{4\pi^2}\nabla\cdot(\theta\mathbf{B}), \tag{1.30}$$

$$\mathbf{j}_\theta = \frac{\alpha c}{4\pi^2}\nabla\times(\theta\mathbf{E}) + \frac{\alpha}{4\pi^2}\frac{\partial}{\partial t}(\theta\mathbf{B}). \tag{1.31}$$

We put θ inside the differentiation, since it is not uniform throughout the whole space: π inside a TI, but 0 outside.

Assume the semi-infinite space below xy-plane is occupied by a TI, such that $\theta(z) = \pi h(-z)$, where $h(z)$ is the Heaviside step function. If one applies an uniform magnetic field along the z-axis (see Fig. 2(a)), then the axion-induced effective charge is,

$$\rho_\theta = \frac{\alpha}{4\pi}\delta(z)B_z. \tag{1.32}$$

That is, there is a thin layer of charges on the surface of the TI. This is consistent with Eq. (1.5).

On the other hand, if one applies an uniform electric field parallel to the surface (see Fig. 2(b)), the the axion-induced effective current density is,

$$\mathbf{j}_\theta = -\frac{\alpha c}{4\pi}\delta(z)\hat{z}\times\mathbf{E}. \tag{1.33}$$

That is, the is a thin layer of current on the surface of the TI, perpendicular to the E-field. This is a Hall current with Hall conductivity $\sigma_H = \alpha c/4\pi = e^2/2h$. Thus, the axion term does produce correct electromagnetic responses of the TI surface state.

Due to the magneto-electric coupling on a TI surface, an electric charge near the surface would induce an image **dyon** – a particle with both electric and magnetic charges (Fig. 3). The magnetic field (outside the TI) generated

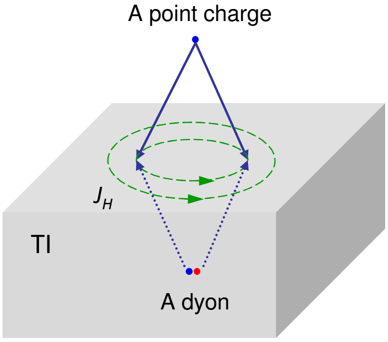

FIG. 3 A point charge outside a TI (a dielectric) has an image charge. The radial electric field also induces Hall current on the surface, which produces a magnetic field that is emanated in effect from an image magnetic monopole.

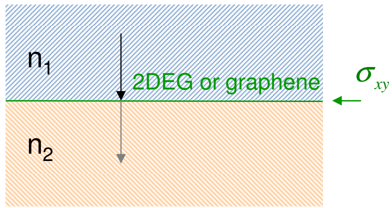

FIG. 4 An EM wave passing through a 2DEG, such as the one in graphene or on the surface of a TI, that is sandwiched between materials with refractive indices n_1, n_2.

by the image monopole (inside the TI) is in fact due to the surface Hall current induced by the electric charge outside. For more details, see Qi *et al.*, 2009; Wilczek, 1987.

In the dynamical range, the magneto-electric coupling would rotate the polarization plane of an optical wave transmitted though (**Faraday effect**) and reflected from (**Kerr effect**) the TI surface (Tse and MacDonald, 2010; Wu *et al.*, 2016). Such rotations are related to the surface Hall current induced by the electric field of the optical wave. Similar effect has been observed in graphene, because it can also have the surface Hall current (Crassee *et al.*, 2011).

In general, an EM wave with circular polarization passing through a 2DEG (along the normal direction, see Fig. 4) has the transmission coefficient (Chiu *et al.*, 1976),

$$t_\pm = \frac{2n_1}{n_1+n_2+\frac{4\pi}{c}\sigma_\pm} = |t_\pm| e^{i\theta_\pm}, \tag{1.34}$$

in which $\sigma_\pm = \sigma_{xx} + i\sigma_{xy}$, and the angle of Faraday rotation is given as,

$$\theta_F = \frac{1}{2}(\theta_+ - \theta_-). \tag{1.35}$$

If $\sigma_{xx} \simeq 0$, the imaginary part of σ_{xy} is small, and $4\pi\sigma_{xy}/c \ll n_1, n_2$, then

$$\theta_F \simeq \frac{4\pi}{c}\frac{\sigma_{xy}}{n_1+n_2}. \tag{1.36}$$

For a graphene suspended in air ($n_1 = n_2 = 1$) with quantum Hall conductance $\sigma_{xy} = \nu e^2/h, \nu \in Z$, we have

$$\theta_F \simeq \nu\alpha, \quad \alpha = \frac{e^2}{\hbar c}. \tag{1.37}$$

That is, the visual transparency of graphene is determined by the fine structure constant (Nair *et al.*, 2008).

C. Axion angle and Berry connection

The axion angle is a coarse-grained description of the electromagnetic response of TI. Like electric permittivity and magnetic permeability, it is a response function that depends on material property. In principle, χ_{ij} can be calculated from the theory of response using Eq. (1.4). This difficult task has been accomplished by Vanderbilt's group (Essin *et al.*, 2010; Malashevich *et al.*, 2010). They showed that the general form of the **magneto-electric susceptibility** is,

$$\chi_{ij} = \tilde{\chi}_{ij} + \chi_\theta \delta_{ij}, \tag{1.38}$$

in which the second term, $\chi_\theta = \frac{e^2}{2hc}\frac{\theta}{\pi}$, is related to the magneto-electric coupling in previous section. The axion angle is given as an integral of Berry connections,

$$\theta = \frac{1}{4\pi}\int_{BZ} d^3k\, \epsilon_{abc}\mathrm{tr}\left(\mathsf{A}_a\partial_b\mathsf{A}_c - \frac{2i}{3}\mathsf{A}_a\mathsf{A}_b\mathsf{A}_c\right). \tag{1.39}$$

The trace is a sum over occupied energy bands, and

$$[\mathsf{A}_a(\mathbf{k})]_{nn'} = i\langle u_{n\mathbf{k}}|\frac{\partial}{\partial k_a}|u_{n'\mathbf{k}}\rangle. \tag{1.40}$$

The reason that the integrand of the axion angle is the **Chern-Simons term** can be understood from the perspective of dimensional reduction. That is, the 3D TI can be considered as a descendent of the 4D quantum Hall effect, which is characterized by the second Chern number. We will explore more about this in Chap. **??**.

The axion angle is defined only up to $2\pi w, w \in Z$. This is proved as follows: Under a gauge transformation (U is an unitary matrix),

$$\mathsf{A}_a \to \mathsf{A}'_a = \mathsf{U}^\dagger\mathsf{A}_a\mathsf{U} + i\mathsf{U}^\dagger\partial_a\mathsf{U}, \tag{1.41}$$

it is left as an exercise to show that,

$$\theta \to \theta' = \theta + \frac{1}{12\pi}\int_{BZ} d^3k\, \epsilon_{abc}\mathrm{tr}\left(\mathsf{U}^\dagger\partial_a\mathsf{U}\mathsf{U}^\dagger\partial_b\mathsf{U}\mathsf{U}^\dagger\partial_c\mathsf{U}\right). \tag{1.42}$$

The second term is an integer multiple of 2π, which we now prove (Nomura, 2013).

For simplicity, we consider SU(2) gauge transformation, $\mathsf{U} = e^{i\frac{\phi}{2}\hat{\mathbf{n}}\cdot\boldsymbol{\sigma}}$. Following Nomura's note, write

$$\begin{aligned}\mathsf{U}(\mathbf{k}) &= \cos\frac{\phi(\mathbf{k})}{2} + i\hat{\mathbf{n}}\cdot\boldsymbol{\sigma}\sin\frac{\phi(\mathbf{k})}{2} &(1.43)\\ &\equiv i m_\mu(\mathbf{k})\sigma_\mu, &(1.44)\end{aligned}$$

where (no need to worry about upper/lower index here)

$$m_\mu = \left(\cos\frac{\phi}{2}, n_x \sin\frac{\phi}{2}, n_y \sin\frac{\phi}{2}, n_z \sin\frac{\phi}{2}\right), m_\mu^2 = 1, \quad (1.45)$$

$$\sigma_\mu = (1/i, \sigma_x, \sigma_y, \sigma_z). \quad (1.46)$$

With the help of $\mathrm{tr}(\sigma_\mu\sigma_\nu^\dagger\sigma_\rho\sigma_\lambda^\dagger) = 2\epsilon_{\mu\nu\rho\lambda}$, it can be shown that,

$$\begin{aligned} & \frac{1}{24\pi^2}\int_{BZ} d^3k\ \epsilon_{abc}\mathrm{tr}\left(\mathsf{U}^\dagger\partial_a\mathsf{U}\mathsf{U}^\dagger\partial_b\mathsf{U}\mathsf{U}^\dagger\partial_c\mathsf{U}\right) & (1.47)\\ = & \frac{1}{24\pi^2}\int_{BZ} d^3k\ \epsilon_{abc}\mathrm{tr}\left(\mathsf{U}\partial_a\mathsf{U}^\dagger\partial_b\mathsf{U}\partial_c\mathsf{U}^\dagger\right) & (1.48)\\ = & \frac{1}{12\pi^2}\int_{BZ} d^3k\ \epsilon_{abc}\epsilon_{\mu\nu\rho\lambda}m_\mu\partial_a m_\nu\partial_b m_\rho\partial_c m_\lambda & (1.49)\\ = & \frac{1}{2\pi^2}\int_{BZ} d^3k\ \epsilon_{\mu\nu\rho\lambda}m_\mu\partial_1 m_\nu\partial_2 m_\rho\partial_3 m_\lambda. & (1.50)\end{aligned}$$

This integral is the winding number w of the mapping $T^3 \to SU(2) \simeq S^3$ (e.g., see Sec. 34 of Gottfried, 1989). Therefore, the axion angle can change by $2\pi w$ under a gauge transformation. It is well defined only within the interval $[0, 2\pi]$.

Recall that in the Qi-Wu-Zhang model (Sec. **??**), we have the winding number of the mapping $T^2 \to S^2$. Here the mapping is $T^3 \to S^3$. The mapping $T^4 \to S^4$ will be encountered in the next chapter while we discuss the second Chern number.

In general, if N energy levels are filled, then the gauge rotation in Eq. (1.47) should be $U(N)$. The winding number of the mapping $S^3 \to U(N) = U(1)\times SU(N)$ is related to the homotopy group,

$$\pi_3(U(N)) = \pi_3(SU(N)). \quad (1.51)$$

The $U(1)$ factor disappears Since $U(1) \simeq S^1$, and $\pi_3(S^1) = 0$. It is known that

$$\pi_3(SU(N)) = Z \text{ for } N \geq 2. \quad (1.52)$$

Therefore, we should still get an integer. When the base space is a T^3, instead of S^3, the $U(1)$ phase would contribute another integer. But overall Eq. (1.47) should still be an integer.

D. Time reversal symmetry and space inversion symmetry

1. Time reversal symmetry

If an insulator has time reversal invariance, then its axion angle can only be 0 or π. This is a reflection of the Z_2 classification discussed in Chaps. **??** and **??**. The proof is as follows (Wang *et al.*, 2010):
Recall that in Chap. **??**, we have

$$\vec{\mathsf{A}}(-\mathbf{k}) = \mathsf{w}(\mathbf{k})\vec{\mathsf{A}}^*(\mathbf{k})\mathsf{w}^\dagger(\mathbf{k}) - i\mathsf{w}(\mathbf{k})\frac{\partial}{\partial\mathbf{k}}\mathsf{w}^\dagger(\mathbf{k}), \quad (1.53)$$

where

$$|u_{-\mathbf{k}\alpha}\rangle = \sum_\beta w^*_{\alpha\beta}(\mathbf{k})|\Theta u_{\mathbf{k}\beta}\rangle. \quad (1.54)$$

Therefore,

$$\begin{aligned}\theta &= \frac{1}{4\pi}\int_{BZ} d^3k\ \epsilon_{abc}\mathrm{tr}\left(\mathsf{A}_a\partial_b\mathsf{A}_c - \frac{2i}{3}\mathsf{A}_a\mathsf{A}_b\mathsf{A}_c\right)_{-\mathbf{k}} & (1.55)\\ &\vdots \\ &= -\frac{1}{4\pi}\int_{BZ} d^3k\ \epsilon_{abc}\mathrm{tr}\left(\mathsf{A}^*_a\partial_b\mathsf{A}^*_c + \frac{2i}{3}\mathsf{A}^*_a\mathsf{A}^*_b\mathsf{A}^*_c\right)_{\mathbf{k}} \\ &+ \frac{1}{12\pi}\int_{BZ} d^3k\ \epsilon_{abc}\mathrm{tr}\left(\mathsf{w}\partial_a\mathsf{w}^\dagger\mathsf{w}\partial_b\mathsf{w}^\dagger\mathsf{w}\partial_c\mathsf{w}^\dagger\right). & (1.56)\end{aligned}$$

The first term is $-\theta^* = -\theta$, since θ is real. Therefore, we have

$$\theta = \frac{1}{24\pi}\int_{BZ} d^3k\ \epsilon_{abc}\mathrm{tr}\left(\mathsf{w}\partial_a\mathsf{w}^\dagger\mathsf{w}\partial_b\mathsf{w}^\dagger\mathsf{w}\partial_c\mathsf{w}^\dagger\right). \quad (1.57)$$

This looks the same as the integral in Eq. (1.47), except that the w here is a $U(2)$ matrix (assuming there are only 2 energy levels). As shown in Wang *et al.*, 2010, the $U(1)$ factor does not lead to non-integrable phase, and we are left with a $SU(2)$ matrix. Thus, like Eq. (1.47), this integral is the winding number of the mapping $T^3 \to \mathrm{SU}(2) \simeq S^3$. As a result,

$$\theta = 0, \pi \mod 2\pi. \quad (1.58)$$

In general, for $2N$ energy levels, the $2N \times 2N$ sewing matrix m can be decomposed as a direct sum of N $SU(2)$ matrices (multiplied by a $U(1)$ phase). Each block contributes an integer winding number, so the conclusion remains the same (Wang *et al.*, 2010).

2. Space inversion symmetry

One can define a sewing matrix for space inversion,

$$s_{\alpha\beta}(\mathbf{k}) = \langle u_{-\mathbf{k}\alpha}|\Pi|u_{\mathbf{k}\beta}\rangle, \quad (1.59)$$

or

$$|u_{-\mathbf{k}\alpha}\rangle = \sum_\beta s^*_{\alpha\beta}(\mathbf{k})\Pi|u_{\mathbf{k}\beta}\rangle. \quad (1.60)$$

It relates $\vec{\mathsf{A}}(-\mathbf{k})$ and $\vec{\mathsf{A}}(\mathbf{k})$ as follows (see the homework of Chap **??**, or Sec. 14.3 of Bernevig and Hughes, 2013),

$$\vec{\mathsf{A}}(-\mathbf{k}) = -\mathsf{s}(\mathbf{k})\vec{\mathsf{A}}(\mathbf{k})\mathsf{s}^\dagger(\mathbf{k}) - i\mathsf{s}(\mathbf{k})\frac{\partial}{\partial\mathbf{k}}\mathsf{s}^\dagger(\mathbf{k}), \quad (1.61)$$

One may wonder if there is a similar Z_2 invariant associated with the SI. Indeed, one can show that, in the presence of SI, θ can only be 0 or π, as in the case with TRS:

$$\theta = \frac{1}{4\pi}\int_{BZ} d^3k\ \epsilon_{abc}\mathrm{tr}\left(\mathsf{A}_a\partial_b\mathsf{A}_c - \frac{2i}{3}\mathsf{A}_a\mathsf{A}_b\mathsf{A}_c\right)_{-\mathbf{k}} \quad (1.62)$$

$$\begin{aligned} &\vdots \\ &= -\frac{1}{4\pi}\int_{BZ} d^3k\ \epsilon_{abc}\mathrm{tr}\left(\mathsf{A}_a\partial_b\mathsf{A}_c - \frac{2i}{3}\mathsf{A}_a\mathsf{A}_b\mathsf{A}_c\right)_{\mathbf{k}} \\ &+ \frac{1}{12\pi}\int_{BZ} d^3k\ \epsilon_{abc}\mathrm{tr}\left(\mathsf{s}\partial_a\mathsf{s}^\dagger\mathsf{s}\partial_b\mathsf{s}^\dagger\mathsf{s}\partial_c\mathsf{s}^\dagger\right). \end{aligned} \quad (1.63)$$

Again the first term is $-\theta$, so we would reach the same conclusion as the TRS case above.

However, unlike TRS, an insulator with SIS and $\theta = \pi$ does not have robust surface state, since the surface itself breaks the SIS. As we have mentioned in Chap **??**, other crystalline symmetries can protect a topological phase. This forms the subject of **topological crystalline insulator** (Fu, 2011; Hsieh *et al.*, 2012).

Exercise

1. (a) Starting from the Lagrangian density $\mathcal{L}_{EM}$, and using the Euler-Lagrange equation, derive the Maxwell equation in Eq. (1.22).
(b) Verify Eq. (1.23), which by the way is related to the **Bianchi identity** in differential geometry.
(c) Show that the Maxwell equations in conventional form are given as Eqs. (1.24), (1.25), (1.26), (1.27).
2. Show that, under the gauge transformation,

$$\mathsf{A}_a \to \mathsf{A}'_a = \mathsf{U}^\dagger\mathsf{A}_a\mathsf{U} + i\mathsf{U}^\dagger\partial_a\mathsf{U}, \quad (1.64)$$

where U is an unitary matrix, the axion angle changes as,

$$\theta \to \theta' = \theta + \frac{1}{12\pi}\int_{BZ} d^3k\ \epsilon_{abc}\mathrm{tr}\left(\mathsf{U}^\dagger\partial_a\mathsf{U}\mathsf{U}^\dagger\partial_b\mathsf{U}\mathsf{U}^\dagger\partial_c\mathsf{U}\right).$$

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