Axion mass in magnetic topological insulators

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Abstract

We study axion in 3D topological insulators with magnetic impurities under finite temperature. We find stable antiferromagnetic ground state and ferromagnetic metastable state. In both magnetic states, the mass of axion is found to be up to eV scale and it approaches to zero near the phase boundary of the magnetic state. This result applies to both normal and topological insulator phases.
1 Introduction

Axion has drawn attention in interdisciplinary fields of particle physics, cosmology, and condensed matter physics. In condensed matter physics, a dynamical axion is predicted in the magnetic topological insulators (TIs) [1]. It is a quasi particle that couples to the electromagnetic fields, which leads to an instability of the electromagnetic fields. It is predicted that the instability causes the total reflection of the incident light [1] or the conversion of the external electric field to magnetic field [2]. On top of that it has been proposed in Refs. [3–5] that the axion in the magnetic TIs can be a possible excitation signal in the detection of particle axion, which is a good candidate for dark matter of the universe. On the other hand, a static axion or constant axion is known as the magnetoelectric effect [6–11]. To understand the properties of both the dynamical and static axions, magnetism plays a crucial role.

In Refs. [12–14], the dynamical axion in the antiferromagnetic (AFM) TIs is described from the partition function given by the path integral. As a result, the mass of the dynamical axion in the AFM TIs is estimated to be about a meV. Ref. [15] has revisited the axion mass in the Hubbard model and reformulated the action of the axion field using Hubbard-Stratonovich transformation. In the formula, the effective potential for the axion field is derived in the topological and normal insulators under the AFM and paramagnetic states. Consequently, both the dynamical and static axions are described consistently and the axion mass is found to be less than $\mathcal{O}(\text{eV})$. Furthermore it can be suppressed near the phase boundary between the AFM and paramagnetic states.

In recent years magnetically doped bismuth selenide or bismuth telluride has caught lots of attention. For example, both the AFM and ferromagnetic (FM) states are predicted in $\text{MnBi}_2\text{Te}_4$ [16–20] or $\text{Mn}_2\text{Bi}_2\text{Te}_5$ [21] by the first-principles calculations. In addition, a rich magnetic topological states in addition to the AFM/FM states are predicted [21]. Since such materials are probable candidates for the detection of the particle axion, it is important to find how to describe the axion in variety of magnetic states.

In this work, we formulate the axion in the TIs with magnetic dopants under finite temperature. For the purpose, we consider the three-dimension (3D) effective TIs model with the interaction term of electrons with magnetic impurities. The grand potential is calculated from the path integral under finite temperature, and consequently the effective potential for the order parameter of the AFM and FM
are derived. Around the stationary points of the effective potential, the mass of dynamical axion is formulated.

This paper is organized as follows. In the next section, we give the Hamiltonian of the model and define the observables including the order parameters. In Sec. 3 the effective potential for the order parameters is derived from the grand potential, which gives rise to the phase diagram of magnetism in Sec. 4. Finally the axion mass is derived in Sec. 5. The conclusion is given in Sec. 6.

2 The model

We consider a effective model for 3D topological insulators (TIs). The basic Hamiltonian is [1,22]\(^{#1}\)

\[ H_{\text{TI}} = \sum_{k} c_{k}^\dagger H_{k}^{\text{TI}} c_{k}, \]  
\[ H_{k}^{\text{TI}} = (\epsilon_{0} - \mu)1 + \sum_{a=1}^{4} d^{a} \Gamma^{a}, \]  

where \( c_{k}^\dagger \) and \( c_{k} \) are creation and annihilation operator of electrons in the wavenumber space and \( \mu \) is the chemical potential, \( k \) is the wavenumber, and \( \Gamma^{a} \) are the Gamma matrices defined in Eq. (A.1) of Appendix A. \( \epsilon_{0} \) is a constant and \( d^{a} \) is parameterized as

\[ (d^{1}, d^{2}, d^{3}, d^{4}) = (A_{2} \sin k_{x} \ell_{x}, A_{2} \sin k_{y} \ell_{y}, A_{1} \sin k_{z} \ell_{z}, \mathcal{M}), \]  

where \( \mathcal{M} = M_{0} - 2B_{1} - 4B_{2} + 2B_{1} \cos k_{z} \ell_{z} + 2B_{2}(\cos k_{x} \ell_{x} + \cos k_{y} \ell_{y}) \). \( M_{0} < 0 \) and \( M_{0} > 0 \) correspond to topological and normal insulators, respectively. We consider a cubic lattice in the later analysis, i.e. \( \ell_{x} = \ell_{y} = \ell_{z} \equiv \ell \), for simplicity. The Hamiltonian has the time-reversal invariance, which is one of the features of the TIs, and it describes Bi\(_{2}\)Se\(_{3}\) family of materials, including Bi\(_{2}\)Te\(_{3}\) and Sb\(_{2}\)Te\(_{3}\) [23]. In the present study, we additionally assume magnetic dopants, such as Fe, Cr, or Mn, in the material and introduce the onsite interaction term between the impurity and electron [24]

\[ H_{J} = \sum_{I}^{N_{s}} [J^{A} \mathbf{S}^{A}(\mathbf{x}_{I}) \cdot \mathbf{s}_{I}^{A} + J^{B} \mathbf{S}^{B}(\mathbf{x}_{I}) \cdot \mathbf{s}_{I}^{B}], \]  

\(^{#1}\)We change the notation of Hamiltonian from one in Ref. [15].
where \( S^A (s^A_I) \) and \( S^B (s^B_I) \) are the local spins of the impurities (spins of electron) at cite \( I \) of the sublattice \( A \) and \( B \), respectively. \( J^A \) and \( J^B \) are the exchange coupling constants and \( N_s \) is the number of the impurities. In the following discussion, we consider the magnetism in \( z \) direction. Then the spins of electron are written as

\[
s^A_{zI} = \frac{1}{2} c^\dagger_I (\Gamma^{12} + \Gamma^5) c_I, \tag{2.5}
\]

\[
s^B_{zI} = \frac{1}{2} c^\dagger_I (\Gamma^{12} - \Gamma^5) c_I, \tag{2.6}
\]

where \( c_I \) is the wavefunction of the electron at cite \( I \) in the lattice space, and \( \Gamma^{12} \) and \( \Gamma^5 \) are given in Appendix A. The similar model, but only with term proportional to \( \Gamma^{12} \) is considered in Refs. [25–27] in different context. In Ref. [27], the same terms as both \( \Gamma^{12} \) and \( \Gamma^5 \) are considered. In the literature, Cr and Mn are doped on the top and the bottom halves of the TI films in superlattice and the exchange couplings with Cr and Mn are taken to be opposite each other. Then the mass of the dynamical axion is estimated to be meV. We will get a different result in Sec. 5.

We apply the mean field approximation (MFA) to \( H_J \). In the MFA, \( H_J \) becomes

\[
H_J \approx \sum_{I}^{N_s} \left[ J^A s^A_z (x_I) \langle s^A_z \rangle + J^B s^B_z (x_I) \langle s^B_z \rangle + J^A S^A_z (x_I) \langle s^A_z \rangle + J^B S^B_z (x_I) \langle s^B_z \rangle \right] - N_s (J^A \langle s^A_z \rangle \langle s^A_z \rangle + J^B \langle s^B_z \rangle \langle s^B_z \rangle). \tag{2.7}
\]

Introducing

\[
M^A = x \langle S^A_z \rangle, \quad M^B = x \langle S^B_z \rangle, \tag{2.8}
\]

\[
m^A = \langle s^A_z \rangle, \quad m^B = \langle s^B_z \rangle, \tag{2.9}
\]

where \( x = N_s / N \) and \( N \) is the number of cite, we get

\[
H_J \approx \sum_{i}^{N_s} \left[ J^A M^A s^A_{zI} + J^B M^B s^B_{zI} \right] + \sum_{I}^{N_s} \left[ J^A m^A S^A_z (x_I) + J^B m^B S^B_z (x_I) \right] - N_s (J^A m^A + J^B m^B). \tag{2.10}
\]

As a result, the total Hamiltonian is linearized as\(^2\)

\[
H^{\text{TI}} + H_J \approx H_e + H_S + H_R, \tag{2.11}
\]

\(^2\text{Although } M^A, M^B, m^A \text{ and } m^B \text{ themselves should be interpreted as the mean field values (or vacuum expectation values), we take them as spurious fields in order to give the effective potential. See later discussion.}\)
where $H_e$ and $H_S$ are the Hamiltonians of the electrons and the local spin defined by

\begin{align}
H_e &= H^{TI} + \sum_i^N [J^A M^A s^A_{zi} + J^B M^B s^B_{zi}] , \\
H_S &= \sum_i^N [J^A m^A S^A_z(x_i) + J^B m^B S^B_z(x_i)] , \\
H_R &= -N(J^A M^A m^A + J^B M^B m^B).
\end{align}

(2.12) (2.13) (2.14)

For later analysis, it is convenient to write down the Hamiltonian by using the following variables

\begin{align}
m_t &= m^A + m^B , \\
m_r &= m^A - m^B , \\
M_f &= \frac{1}{2}(J^A M^A + J^B M^B) , \\
M_5 &= \frac{1}{2}(J^A M^A - J^B M^B).
\end{align}

(2.15) (2.16) (2.17) (2.18)

$M_f$ and $M_5$ plays the order parameters of the FM and AFM, respectively. In terms of $M_f$ and $M_5$ the Hamiltonian of electrons is given by

\begin{equation}
H_e = \sum_k c_k^\dagger \mathcal{H}_{ek} c_k ,
\end{equation}

(2.19)

where

\begin{align}
\mathcal{H}_{ek} &= \mathcal{H}^{TI}_k + \mathcal{H}^m_k , \\
\mathcal{H}^m_k &= M_f \Gamma^{12} + M_5 \Gamma^5.
\end{align}

(2.20) (2.21)

We note that two terms proportional to $\Gamma^{12}$ and $\Gamma^5$ have appeared in the Hamiltonian for the electrons. Those terms describe the magnetism of the materials and they are consistent with the symmetry of the crystal structure of the materials, such as Bi$_2$Se$_3$ and Bi$_2$Te$_3$ [23]. Diagonalizing $\mathcal{H}_{ek}$ gives four energy bands. They are given by $E_{jk} = \epsilon_0 - \mu \pm e_{jk} (j = 1, 2)$, where

\begin{align}
e_{1k} &= \sqrt{d_0^2 + M_f^2 + M_5^2 + 2M_f \sqrt{d_s^2 + M_5^2}} , \\
e_{2k} &= \sqrt{d_0^2 + M_f^2 + M_5^2 - 2M_f \sqrt{d_s^2 + M_5^2}} .
\end{align}

(2.22) (2.23)

#3 $M_5$ corresponds to $\phi$ in Ref. [15].
where \( d_0 \equiv \sqrt{\sum_{a=1}^{4} d^a d^a} \) and \( d_s \equiv \sqrt{(d^3)^2 + (d^4)^2} \).

In the following discussion, we consider the half-filling case since we are interested in the insulator in the bulk. In addition we assume that the temperature is sufficiently smaller than the energy scale of the electron. This is a good approximation since we consider temperature up to \( \mathcal{O}(10^2 \text{ K}) \). Then the chemical potential should be chosen as \( \mu \simeq \epsilon_0 \), and the relevant energy bands in the following discussion are going to be \(-e_{1k}\) and \(-e_{2k}\).

3 The effective potential from the grand potential

While the mean field values for each variables can be derived from the Hamiltonian, the grand potential is useful to derive the effective action for the order parameters \( M_f \) and \( M_5 \). The grand potential is given by\(^4\)

\[
\Omega = -\beta^{-1} \ln Z, \tag{3.1}
\]

where \( \beta = 1/T \) is the inverse temperature and \( Z \) is the partition function given by

\[
Z = \int \mathcal{D}c^\dagger \mathcal{D}c \mathcal{D}M \ e^{-S_E}. \tag{3.2}
\]

Here \( c \) is the wavefunction of electrons, \( M \) represents \( S^A_2 \) and \( S^B_2 \), and \( S_E \) is the action of the system in the Euclidean space.\(^5\) The Hamiltonian of electrons and local spins are linearized under the MFA as seen in the previous section. Then, the Euclidean action is given by \( S_E = S_e + S_S + S_R \) where

\[
S_e = \int_0^\beta d\tau \sum_i \nabla_i^\dagger [\partial_\tau + \mathcal{H}_e]c_i, \tag{3.3}
\]

\[
S_S = \int_0^\beta d\tau H_S, \tag{3.4}
\]

\[
S_R = \int_0^\beta d\tau H_R = \beta H_R. \tag{3.5}
\]

Consequently, the grand potential is obtained as

\[
\Omega = \Omega_e + \Omega_S + H_R. \tag{3.6}
\]

\(^4\)Since we consider the half-filling case, the grand potential corresponds to the Helmholtz free energy.

\(^5\)In the derivation of the kinetic term of the dynamical axion, we promote \( M_5 \) to a dynamical field. See later discussion and Appendix D.
where $\Omega_e$ is the grand potential for the electrons and $\Omega_S$ is the one for the local spins given by

$$\Omega_S = -\beta^{-1}N S \left[ \ln \left( \frac{\sinh(S + 1/2)\beta J^A m^A}{\sinh \beta J^A m^A/2} \right) + (A \to B) \right].$$

(3.7)

Here $S$ is the absolute value of the local spin. $\Omega_e$, on the other hand, is computed as

$$\Omega_e = -\beta^{-1} \ln e^{-S_e},$$

(3.8)

$$S_e = -\ln \det[\partial_e + \mathcal{H}_e].$$

(3.9)

Here the determinant is obtained by

$$\det[\partial_e + \mathcal{H}_e] = \prod_{n, j, k} (-i\omega_n + E_{jk}),$$

(3.10)

where $\omega_n = (2n + 1)\pi/\beta$ is the Matsubara frequency for fermion.

From the grand potential, the mean field (MF) values for $m^A$, $m^B$, $M^A$, and $M^B$ are obtained as

$$m_{\text{MF}}^A = \frac{1}{N} \frac{\partial \Omega_e}{\partial J^A m^A},$$

(3.11)

$$m_{\text{MF}}^B = \frac{1}{N} \frac{\partial \Omega_e}{\partial J^B m^B},$$

(3.12)

$$M_{\text{MF}}^A = \frac{1}{N} \frac{\partial \Omega_S}{\partial J^A m^A},$$

(3.13)

$$M_{\text{MF}}^B = \frac{1}{N} \frac{\partial \Omega_S}{\partial J^B m^B}.$$  

(3.14)

They are also derived from $\partial \Omega/\partial M^A = \partial \Omega/\partial M^B = \partial \Omega/\partial m^A = \partial \Omega/\partial m^B = 0$. In terms of $m_t$, $m_r$, $M_f$ and $M_5$, the MF values are given as

$$m_{t,\text{MF}} = \frac{1}{N} \frac{\partial \Omega_e}{\partial M_f} = -\frac{1}{N} \sum_k \left[ \frac{M_f + \sqrt{d_s^2 + M_5^2}}{e_{1k}} n_F(E_{1k}) + \frac{M_f - \sqrt{d_s^2 + M_5^2}}{e_{2k}} n_F(E_{2k}) \right],$$

(3.15)

$$m_{r,\text{MF}} = \frac{1}{N} \frac{\partial \Omega_e}{\partial M_5} = -\frac{1}{N} \sum_k M_5 \left[ \frac{1 + M_f/\sqrt{d_s^2 + M_5^2}}{e_{1k}} n_F(E_{1k}) + \frac{1 - M_f/\sqrt{d_s^2 + M_5^2}}{e_{2k}} n_F(E_{2k}) \right],$$

(3.16)

$$M_{f,\text{MF}} = -\frac{1}{2} e S \left[ J^A B_S (S \beta J^A m^A) + J^B B_S (S \beta J^B m^B) \right],$$

(3.17)

$$M_{5,\text{MF}} = -\frac{1}{2} e S \left[ J^A B_S (S \beta J^A m^A) - J^B B_S (S \beta J^B m^B) \right].$$

(3.18)
where $n_F(E) = 1/(1 + e^{\beta E})$ is the Fermi distribution function and $B_S$ is the Brillouin function.

Since we are interested in the dynamics with respect to $M_f$ and $M_5$ around possible stationary points, we put the MF values for the electron spins $m_t$ and $m_r$ and define the effective action for $M_f$ and $M_5$ as

$$\Omega|_{m_t=m_t, MF, m_r=m_r, MF} \equiv -\beta^{-1} \ln e^{-S_{\text{eff}}}.$$ (3.19)

Consequently the effective potential for $M_f$ and $M_5$ is given by

$$V_{\text{eff}}(M_f, M_5) = \frac{1}{\beta V} S_{\text{eff}} = \frac{1}{V} \Omega|_{m_t=m_t, MF, m_r=m_r, MF},$$ (3.20)

where $V$ is the volume of the system. Here we have omitted the kinetic terms for the fluctuation around the stationary values for $M_f$ and $M_5$. Derivation of the kinetic term is given in the Appendix D. We will use the effective potential and the kinetic term to calculate the axion mass in Sec. 5.

4 Magnetic states

Let us see possible magnetic states, which is determined by the grand potential or equivalently the effective potential given in Eq. (3.20). Fig. 1 shows the effective potential on $(M_f, M_5)$ plane for various values of temperature. In the calculation we take the model parameters as those proposed by the first-principles calculation [1,22, 25,29] and the values are given in the figure caption. In the figure we plot the effective potential normalized as $\tilde{V}_{\text{eff}} \equiv (V_{\text{eff}}(M_f, M_5) - V_{\text{eff}}(0,0))\ell^3$. For $J^A = J^B > 0$ we found that the global minimum of the potential corresponds to $M_f = 0$ and nonzero $M_5 = M_{50}$. Here $M_{50}$ is the stationary value for $M_5$. At the zero temperature limit, $|M_{50}| = xSJ^A$ is expected from Eq. (3.18), which is consistent with the figure. It is also clear that the minimum is stable. This is also checked analytically, which is shown in Appendix C. At the minimum $m_A \simeq -m_B$ is realized, which means that the magnetic order of the electrons is the AFM. The same is true for $M^A$ and $M^B$, i.e. $M^A \simeq -M^B$. The AFM disappears for temperature above the critical temperature $T_{c}^{\text{AFM}}$, which is around 80 K in the figure. In the region $T > T_{c}^{\text{AFM}}$, the global minimum is at the origin. Namely all the MF values are zero and the insulator becomes paramagnetic state.

#6In Appendix B we give another aspect of the definition of the effective action.
for potential as function of $M$. When the temperature gets even higher, the global minimum eventually reduces to $M = 0$ at a sufficiently low temperature and it disappears for $T \gtrsim 10$ K. When the temperature gets even higher, the global minimum eventually reduces to $(M_f, M_5) = (0, 0)$. We note that the result that the AFM state is the ground state while there is a metastable FM state is consistent with the first-principles’ calculation for Mn$_2$Bi$_2$Te$_5$ [21].
The result that the AFM state is lower than the FM one can be confirmed analytically as follows. The total energy is calculated from the free energy,
\[ E = \frac{\partial}{\partial \beta} \beta \Omega + \mu N n = E_e + E_S + H_R, \]  
where \( N n = - \frac{\partial \Omega}{\partial \mu} \) and
\[ E_e = \sum_{j,k} (E_{j,k} + \mu) n_F(E_{j,k}), \]  
\[ E_S = -N_S S \left[ J^A m^A B_S (S \beta J^A m^A) + J^B m^B B_S (S \beta J^B m^B) \right]. \]  
Taking the MF values for \( M^A \) and \( M^B \) at zero temperature limit, it is simply given by
\[ E = E_e = -\sum_k (e_{1k} + e_{2k}). \]  
From Eqs. (2.22) and (2.23), it is straightforward to check that \( E|_{M_f=0,M_5=M} - E|_{M_f=M, M_5=0} < 0 \) for any values of \( M \) and \( k \). This is why the AFM is the lowest energy state.

To get the whole picture, we plot the phase diagram regarding the magnetic order on \((M_0,T)\) plane in Fig. 3. Shaded region shows the AFM or FM states. In
Figure 3: Phase diagram of the magnetic state. The AFM state and metastable FM state are indicated as “AFM” and “FM*”, respectively. Here $J^A, J^B, S, x, A_i$, and $B_i (i = 1, 2)$ are taken as the same as Fig. 1. $T_c^{AFM}$ is the critical temperature of the AFM state and the region $T < T_c^{AFM}$ the AFM state becomes the global minimum. $T_c^{FM*}$ is the critical temperature between the metastable FM state and the AFM state. As a reference, we indicate the topological and normal phases of insulator as ‘TI’ and ‘NI’, respectively, which is separated by a vertical line $M_0 = 0$ (green dashed).

the low temperature below $\mathcal{O}(10^2 \text{K})$, the magnetic state is the AFM. On the other hand, at sufficiently low temperature that is less than $\mathcal{O}(10 \text{K})$, the metastable FM state appears. Here we denote $T_c^{FM*}$ as the critical temperature. We note that the stable AFM state also exists at the temperature, which indicates a possible phase transition between the metastable FM state and the AFM state. While the critical temperatures $T_c^{AFM}$ and $T_c^{FM*}$ depend on the value of $M_0$, the sign of $M_0$, i.e., topological phase or not, does not have a significant impact on them. In the next section, we compute the mass of dynamical axion for the AFM and the FM states.

5 Axion mass

As discussed in Ref. [15], the dynamical axion field is defined as the quantum fluctuation around the minimum of the potential in $M_5$ direction. As shown in the
previous section there are two possible minima; the AFM and metastable FM states. Expanding $M_5$ as $M_5 \equiv M_{50} + \varphi$ around the minima, the axion field $a$ is defined as

$$V_{\text{eff}} = V_{\text{eff}}(M_{f0}, M_{50}) + \frac{1}{2} g^2 \frac{\partial^2 V_{\text{eff}}}{\partial M_5^2} \bigg|_{M_f=M_{f0}, M_5=M_{50}} a^2 + O(a^4). \quad (5.1)$$

Here $g = d\Phi/d\theta \big|_{\theta=\theta_0}$ where $\Phi(\theta) = M_5$ is the inverse function of $\theta$ defined by [1]

$$\theta(M_5) = \frac{1}{4\pi} \int d^3k \sum_{\alpha=1}^5 d^2 \phi_\alpha \epsilon^{ijkl} d^i \partial_{k_x} d^j \partial_{k_y} d^k \partial_{k_z} d^l. \quad (5.2)$$

In the expression we define $|d|^2$ as $|d|^2 \equiv \sum_{\alpha=1}^5 d^a d^a$ where $d^a = M_5$ and $\epsilon^{ijkl}$ is Levi-Civita symbol with $i, j, k, l$ being 1, 2, 3, and 5. A parameter $\theta_0$ satisfies $\Phi(\theta_0) = M_{50}$. Then the mass $m_a$ of the dynamical axion is given by

$$K_\alpha m_a^2 = \frac{1}{2V} \sum_k \frac{d_0^2}{(d_0^2 + M_{50}^2)^{5/2}}, \quad (5.3)$$

where $K_\alpha$ is the stiffness. For reference, see Appendix C for the analytic expression of the second derivative of $V_{\text{eff}}$ in the zero temperature limit, which we have checked the consistency with the spin susceptibility. The stiffness is given by the perturbative expansion with respect to $\varphi$. The details are given in Appendix D and the result is

$$K_\alpha = \frac{1}{V} \sum_k \frac{d_0^2}{4(d_0^2 + M_{50}^2)^{5/2}}, \quad (5.4)$$

for the AFM states and

$$K_\alpha = \frac{1}{V} \sum_k \frac{(d_0^2 - d_5^2 + M_{f0}^2)(e_{2k} - e_{1k}) + dsM_{f0}(e_{1k} + e_{2k})}{8ds^3M_{f0}e_{1k}e_{2k}}, \quad (5.5)$$

for the FM states. It is clear that the functions in the summation are positive, irrespective of the wavenumber. From Eqs. (5.3), (5.4), and (5.5), we evaluate the axion mass.

As shown in the previous section, there are two possible magnetic states, the AFM state and metastable FM state. Thus we evaluate the axion mass for both states. Fig. 4 shows the axion mass on $(M_0, T)$ plane for the AFM state and the metastable FM state. We found that the axion mass is $O(eV)$ for both states, except for the phase boundaries. This result is consistent with Ref. [15] where only the AFM state is considered at the zero temperature in the Hubbard model. Here we see a mild dependence of the mass on the sign of $M_0$. At the phase boundaries, the axion mass approaches to zero from the AFM state to paramagnetic state or from the metastable
Figure 4: Color map of the axion mass under the AFM state (left) and the metastable FM state (right). Here $J^A$, $J^B$, $S$, $x$, $A_i$, and $B_i$ ($i = 1, 2$) are taken as the same as Fig. 1. As Fig. 3, topological and normal phases are indicated as “TI” and “NI”, respectively.

FM state to the AFM state. Therefore the axion mass can be in principle various value by optimizing the temperature. This result is quantitatively consistent with Ref. [27], meanwhile typical value of the axion mass is different. The typical energy of the mass given is determined by the energy band, and it is not sensitive to the value of the band gap, which is a different feature from the results in the Hubbard model [15].

It is worth noting that there are two types of axion for the AFM and FM states. They could be utilized in the future particle axion search. For example, we speculate that in the circumstance of the FM state, particle axion induces an excitation of the dynamical axion and it may cause the phase transition to the AFM state, which can be a possible signal of the axion detection.

As we mentioned, the axion mass is not severely influenced by the topology of the insulators. This is true for both the AFM and the metastable FM states. Therefore, various insulators that are not in the topological phase are also possible candidates of material for the searches of particle axion and axion-like particles.
6 Conclusion

In this study we have formulated the mass of the dynamical axion in the magnetically doped topological insulators. To this end, we consider the 3D effective model of TIs with the interaction terms between the electrons and the impurities. We have found that the antiferromagnetic state is the ground state at low temperature. Besides, the ferromagnetic state appears as metastable state under sufficiently low temperature. In both magnetic states, the axion mass is found to be $\mathcal{O}(\text{eV})$ and it goes to zero as the temperature approaches to the critical temperature, i.e. the phase boundary. In addition, we have found a mild dependence of the axion mass on the topology of insulators; it tends to be suppressed in the topological insulator phase.

The fact that the axion mass can be controlled by temperature is suitable for the detection of particle axion. Especially the phase boundary has a potential to search particle axion with a suppressed mass. In addition, there can be various magnetic states indicated in first-principles’ calculation, for example, in MnBi$_2$Te$_4$ [16–20] or Mn$_2$Bi$_2$Te$_5$ [21]. In order to describe such rich magnetic states rather than the AFM or FM, we need further extension of the model, which would be another interesting research to find out the mass of the dynamical axion in a more complicated phase diagram. We leave it for the future work.

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A Gamma matrices

The Gamma matrices $\Gamma^a$ ($a = 1, \cdots, 4$) in Eq. (2.2) are defined as

$$
\Gamma^1 = \begin{pmatrix} 0 & \sigma^1 \\ \sigma^1 & 0 \end{pmatrix}, \quad \Gamma^2 = \begin{pmatrix} 0 & \sigma^2 \\ \sigma^2 & 0 \end{pmatrix}, \quad \Gamma^3 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \Gamma^4 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.
$$

(A.1)
Γ⁵ is defined by Γ⁵ = −Γ¹Γ²Γ³Γ⁴. In addition we define Γ^{ab} = [Γ^a, Γ^b]/(2i). To be explicit, they are given by

\begin{align*}
Γ^5 &= \begin{pmatrix} 0 & σ^3 \\ σ^3 & 0 \end{pmatrix}, \quad Γ^{12} = \begin{pmatrix} σ^3 & 0 \\ 0 & σ^3 \end{pmatrix}.
\end{align*}

(A.2)

In the sublattice basis, the Gamma matrices are given by

\begin{align*}
Γ^{1'} &= \begin{pmatrix} σ^1 & 0 \\ 0 & -σ^1 \end{pmatrix}, \quad Γ^{2'} = \begin{pmatrix} σ^2 & 0 \\ 0 & -σ^2 \end{pmatrix}, \quad Γ^{3'} = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad Γ^{4'} = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix},
\end{align*}

(A.3)

\begin{align*}
Γ^{5'} &= \begin{pmatrix} σ^3 & 0 \\ 0 & -σ^3 \end{pmatrix}, \quad Γ^{12'} = \begin{pmatrix} σ^3 & 0 \\ 0 & σ^3 \end{pmatrix}.
\end{align*}

(A.4)

\section*{B Effective action}

Since we consider the half-filling case, i.e., the number of electrons is fixed, the grand potential \(Ω_e(M^A, M^B)\) of the electron part corresponds to the Helmholtz free energy \(F_e(M^A, M^B)\). The Gibbs free energy \(G_e(m^A, m^B)\) is then given by the Legendre transformation:

\begin{align*}
G_e(m^A, m^B) &= - \sum_{I=A,B} \frac{\partial F_e}{\partial M^I} M^I + F_e \\
&= -N \sum_{I=A,B} J^I m^I M^I + F_e, \quad (B.1)
\end{align*}

where \(m^I \equiv (1/N) \partial F_e/\partial J^I M^I\) (\(I = A, B\)). This definition is equivalent to the MF values for \(m^A\) and \(m^B\) given in Eqs. (3.11) and (3.12). In addition \(G_e(m^A, m^B)\) is equivalent to \(Ω_e + H_R\) where \(m^I\) are taken to be their the MF values. Since the Gibbs free energy corresponds to the effective action in the quantum field theory, Eq. (3.19) is considered as the effective action. In our analysis we give Eq. (3.19) as function of \(M_f\) and \(M_5\), i.e., \(m^I = m^I(M^I)\), instead of \(m^I\) itself since we are interested in the dynamical field around the minimum \((M_{f0}, M_{50})\).
C  The mass at zero temperature and spin susceptibility

At the zero temperature, the curvature around the minimum is computed analytically. The results are

\[
\frac{1}{2} \left. \frac{\partial^2 V_{\text{eff}}}{\partial M_f^2} \right|_{M_f=M_{f0},M_5=M_{50}} = \frac{1}{2} \sum_k \left( d_0^2 - d_s^2 \right) \left[ \frac{1}{e_{1k}^3} + \frac{1}{e_{2k}^3} \right] M_{f0},M_{50} = M_{f0},M_{50}. \tag{C.1}
\]

\[
\frac{1}{2} \left. \frac{\partial^2 V_{\text{eff}}}{\partial M_5^2} \right|_{M_f=M_{f0},M_5=M_{50}} = \frac{1}{2} \sum_k \left[ \frac{1 + M_f/d_s}{e_{1k}} + \frac{1 - M_f/d_s}{e_{2k}} \right] M_{f0},M_{50} = M_{f0},M_{50}. \tag{C.2}
\]

It is clear that both quantities are positive and we have checked that \( \frac{\partial^2 V_{\text{eff}}}{\partial M_f \partial M_5} \bigg|_{M_f=0,M_5=0} = 0 \) at the minimum. Therefore, the minimum is stable.

Above results can be confirmed by the spin susceptibility of electron computed in the linear response theory. In the magnetic TIs, the local spins have effective interaction via electrons. In the present case it corresponds to \( -\tilde{J}_f^e M_f M_5 \) and \( -\tilde{J}_5^e M_5 M_5 \), where normalized effective exchange couplings are given by \( \tilde{J}_f^e = -\chi_f^e \) and \( \tilde{J}_5^e = -\chi_5^e \) [28]. Here \( \chi_f^e \) and \( \chi_5^e \) are the Van Vleck type spin susceptibility for a band insulator. Namely \( \chi_f^e \) and \( \chi_5^e \) correspond to the squared mass parameters.

By taking \( \mathcal{H}_k^n \) as perturbation in the linear response theory they are calculated as

\[
\chi_f^e = \sum_{k,m,n} \left( n_F(E_{nk}) - n_F(E_{mk}) \right) \frac{\langle u_{nk} | \Gamma^{12} | u_{mk} \rangle \langle u_{mk} | \Gamma^{12} | u_{nk} \rangle}{E_{mk} - E_{nk}}, \tag{C.3}
\]

\[
\chi_5^e = \sum_{k,m,n} \left( n_F(E_{nk}) - n_F(E_{mk}) \right) \frac{\langle u_{nk} | \Gamma^5 | u_{mk} \rangle \langle u_{mk} | \Gamma^5 | u_{nk} \rangle}{E_{mk} - E_{nk}}, \tag{C.4}
\]

where \( |u_{nk}\rangle \) is the energy eigenstates of the electron. Therefore we expect that the curvatures at the origin in \( M_f \) and \( M_5 \) directions agrees with the susceptibilities \( \chi_f^e \) and \( \chi_5^e \), respectively. In fact we have checked that

\[
\frac{1}{2} \left. \frac{\partial^2 V_{\text{eff}}}{\partial M_f^2} \right|_{M_f=0,M_5=0} = \frac{1}{2} \sum_k \frac{1 - d_s^2/d_0^2}{d_0}, \tag{C.5}
\]

\[
\frac{1}{2} \left. \frac{\partial^2 V_{\text{eff}}}{\partial M_5^2} \right|_{M_f=0,M_5=0} = \frac{1}{2} \sum_k \frac{1}{d_0}. \tag{C.6}
\]


D Propagator and the stiffness

The stiffness is given by the coefficient of the axion kinetic term.\footnote{Ref. \cite{30} gives a similar calculation using Hubbard-Stratonovich transformation but to discuss topological superconductors and superfluids. See also Ref. \cite{31} for the renormalization group approach.} In order to give the kinetic term we consider a fluctuation of $M_5$ around the stationary point by promoting $M_5$ as a dynamical degree of freedom. To make the discussion generic, we take $M_5 = M_{50} + \varphi$. The kinetic term is obtained by expanding $S_e$ with respect to $\varphi$. To this end, we write $H_e = H + \delta H$. In the wavenumber space, they are defined as

$$H_k = H_k^{\text{TI}} + M_{f0} \Gamma^{12} + M_{50} \Gamma^5,$$

$$\delta H_k = \varphi \Gamma^5.$$

Using $\ln \det(\partial_\tau + H_e) = \text{Tr} \ln(\partial_\tau + H_e)$ and

$$\text{Tr} \ln(\partial_\tau + H + \delta H) = \text{Tr} \ln(-G^{-1}) - \sum_{n=1}^\infty \text{Tr}(G\delta H)^n,$$

where $G^{-1} = -\partial_\tau - H$, the kinetic term is obtained from the quadratic term in the second term of Eq. (D.3):

$$\text{Tr}(G\delta H)^2 = \frac{V^2}{N^2} \int_0^\beta d\tau_i \int_0^\beta d\tau_j \sum_{x_i, x_j} \text{Tr}[G(x_i - x_j) \delta H(x_j) G(x_j - x_i) \delta H(x_i)].$$

Here the arguments of $G$ and $\delta H$ represent $x_i = (\tau_i, x_i)$. The propagator and the field $\delta H$ are expanded as

$$G(x_i - x_j) = \frac{1}{\beta V} \sum_{i\omega_n} \sum_k \tilde{G}(k) e^{-i\omega_n(\tau_1 - \tau_2) + ik \cdot (x_i - x_j)},$$

$$\delta H(x_i) = \frac{1}{\beta V} \sum_{i\omega_n} \sum_k \tilde{\delta H}(k) e^{-i\omega_n \tau + ik \cdot x_i},$$

where $G^{-1}(k) = i\omega_n - H_k$. Similarly to $x_i$, we take the argument $k_i$ of $\tilde{G}$ and $\tilde{\delta H}$ as $k_i = (i\omega_n, k_i)$. Then

$$\text{Tr}(G\delta H)^2 = \frac{1}{\beta^2 V^2} \sum_{i\omega_n} \sum_{i\omega_n} \sum_{k_1, k_2} \text{Tr}[\tilde{G}(k_1) \tilde{\delta H}(k_2) \tilde{G}(k_1 - k_2) \delta H(-k_2)].$$

We find the propagator $\tilde{G}$ in the momentum space is given by

$$\tilde{G}(i\omega_n, q) = \frac{1}{F} \left[ (i\omega_n - \epsilon) g_0 + \sum_{a=1}^5 g_1^a \Gamma^a + \sum_{a=1}^4 g_2^a \Gamma^5 + \sum_{ab} g_{ab} \Gamma^{ab} \right].$$
where $\epsilon = \epsilon_0 - \mu$ and

\[
\begin{align*}
g_0 &= (i\omega_n - \epsilon)^2 - d_0^2 - M_{50}^2 - M_{f0}^2, \\
g_1^a &= -d^a\{-(i\omega_n - \epsilon)^2 + d_0^2 + M_{50}^2 + M_{f0}^2\} \quad (a = 1, 2), \\
g_2^a &= -d^a\{-(i\omega_n - \epsilon)^2 + d_0^2 + M_{50}^2 - M_{f0}^2\} \quad (a = 3, 4, 5), \\
g_1^2 &= 2id^2M_{50}M_{f0}, \\
g_2^2 &= -2id^1M_{50}M_{f0}, \\
g_3^2 &= 2i(i\omega_n - \epsilon)d^4M_{f0}, \\
g_4^2 &= -2i(i\omega_n - \epsilon)d^3M_{f0}, \\
g^{12} &= \{(i\omega_n - \epsilon)^2 - (d^1)^2 - (d^2)^2 + (d^3)^2 + (d^4)^2 + M_{50}^2 - M_{f0}^2\}M_{f0}, \\
g^{34} &= 2(i\omega_n - \epsilon)M_{50}M_{f0} \\
g^{33} &= 2d^1d^3M_{f0}, \\
g^{13} &= -2d^2d^3M_{f0}, \\
g^{14} &= -2d^2d^4M_{f0}, \\
g^{24} &= 2d^3d^4M_{f0}, \\
F &= \{(i\omega_n - \epsilon)^2 - |d_0|^2 - (M_{f0} - M_{50})^2\}\{(i\omega_n - \epsilon)^2 - |d_0|^2 - (M_{f0} + M_{50})^2\} - 4d_s^2M_{f0}^2. 
\end{align*}
\]

Using the propagator, the stiffness is given by

\[
K_a = -\frac{1}{2\beta V} \frac{\partial^2}{\partial(i\omega_n k)^2} \sum_{i\omega_n k} \text{Tr}[\tilde{G}(i\omega_n, k\epsilon)\Gamma^5\tilde{G}(i\omega_n + \epsilon, qk)\Gamma^5]|_{i\omega_n = 0}. 
\]

Here we have redefined $k_1$ and $k_2$ as $k_1 = q$ and $k_2 = -k$ and taken $k = 0$ in $\tilde{G}(q+k)$. This expression can be checked by taking $M_{f0} = 0$ to get

\[
K_a = \frac{1}{V} \sum_{q} \frac{d_0^2}{4(|d_0|^2 + M_{50}^2)^{5/2}}, 
\]

in the zero temperature limit, which agrees with one given in Ref. [15]. This is the expression of the stiffness for the AFM state. The FM state corresponds to nonzero $M_{f0}$ and $M_{50} = 0$. In that case, we find in the zero temperature limit

\[
K_a = \frac{1}{V} \sum_{q} \frac{(d_0^2 - d_s^2 + M_{f0}^2)(e_{2q} - e_{1q}) + dsM_{f0}(e_{1q} + e_{2q})}{8ds^3M_{f0}e_{1q}e_{2q}}, 
\]

where $M_s = 0$ is taken in $e_{1q}$ and $e_{2q}$. We note that the zero temperature limit is a good approximation since we discuss the system at up to $\mathcal{O}(10^2)$ K which is smaller than the typical energy scale of the electron energy.
The formalism given in the discrete space can be written in the continuum case by the following replacements,

\[
\frac{1}{N} \sum_i \rightarrow \frac{1}{V} \int d^3 x, \quad \frac{1}{V} \sum_k \rightarrow \int \frac{d^3 k}{(2\pi)^3},
\]  \hspace{1cm} (D.26)

\[
\sqrt{N} c_i \rightarrow \sqrt{V} \psi(x), \quad N n_i \rightarrow V n(x).
\]  \hspace{1cm} (D.27)

Here \( \psi \) is the wavefunction of electrons in the continuum space, \( n = \psi^\dagger \psi \), and \( n_i = c_i^\dagger c_i \).

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