Supplementary Material: Large dynamical axion field in topological antiferromagnetic insulator $Mn_2Bi_2Te_5$

Jinlong Zhang(张金龙),[1] Dinghui Wang(王丁辉),[2] Minji Shi(施敏吉),[2] Tongshuai Zhu(朱同帅),[2] Haijun Zhang(张海军),[2,3,*] and Jing Wang(王靖)[1,3,4,†]

[1] *State Key Laboratory of Surface Physics, Department of Physics, Fudan University, Shanghai 200433, China*
[2] *National Laboratory of Solid State Microstructures, School of Physics, Nanjing University, Nanjing 210093, China*
[3] *Collaborative Innovation Center of Advanced Microstructures, Nanjing 210093, China*
[4] *Institute for Nanoelectronic Devices and Quantum Computing, Fudan University, Shanghai 200433, China*

(Dated: June 16, 2020)

I. 100AFM CONTRIBUTION TO θ

The low energy physics of $Mn_2Bi_2Te_5$ is described by the massive Dirac model, which is similar to Eq. (1) of the main text. Therefore, in the following we use the notation in Eq. (1). From the discussion in the main text, we see that the Γ^5 term represents the staggered Zeeman field along z axis. There are other leading order $\mathcal{T},\mathcal{P}$-breaking perturbations such as $\sum_{i=1}^{3} m_i\Gamma^i$. In fact, the $m_{1,2}$ is from the in-plane AFM order, namely, from 100AFM and 010AFM. By taking these terms into account, now up to the quadratic term in $\mathbf{k}$, the effective model is

$$\mathcal{H}_{\text{Dirac}} = \epsilon_0(\mathbf{k}) + \sum_{a=1}^{5} d_a(\mathbf{k})\Gamma^a, \tag{1}$$

where $d_{1,2,3,4,5}(\mathbf{k}) = (Ak_x + m_1, Ak_y + m_2, Ak_z + m_3, m_4(\mathbf{k}), m_5)$. From the formula of θ of this model, m_5 gives the linear order contribution to θ as discussed in the main text. While the other masses $m_{1,2,3}$ give rise to high-order contribution to θ, as shown in Fig. 1. For simplicity, we set $m_1 = m_2 = m_3$. One can see that a nonzero m_5 deviates

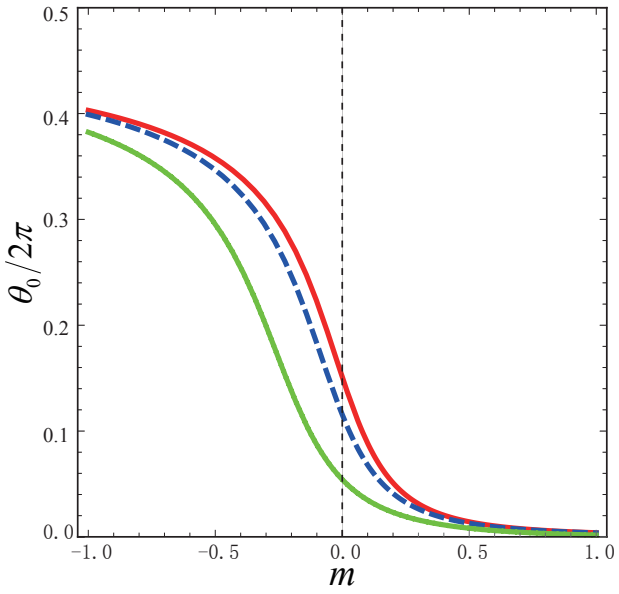

FIG. 1. Higher-order contribution to θ_0 from $m_{1,2,3}$ with finite m_5. The red, blue and green lines have $m_{1,2,3} = 0.0, 0.2, 0.4$. Other parameters are $m_5 = 0.2$, $A = 1.0$, $B = 0.5$.

* zhanghj@nju.edu.cn
† wjingphys@fudan.edu.cn

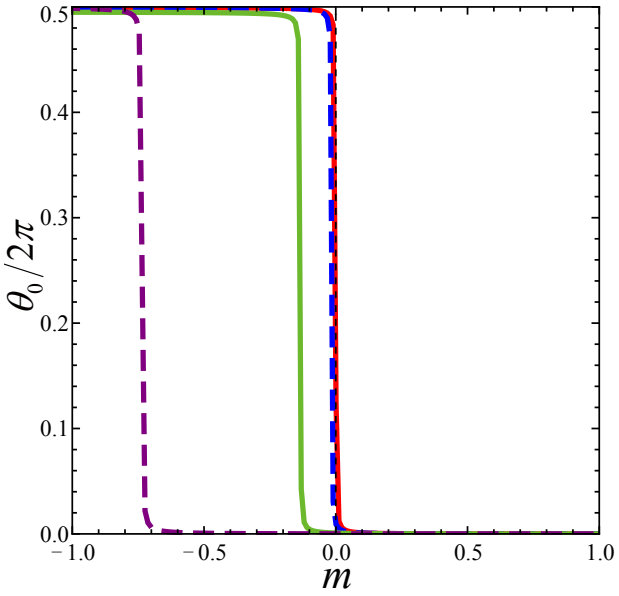

FIG. 2. Higher-order contribution to θ_0 from $m_{1,2,3}$ with vanishing m_5. The red, blue, green, purple lines have $m_{1,2,3} = 0.0, 0.1, 0.3, 0.7$. Other parameters are $A = 1.0$, $B = 0.5$.

θ_0 from π and 0 dramatically (red line), while adding the same finite magnitude of $m_{1,2,3}$ (blue line), θ_0 is almost the same as $m_{1,2,3} = 0$. Further increasing m_1 to be twice of m_5 leads to a small change of θ_0, compared to the θ_0 (from nonzero m_5) deviating from π.

We further set $m_5 = 0$ to see the deviating from π and 0 of θ_0 from $m_{1,2,3}$, which is shown in Fig. 2. One can see that $m_{1,2,3}$ shift the topological phase transition point from $m = 0$ to $m = -B(m_1^2 + m_2^2 + m_3^2)/A^2$. Besides of this, $m_{1,2,3}$ does not change the shape of θ_0 vs m. Further confirming the higher-order contributions to θ_0.

Moreover, we consider the effects from higher-order terms in $\mathcal{H}$ by setting $k \to \sin k$ and $k^2/2 \to 1 - \cos k$. These higher-order k terms only gives small quantitative changes to θ_0 and $1/g$. The conclusion of the main text remains valid.

II. FIRST-PRINCIPLES CALCULATIONS FOR ELECTRONIC AND MAGNETIC PROPERTIES

The first-principles calculations are performed with the Vienna ab initio simulation package (VASP) with projector augmented wave pseudopotentials [1, 2]. The exchange-correlation energy is described by the generalized gradient approximation (GGA) in the Perdew-Burke-Ernzerhof (PBE) parametrization. We set the energy cutoff to 410 eV for the plane-wave expansion. The optB86b-vdW van der Waals correction [3] is used to fully relax the primitive cells. A 10×10×6 **k**-mesh is used for the relaxation with the total energy tolerance 10^{-7} eV, and a $16 \times 16 \times 8$ **k**-mesh is used for self-consistent calculations. Spin-orbit coupling effect is included in self-consistent. To consider strongly correlated $3d$ electrons of Mn and $4f$ electrons of Eu, we use LSDA+U approach [4] in all calculations with the on-site Coulomb interaction U 3 eV for Mn and 7 eV for Eu.

The fitting parameter for 001AFM $Mn_2Bi_2Te_5$ is $C_0 = -7.033 \times 10^{-5}$ eV, $C_1 = -1.886$ eV·Å^2, $C_2 = 14.723$ eV·Å^2, $M_0 = -0.036$ eV, $M_1 = 14.26$ eV·Å^2, $M_2 = 0.142$ eV·Å^2, $A_1 = 1.618$ eV·Å, $A_2 = 2.729$ eV·Å, $B_0 = 0.0149$ eV.

III. AXION ELETRODYNAMICS

The 001AFM order in $Mn_2Bi_2Te_5$ can be obtained naturally from the strong screened Coulomb interaction of electrons. It can be modelled by an interacting Hamiltonian [5], in the basis of $(|\alpha,\uparrow\rangle, |\alpha,\downarrow\rangle, |\beta,\uparrow\rangle, |\beta,\downarrow\rangle)$, it can be written as

$$\mathcal{H}_{int} = U \sum_i (n_{i\alpha\uparrow} n_{i\alpha\downarrow} + n_{i\beta\uparrow} n_{i\beta\downarrow}) + V \sum_i n_{i\alpha} n_{i\beta}. \tag{2}$$

This first term represents the effective on-site repulsion U, and the second term is the effective inter-site repulsion V. Since the on-site and inter-site repulsions are from the Mn atoms, here the U and V is the effective interaction from Mn atoms projected on $|\alpha\rangle$ and $|\beta\rangle$. In the mean field approximation, the 001AFM order is developed if U dominates over V, which leads to $M_5 = -(2/3)UM_z^-$, where $M_z^- = (1/2)(\langle \mathbf{s}_{i\alpha}\rangle - \langle \mathbf{s}_{i\beta}\rangle)$ is the AFM order parameter.

The 001AFM phase also has amplitude and spin-wave excitations, which can induce the fluctuations of the axion field. The fluctuation of the Néel vector $\mathbf{M}^-$ can be generally written as $\mathbf{M}^- = \left(M_0^- + \delta M_z(\mathbf{r},t)\right)\hat{\mathbf{z}} + \delta M_x(\mathbf{r},t)\hat{\mathbf{x}} + \delta M_y(\mathbf{r},t)\hat{\mathbf{y}}$. To the linear order, it can be shown from symmetry analysis that the fluctuation of axion field only depends on δM_z, since θ is a pseudo-scalar. In other words, we have $\delta\theta(\mathbf{r},t) = \delta m_5(\mathbf{r},t)/g = -(2/3)U\delta M_z(\mathbf{r},t)/g$. The dispersion of the amplitude mode $\delta M_z(\mathbf{r},t)$ can be obtained in standard random-phase-approximation, leading to a massive axion field $\delta\theta(\mathbf{r},t)$. The effective action is

$$\begin{aligned}
&\mathcal{S}_{\rm tot} = \mathcal{S}_{\rm Maxwell} + \mathcal{S}_\theta + \mathcal{S}_{\rm axion} \\
&= \frac{1}{8\pi}\int d^3rdt(\epsilon\mathbf{E}^2 - \frac{1}{\mu}\mathbf{B}^2) + \frac{1}{2\pi}\frac{e^2}{h}\int d^3rdt\theta(\mathbf{r},t)\mathbf{E}\cdot\mathbf{B} \\
&+g^2J\int d^3rdt\left[(\partial_t\delta\theta)^2 - (v_i\partial_i\delta\theta)^2 - m_\theta^2\delta\theta^2\right],
\end{aligned} \tag{3}$$

where J, v_i and m_θ are the stiffness, velocity and mass of the spin wave mode δM_z. The third term describes the dynamics of the massive axion. Within the model we have adopted, the parameters J and m are given by

$$J = \int \frac{d^3k}{(2\pi)^3}\frac{d_i(\mathbf{k})d^i(\mathbf{k})}{16|d|^5}, \tag{4}$$

$$Jm_\theta^2 = \left(\frac{2}{3}UM_z^-\right)^2\int\frac{d^3k}{(2\pi)^3}\frac{1}{4|d|^3}, \tag{5}$$

where $|d| = \sqrt{\sum_{a=1}^5 d_a d^a}$ and the repeated index indicates summation with $i = 1,2,3,4$.

IV. EXPERIMENTAL PROPOSALS

The classical equation of motion for axion field can be obtained by variation in the action over θ as

$$\left(\partial_t^2 - v_i^2\partial_i^2 + m_\theta^2\right)\delta\theta + \frac{e^2}{h}\frac{1}{g^2J}\mathbf{E}\cdot\mathbf{B} = 0, \tag{6}$$

with $\mathbf{B} = \mathbf{B}_0$, $\mathbf{E}(t) = \mathbf{E}_{\rm ac}\sin(\omega t)\Theta(t)$. $\Theta(t)$ is a stepwise function. The initial condition $\delta\theta(0) = 0$, the solution is

$$\delta\theta(t) = \frac{1}{\omega^2 - m_\theta^2}\frac{e^2}{h}\frac{1}{g^2J}\mathbf{E}_{\rm ac}\cdot\mathbf{B}_0\sin(\omega t). \tag{7}$$

Therefore, the topological magnetization is

$$\begin{aligned}
\mathbf{M}_t &= -\frac{\theta}{2\pi}\frac{e^2}{h}\mathbf{E} \\
&= -\frac{1}{2\pi}\frac{e^2}{h}(\theta_0 + \delta\theta)\mathbf{E}_{\rm ac}\cdot\mathbf{B}_0\mathbf{E}_{\rm ac}\sin(\omega t) \\
&= a_1\sin(\omega t) + a_2\cos(2\omega t),
\end{aligned} \tag{8}$$

with

$$a_1 = -\frac{1}{2\pi}\frac{e^2}{h}\theta_0\mathbf{E}_{\rm ac}\cdot\mathbf{B}_0\mathbf{E}_{\rm ac}, \tag{9}$$

$$a_2 = \frac{1}{4\pi}\left(\frac{e^2}{h}\right)^2\frac{1}{\omega^2 - m_\theta^2}\frac{1}{g^2J}\left(\mathbf{E}_{\rm ac}\cdot\mathbf{B}_0\right)^2\mathbf{E}_{\rm ac}. \tag{10}$$

We can see that the amplitude of 2ω contribution is frequency dependent, which is divergent when $\omega \sim m_\theta$. This frequency dependent response will further distinguish DAF from static AFM order.

The AFM resonance frequency can be calculated by the equation of motion of the biparticle AFM system [6]. Here we only comment that since the microwave magnetic field used in AFM resonance is usually much smaller than the

magnetic anisotropy field. The AFM spins are always precessing around the easy z axis, which does not depend on the direction of the applied resonance magnetic field. This will always induce a change of δm^z, which further excites the axion dynamics.

The CME with a polarization current induced by AFM resonance is

$$\mathbf{j}(t) = -\frac{e^2 U}{3\pi g h}\mathbf{B}\sum_{j=\pm}\omega_j \delta m_j^z \sin(\omega_j t). \tag{11}$$

The maximum value of the CME is $|\mathbf{j}_{\max}| = (e^2U)/(3\pi gh)\mathbf{B}\omega_\pm \delta m_\pm^z$. For an estimation, with $\delta m^z/m_z \sim 0.02$, $\omega_\pm/2\pi = 300$ GHz, $B = 1$ T, $U = 25$ meV, $1/g = 0.03$ meV^{-1}, we have $|\mathbf{j}_{\max}| \sim 12$ A/cm^2, which is feasible in experiments.

[1] G. Kresse and J. Hafner, Phys. Rev. B **47**, 558 (1993).
[2] G. Kresse and D. Joubert, Phys. Rev. B **59**, 1758 (1999).
[3] J. Klimeš, D. R. Bowler, and A. Michaelides, J. Phys. Condens. Mattter **22**, 022201 (2009).
[4] S. Dudarev, G. Botton, S. Savrasov, C. Humphreys, and A. Sutton, Phys. Rev. B **57**, 1505 (1998).
[5] R. Li, J. Wang, X. L. Qi, and S. C. Zhang, Nature Phys. **6**, 284 (2010).
[6] A. Sekine and K. Nomura, Phys. Rev. Lett. **116**, 096401 (2016).