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Reply to "Comment on 'Chiral gauge field and axial anomaly in a Weyl semimetal'"

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Recently, the Comment by Zhang et.al. questions our results of anomaly equations. In this Reply, we provide detailed derivation of anomaly equations from microscopic models and explain the reason why we respectfully disagree with the derivation and argument in the Comment.

In the Comment by Zhang *et al*, the authors proposed an alternative form for the anomaly equations (Eqs. (5)) and (6) in the Comment), which is based on the effective theory of Weyl fermions. Unfortunately, we found their derivation unconvincing. The correct form of the anomaly equation should coincide with the prediction of electromagnetic response from the microscopic theory (at ultraviolet cut-off) of Wevl semi-metals. Different from high energy physics in which the microscopic theory at the ultraviolet cut-off scale is unknown, the microscopic theory for Weyl semi-metals as condensed matter systems is well-defined and well-known. Therefore, the most unambiguous way to determine the response properties is to study the microscopic theory. The Hamiltonian of the four-band model shown by Eq. (4), as well as Appendix A in our paper¹ can be used to describe such a type of microscopic theory. Below, we provide our reply by employing this "microscopic" model to derive the effective magneto-electric response for Weyl fermions below and demonstrate the physics of anomaly equations directly from microscopic Hamiltonian.



FIG. 1. The energy dispersion of Weyl semi-metals is shown along the k_z direction. Weyl fermions are located at $\pm K_0$ and the momentum regions I and II are labelled.

We consider a simplified Hamiltonian (the Hamiltonian

(A1) in the appendix)

$$H = \mathcal{M}\Gamma_5 + L_1k_z\Gamma_4 + L_2(k_y\Gamma_1 - k_x\Gamma_2) + U\Gamma_{12}, \ (1)$$

where $\mathcal{M} = M_0 + M_1 k_z^2 + M_2 (k_x^2 + k_y^2)$, $\Gamma_{1,2,3} = \sigma_{x,y,z} \tau_x$, $\Gamma_4 = \tau_y$, $\Gamma_5 = \tau_z$ and $\Gamma_{ab} = [\Gamma_a, \Gamma_b]/2i$ $(a, b = 1, \dots, 5)$. Here the magnetization is only assumed along the z direction, given by the U term, where $U = U_0 + \delta_z$ for a constant magnetization U_0 and a magnetic fluctuation δ_z along the z direction $(|\delta_z| \ll |U_0|)$. The eigen-energy of the Hamiltonian (1) is given by

$$E_{st} = s\sqrt{L_2^2(k_x^2 + k_y^2) + \left(\sqrt{\mathcal{M}^2 + L_1^2 k_z^2} + t|U|\right)^2}$$
(2)

with $s, t = \pm$. The band gap of the above Hamiltonian closes at $k_x = k_y = 0$ when the condition $\mathcal{M}^2 + L_1^2 k_z^2 = U^2$ is satisfied. This requires $|U_0| > |M_0|$. In this regime, the energy dispersion for two low energy bands is shown in Fig. 1. Two Weyl points are located at $K_0 = \frac{1}{L_1}\sqrt{U^2 - M_0^2}$. Thus, we can divide the whole momentum space into two regions (I and II shown in Fig. 1). In the region-I, the energy dispersion behaves linearly and can be well described by the effective model of Weyl fermions. Here we have assume that the energy dispersion in the x-y plane is well described by linear dispersion up to the large momentum cut-off Λ_{∞} (M₂ is small). The details of projecting the Hamiltonian into the low energy space to obtain Weyl fermions as an effective model has been well discussed in the appendix A of the paper¹. In the region-II, the quadratic term (k_z^2) is larger than the linear term and thus we cannot use the effective Hamiltonian of Weyl fermions to describe this system. This corresponds to the high energy part. We choose the momentum that separates the region-I and II as Λ_0 . Thus, the region-I includes the momentum range $k_z \in [-K_0 - \Lambda_0, -K_0 + \Lambda_0]$ and $k_z \in [K_0 - \Lambda_0, K_0 + \Lambda_0]$, while the region-II includes the momentum range $k_z \in [-\Lambda_{\infty}, -K_0 - \Lambda_0]$ and $k_z \in [-K_0 + \Lambda_0, K_0 - \Lambda_0]$ and $k_z \in [K_0 + \Lambda_0, \Lambda_\infty]$. We assume $K_0 \gg \Lambda_0$, which means two Weyl points are well separated so that the low energy description of Weyl fermions is valid. Now let's consider the chemical potential is quite close to the Weyl points, and thus only crosses the bands in the region-I and lies in the band gap of the region-II. The total charge and current of the

system can be written as:

$$j_{\rm tot}^{\mu} = j_I^{\mu} + j_{II}^{\mu},$$
 (3)

where $\mu = 0$ labels the charge density and $\mu = 1, 2, 3$ labels the spatial components of the current, while j_{I}^{μ} and j_{II}^{μ} give the contribution from the region-I and II, respectively. The current j_{μ} in our paper is exactly j_{I}^{μ} here. Although the chemical potential in the region-II lies in the band gap, the adiabatic charge and current response, which comes from the contribution from the occupied bands below the energy gap, still exist and direct calculation shows that

$$j_{II}^{\mu} = \frac{e^2}{h} (2K_0 - 2\Lambda_0) \epsilon^{\mu\nu\lambda} \partial_{\nu} A_{\lambda}, \qquad (4)$$

where $\mu, \nu, \lambda = 0, 1, 2$. This contribution from the high energy part of the Weyl semi-metals is nothing but the anomalous Hall effect and the chiral magnetic effect, described in literature^{2,3}. We further expand K_0 for a small δ_z and find

$$K_0 = \frac{1}{L_1} \sqrt{U_0^2 - M_0^2} + \frac{U_0}{L_1 \sqrt{U_0^2 - M_0^2}} \delta_z.$$
 (5)

We define $a_3 = -\frac{2\pi U_0}{L_1\sqrt{U_0^2 - M_0^2}}\delta_z$ and $C_3 = -\frac{2\pi}{L_1}\sqrt{U_0^2 - M_0^2}$, where C_3 is a constant while a_3

fluctuates in space-time. Thus, we have

$$\partial_{\mu}j_{II}^{\mu} = -\frac{1}{2\pi^{2}}\epsilon^{\mu\nu\lambda}\partial_{\mu}a_{3}\partial_{\nu}A_{\lambda}$$
$$= -\frac{1}{8\pi^{2}}\epsilon^{\mu3\nu\lambda}f_{\mu3}F_{\nu\lambda}, \qquad (6)$$

where we add an additional superscript 3 into the Levi-Civita symbol. Furthermore due to the total charge conservation:

$$\partial_{\mu}j^{\mu}_{\rm tot} = 0 \tag{7}$$

we have

$$\partial_{\mu}j_{I}^{\mu} = -\partial_{\mu}j_{II}^{\mu} = \frac{1}{8\pi^{2}}\epsilon^{\mu3\nu\lambda}f_{\mu3}F_{\nu\lambda},\qquad(8)$$

This is nothing but our anomaly equation for the effective model of Weyl fermions by noting that j_I^{μ} is exactly j_{μ} in Ref. 1. The axial gauge field $(a_3 \text{ field})$ is proportional to the \hat{z} -directional magnetic fluctuation. More generally, when \hat{x} and \hat{y} direction magnetic fluctuations exist, similar derivation can give rise to the full anomaly equation

$$\partial_{\mu}j_{I}^{\mu} = -\partial_{\mu}j_{II}^{\mu} = \frac{1}{8\pi^{2}}\epsilon^{\mu\rho\nu\lambda}f_{\mu\rho}F_{\nu\lambda}.$$
(9)

Our itemized responses to the Comment by Zhang et al are listed below.

1) The main misunderstanding in the Comment is the charge conservation in Weyl semi-metals. Obviously, the charge conservation should be satisfied in the level of "*mi*croscopic" model, as illustrated in the above derivation and Eq. (7). However, if we consider the low energy effective theory of Weyl fermions (the Weyl Hamiltonian Eq. (1) in our paper¹), it is not necessary for charge to be conserved since the high energy states in Weyl semi-metal materials, which is *not* included in the long-wavelength effective Weyl Hamiltonian, can also contribute to charge and current response. In other words, the full electronic transport of Weyl semimetals should be contributed by both low-energy part in region-I (described by the two Weyl points as well as their Dirac-type Hamiltonian) and the high-energy parts in region-II from occupied bands. The anomalous Hall contribution from the high-energy parts is general for Weyl semimetals, as discussed in Ref. 2. Normally, such high energy contribution is taken into account through regularization procedure, which, in any case, should be consistent with the results from the microscopic model in order to correctly describe Weyl semimetals, in particular the Hall current contributions of the Weyl semi-metals. The Comment does not give any derivation of the anomalous Hall current, but refers to the Ref. 3 (Ref. [5] in the Comment) for the anomalous Hall contribution. The Eqs. (34) and (35) in Ref. 3 is consistent with our derivation when axial gauge potential $(b_{\mu}$ field in Ref. 3) is a constant, but this paper does not concern the case when axial gauge potential has smooth spatial and temporal dependence. Our derivation suggests that the Eqs. (34) and (35) in Ref. 3 remain valid even when axial gauge field strength exists. Physically, the spatial part of axial gauge field is proportional to the distance between two Weyl points, and its variation in space-time can give rise to the change of Hall response in the region-II. Since the total current should be conserved. the magnetoelectric response of Weyl fermions (region-I) should vary accordingly. Such type of response is missing in the anomaly equation (5) in the Comment.

2) The authors of the Comment derive their anomaly equations from the Fujikawa's method. However, we find that their derivation is confusing and the description is unclear. Let us address several issues below: (a). The authors of the Comment only derived the axial current, but did not show any derivation of the charge current part. (b). The anomaly equation of Eq. (10) in the Comment includes η and is not topological. The authors only argue that this term should not exist, but did not show any rigorous derivation about that.

3) The discussion about axial electric field in the last two paragraphs of the Comment is confusing. The authors seem to admit that the axial field can contribute to anomalous Hall current, according to the statement "Instead, the cross coupling between vector gauge fields A_{μ} and axial gauge fields a_{μ} should contribute to normal charge currents" and "but the axial gauge fields can change the strength of these effects". However, it is clear that the anomaly equation (5) in the Comment cannot describe these effects. On the other hand, such type of electromagnetic response can be included in our anomaly equation. As we stated at the beginning, a correct form of anomaly equation from effective theory should reproduce

the prediction from the microscopic theory. Thus, we believe the electromagnetic reponse of Weyl semi-metals

should be correctly described by the anomaly equation in our original paper.

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