

Supplementary Information: Emergent chirality-dependent electromotive force in Weyl semimetals enabled by generalized unitary transformation

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1 S1: Detailed derivation of the generalized unitary transformation

The original Hamiltonian describing low-energy electrons around the Weyl nodes is:

$$H = sv_f(\vec{p} \cdot \vec{\sigma}) - J\vec{M}(\vec{r}, t) \cdot \vec{\sigma} \quad (1)$$

1.1 S1.1: Spin-rotation transformation U_θ

Using the unitary transformation operator in the form

$$U_\theta = \exp\left(\frac{-i\theta(x)\sigma_x}{2}\right), \quad (2)$$

gives the transformed wave-function as

$$\psi' = U_\theta\psi, \quad (3)$$

then the original Schrödinger equation

$$H\psi = i\hbar \frac{\partial}{\partial t} \psi, \quad (4)$$

can be converted to

$$\begin{aligned} U_\theta H U_\theta^{-1} \psi' &= i\hbar U_\theta \frac{\partial}{\partial t} (U_\theta^{-1} \psi') \\ &= i\hbar U_\theta \left(\frac{\partial U_\theta^{-1}}{\partial t} \right) \psi' + i\hbar U_\theta U_\theta^{-1} \frac{\partial \psi'}{\partial t} \\ &= i\hbar U_\theta U_\theta^{-1} \frac{i\sigma_x}{2} \frac{\partial \theta}{\partial t} \psi' + i\hbar \frac{\partial \psi'}{\partial t}, \end{aligned} \quad (5)$$

we can write

$$\begin{aligned} U_\theta H U_\theta^{-1} \psi' &= \\ U_\theta \left[s v_f (p_x \sigma_x + p_y \sigma_y + p_z \sigma_z) - J M \hat{n} \cdot \sigma \right] U_\theta^{-1} \psi' \\ &= -\hbar \frac{\sigma_x}{2} \frac{\partial \theta}{\partial t} + i\hbar \frac{\partial \psi'}{\partial t} \end{aligned} \quad (6)$$

$$\begin{aligned} &\left[s v_f \left(e^{-\frac{i\sigma_x \theta}{2}} p_x \sigma_x e^{\frac{i\sigma_x \theta}{2}} + e^{-\frac{i\sigma_x \theta}{2}} p_y \sigma_y e^{\frac{i\sigma_x \theta}{2}} + \left(e^{-\frac{i\sigma_x \theta}{2}} p_z \sigma_z e^{\frac{i\sigma_x \theta}{2}} \right) - J M \sigma_z \right] \psi' \\ &= \frac{-\hbar}{2} \sigma_x \frac{\partial \theta}{\partial t} \psi' + i\hbar \frac{\partial \psi'}{\partial t} \end{aligned} \quad (7)$$

Transformation operator U_θ is supposed in a way that rotates spins at point x inside the wall that converts the non-collinear magnetic configuration to the collinear magnetic structure along the z axis:

$$U_\theta \sigma \cdot n(x) U_\theta^{-1} = \sigma_z \quad (8)$$

Consequently, the other terms of Hamiltonian under the transformation become:

$$\begin{aligned} U_\theta p_x \sigma_x U_\theta^{-1} &= e^{-\frac{i\sigma_x \theta}{2}} p_x \sigma_x e^{\frac{i\sigma_x \theta}{2}} \\ &= e^{-\frac{i\sigma_x \theta}{2}} p_x e^{\frac{i\sigma_x \theta}{2}} \sigma_x \\ &= \left(\frac{\hbar}{2} \cdot \frac{\partial \theta}{\partial x} \sigma_x + p_x \right) \sigma_x \end{aligned} \quad (9)$$

$$\begin{aligned} U_\theta p_y \sigma_y U_\theta^{-1} &= p_y e^{-\frac{i\sigma_x \theta}{2}} \sigma_y e^{\frac{i\sigma_x \theta}{2}} \\ &= p_y (\sin \theta \sigma_z + \cos \theta \sigma_y) \end{aligned} \quad (10)$$

$$\begin{aligned}
U_\theta p_z \sigma_z U_\theta^{-1} &= p_z e^{\frac{-i\sigma_x \theta}{2}} \sigma_z e^{\frac{i\sigma_x \theta}{2}} \\
&= p_z (\cos \theta \sigma_z - \sin \theta \sigma_y)
\end{aligned} \tag{11}$$

Substituting Eqs. (9)–(11) into Eq. (7), the transformed Schrödinger equation becomes:

$$\begin{aligned}
\left[sv_f \left(\frac{\hbar}{2} \cdot \frac{\partial \theta}{\partial x} \sigma_x + p_x \right) \sigma_x + p_y (\sin \theta \sigma_z + \cos \theta \sigma_y) + p_z (\cos \theta \sigma_z - \sin \theta \sigma_y) - JM \sigma_z \right] \psi' \\
= -\hbar \frac{\sigma_x}{2} \frac{\partial \theta}{\partial t} + i\hbar \frac{\partial \psi'}{\partial t}
\end{aligned} \tag{12}$$

1.2 S1.2: Dimensionality-reduction transformation U_λ

In contrast to the exchange interaction, which has been transformed into a collinear effective Hamiltonian, the nature of spatial dependence of θ means that the U_θ -transformation cannot change the spin-momentum coupling term into a collinear diagonalizable operator. Nonetheless, we can address the transverse direction in momentum space by applying a new transformation, U_λ , which removes the p_y and p_z dependent component of the Hamiltonian. This transformation is defined as:

$$U_\lambda = \exp(i\lambda(p_y y + y p_y + p_z z + z p_z)) \tag{13}$$

$$\psi'' = \exp(i\lambda(p_y y + y p_y + p_z z + z p_z)) \psi' \tag{14}$$

As a result

$$\psi' = \exp(-i\lambda(p_y y + y p_y + p_z z + z p_z)) \psi'' \tag{15}$$

It can be shown that:

$$\begin{aligned}
U_\lambda p_i U_\lambda^{-1} &= e^{i\lambda(p_i r_i + r_i p_i)} p_i e^{-i\lambda(p_i r_i + r_i p_i)} \\
&= p_i + i\lambda(2i\hbar p_i) + \frac{(i\lambda)^2}{2!} (2i\hbar)^2 p_i + \frac{(i\lambda)^3}{3!} (2i\hbar)^3 p_i + \dots \\
&= \left(1 - 2\hbar\lambda + \frac{(2\hbar\lambda)^2}{2!} - \frac{(2\hbar\lambda)^3}{3!} + \dots \right) p_i \\
&= e^{(-2\hbar\lambda)} p_i,
\end{aligned} \tag{16}$$

where $i = y, z$ and $r_i = y, z$.

Owing to this fact, one can realize at the large positive λ that $U_\lambda p_y U_\lambda^{-1} \simeq 0$ and $U_\lambda p_z U_\lambda^{-1} \simeq 0$. Accordingly, it can be realized that:

$$(sv_f \left(\frac{\hbar}{2} \cdot \frac{\partial \theta}{\partial x} \sigma_x + p_x \right) \sigma_x + JM \sigma_z) \psi'' = i\hbar \frac{\partial \psi''}{\partial t} \tag{17}$$

Accordingly, the effective Hamiltonian can be given by:

$$H' = sv_f p_x \sigma_x + \left(\frac{\hbar}{2} \cdot \frac{\partial \theta}{\partial x}\right) \sigma_x - JM \sigma_z \quad (18)$$

2 S2: Berry phase calculation

Applying the reversed transformations defined in Section S1, eigenfunctions of the original Hamiltonian are given as:

$$\psi_{k_x^\pm} = e^{ik_x x} e^{\frac{i\sigma_x \theta}{2}} e^{-i\lambda(p_y y + y p_y + p_z z + z p_z)} \psi_{k_x^\pm}'' \quad (19)$$

Berry phase is defined as $\gamma^\pm = i \oint \langle \psi_\pm | \frac{\partial}{\partial r} | \psi_\pm \rangle dr$, where $i \langle \psi_\pm | \frac{\partial}{\partial r} | \psi_\pm \rangle$ is the Berry connection $A^\pm(\vec{r})$ and $\vec{r}$ is the atomic position. For each of the eigenstates, considering that integration is computable on a closed route including the magnetic wall along the system and a semicircular contour outside the system, and since only the routes with spatial variations of magnetization can contribute in the integration, the semicircular path does not contribute. Then we can write:

$$\gamma^\pm = i \int_c (\alpha_\pm^*, \beta_\pm^*) \left(ik_x + \frac{i\sigma_x}{2} \cdot \frac{\partial \theta}{\partial r} \right) \begin{pmatrix} \alpha_\pm \\ \beta_\pm \end{pmatrix} dr + i \int_0^L (\alpha_\pm^*, \beta_\pm^*) \left(ik_x + \frac{i\sigma_x}{2} \cdot \frac{\partial \theta}{\partial x} \right) \begin{pmatrix} \alpha_\pm \\ \beta_\pm \end{pmatrix} dx \quad (20)$$

Contribution of the first term in the integral is equal to zero and finally the Berry phase reads:

$$\gamma^\pm = -k_x L - (\alpha_\pm, \beta_\pm) [\theta(L, t) - \theta(0, t)] \quad (21)$$

In which L is the dimension of system along the x direction.

3 S3: Detailed SMF integration over occupied states

The spin-dependent motive force is:

$$\varepsilon^\pm = -\frac{\hbar}{e} \cdot \frac{d\gamma^\pm}{dt} \quad (22)$$

Supposing that the magnetic wall of substrate moves with velocity v_D and dynamics of the wall is considered by $x_0(t) = v_D t$, the SMF for a single state reads:

$$\varepsilon_{k_x, s}^+ = \frac{\hbar^2 s v_f k_x}{e} \cdot \frac{JM + E_{k_x}}{s^2 v_f^2 \hbar^2 k_x^2 + (JM + E_{k_x})^2} \cdot \frac{v_D}{d} \cdot \left(\text{sech}\left(\frac{L - v_D t}{d}\right) - \text{sech}\left(\frac{-v_D t}{d}\right) \right) \quad (23)$$

In large scale of system, $L \rightarrow \infty$, expression $\text{sech}\left(\frac{L - v_D t}{d}\right) \sim 0$, then the result can be written as:

$$\varepsilon_{k_x, s}^+ = \frac{\hbar^2 s v_f k_x}{e} \cdot \frac{JM + E_{k_x}}{s^2 v_f^2 \hbar^2 k_x^2 + (JM + E_{k_x})^2} \cdot \frac{v_D}{d} \cdot [-\text{sech}\left(\frac{-v_D t}{d}\right)] \quad (24)$$

The total spin-motive force is obtained by taking into account the occupied states of the band energy:

$$\begin{aligned}\varepsilon_{tot,s}^+ &= \sum_{k_x} \varepsilon_{k_x}^+ \\ &= \int \frac{L}{2\pi} dk_x \frac{\hbar^2 s v_f k_x}{e} \cdot \frac{JM + E^+}{(s v_f \hbar k_x)^2 + (JM + E^+)^2} \frac{v_D}{d} \cdot \text{sech}\left(\frac{v_D t}{d}\right)\end{aligned}\quad (25)$$

Considering $s^2 = 1$ and using the fact that $E_{k_x}^2 = \hbar^2 k_x^2 s^2 v_f^2 + J^2 M^2$ it can be understood that:

$$\begin{aligned}\varepsilon_{tot,s}^+ &= \int_0^{E_f} \frac{L dk_x}{2\pi} \cdot \frac{\hbar^2 s v_f k_x}{e} \frac{v_D}{d} \frac{JM + E^+}{E_{k_x,s}^2 - J^2 M^2 + (JM + E_{k_x,s})^2} \cdot (-\text{sech}\left(\frac{-v_D t}{d}\right)) \\ &= \frac{Ls}{2\pi e d} \cdot \frac{v_D}{v_f} \cdot \text{sech}\left(\frac{-v_D t}{d}\right) \int_0^{E_f} \frac{dE_{k_x}}{2}\end{aligned}\quad (26)$$

At the limit of steady state, time scale $t \sim \frac{L}{v_D}$, the final expression of spin-motive force of system is:

$$\varepsilon_{tot,s}^+ = \frac{s E_f}{2\pi e d} \frac{v_D}{v_f} e^{-\frac{L}{d}} \quad (27)$$