Supplemental Material: Gate-Tunable Lifshitz Transition of Fermi Arcs and Its Transport Signatures

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I. LATTICE MODEL FOR NUMERICAL CALCULATION

In this Section, we elucidate the model and parameters for the device sketched in Fig. 3(a) of the main text.

The numerical calculations reported in the main text are performed based on a lattice model derived from Eq. (1) in the main text. Such minimal model is firstly rotated by an angle θ about the y axis, or explicitly, $\tilde{H}(\boldsymbol{k}) = H(U_y^{-1}\boldsymbol{k})$ with $U_y(\theta) = \begin{pmatrix} \cos\theta & 0 & -\sin\theta \\ 0 & 1 & 0 \\ \sin\theta & 0 & \cos\theta \end{pmatrix}$. Then the mapping to a square lattice is obtained by $k_{i=x,y,z} \to a^{-1}\sin k_i a$ and $k_i^2 \to 2a^{-2}(1-\cos k_i a)$, with a the lattice constant of the fictitious cubic lattice. Performing Fourier transformation in both the x and y directions yields

$$H_W^{\text{latt}} = \sum_i \psi_i^\dagger H_{ii}\psi_i + \sum_i \psi_i^\dagger H_{i,i+\hat{x}}\psi_{i+\hat{x}} + \sum_i \psi_i^\dagger H_{i,i+\hat{y}}\psi_{i+\hat{y}} + H.c., \tag{S1}$$

where $\psi_i = (\psi_{1,i}, \psi_{2,i})^{\mathrm{T}}$ are the Fermi operators with two pseudospin components, and the on-site and nearest-neighbor hopping matrices are

$$\begin{aligned} H_{ii} &= M_2(k_0^2 - \frac{4}{a^2} + \frac{2}{a^2}\cos k_z a\cos^2\theta)\sigma_z \\ &+ M_1(k_1^2 - \frac{2}{a^2} + \frac{2}{a^2}\cos k_z a\sin^2\theta)\sigma_x, \\ H_{i,i+\hat{x}} &= \frac{M_2}{a^2}(\sin^2\theta + i\sin k_z a\sin\theta\cos\theta)\sigma_z \\ &+ \frac{M_1}{a^2}(\cos^2\theta - i\sin k_z a\sin\theta\cos\theta), \\ H_{i,i+\hat{y}} &= \frac{M_2\sigma_z}{a^2} + \frac{v_y\sigma_y}{2ai}. \end{aligned} \tag{S2}$$

Note that k_z is conserved during scattering which is treated as a parameter. Similarly, the lattice models for the normal metal is

$$H_N^{\text{latt}} = \sum_i (\frac{6C}{a^2} - \frac{2C}{a^2}\cos k_z a - \mu_N)c_i^\dagger c_i - \sum_i \frac{C}{a^2}(c_i^\dagger c_{i+\hat{x}} + c_i^\dagger c_{i+\hat{y}}) + \text{H.c.}, \tag{S3}$$

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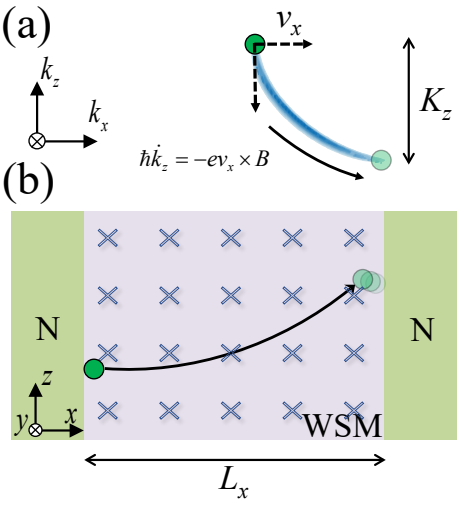

FIG. S1. (a) Electrons slide along the FA and pushed into the Weyl node by the Lorentz force. (b) The electron trail in real space of the critical case that the incident electrons with k_z at a Weyl node are pushed into the other Weyl node just before reaching the right electrode, corresponding to (a).

where c_i is the electron operator for the normal metal. The coupling between the outmost layers of the WSM and the N is described as

$$H_T = \sum_i t_N[c_i^\dagger\psi_{1,i+\hat{y}} + c_i^\dagger\psi_{2,i+\hat{y}}] + \text{H.c.}. \tag{S4}$$

II. THE QUANTITATIVE DESCRIPTION OF THE MAGNETIC FIELD EFFECTS

In this section, we will estimate the critical magnetic field B_0 in a semi-classical picture.

As shown in Fig. S1(a), once the magnetic field is employed, the incident electrons in the right-moving channels will be driven by the Lorentz force and slide along the Fermi arc. K_z is the span of the Fermi arc in the k_z-direction and B_0 is the critical value that all incident electrons at the top surface reach the Weyl node and penetrate into the chiral Landau bands of the bulk states. The semiclassical equation of motion is given by

$$\hbar\dot{k}_z = (-e)v_x \times B \tag{S5}$$

where v_x is the x-direction velocity. Integrating the equation on both sides yields $\hbar\Delta k_z = -e\Delta x B$, which relates

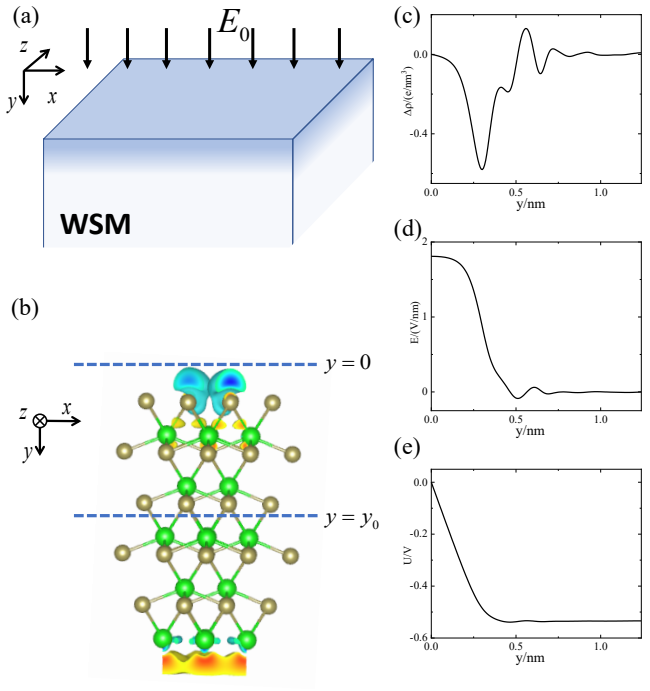

FIG. S2. (a) Scheme of the potential resulting from the difference of charge density near the surface of WSM, the external electric field E_0 is imposed perpendicular to the open surface of ZrTe. (b) The difference of charge density between $E_0 = 0.05$ V/nm and $E_0 = 0$ condition, the yellow and blue parts near the surface represent the increase and decrease of charge density respectively, the zero electric field reference surface is taken as $y_0 \approx 1.24$ nm. (c)-(e) The calculation of surface electrostatic potential induced by the external electric field, with (c) the distribution of charge density difference (d) the electric field intensity and (e) the electric potential along the y direction.

the change of the momentum k_z in the z direction and the displacement Δx in the x direction. The saturated magnetic field can thus be obtained by

$$B_0 = \frac{\hbar K_z}{eL_x}. \tag{S6}$$

III. THE DISCUSSION ON THE EXPERIMENTAL IMPLEMENTATION

We discuss the experimental implementation of our proposal. In the previous discussion, all results are obtained based on the minimal model of the WSM and the effect of the surface gate is introduced phenomenologically by the potential U. From Fig.2 in the main text, one can see that the Lifshitz transition of FAs can be driven by a surface potential with $U_c \sim 0.3$ eV. In the following, we show that such a surface potential can be achieved in real WSMs. In reality, the establishment of the surface potential by the gate voltage is sketched in Fig. S2(a). A surface gate creates a vertical electric field, which drives free charges to the sample boundary, where these charges rearrange and achieve equilibrium again due to the screening effect. As a result, a finite accumulation of the charge density and thus that of the electric potential are induced by the surface gate, which leads to a potential difference between the surface and bulk electrons. This is the physical origin of the parameter U in the previous calculation.

We show that the strength of the surface potential $U_c \sim 0.3$ eV required by the Lifshitz transition of the FAs can be realized in real WSMs. We here take a typical WSM, ZrTe [1] as an example, and perform first-principles calculations on the charge density difference induced by an external electric field using VASP software package [2, 3]. The calculation is performed on a three-layer ZrTe slab with a 1.4 nm vacuum, and an external electric field E_0 is applied perpendicular to the open surface, which is created by a surface gate in the experiment. The sampling of the Brillouin zone in the self-consistent process is taken as the grid of $18 \times 18 \times 13$, and the exchange-correlation potential is treated within the generalized gradient approximation [4] of the Perdew-Burke-Ernzerhof type [5]. The difference of the charge density distribution between $E_0 = 0.05$ V/nm and $E_0 = 0$ is plotted in Fig. S2(b). As is shown, negative and positive charge density difference is accumulated on the top and bottom boundaries, respectively. The fluctuation of the charge density on the atomic scale in the x-z plane is not important so that we take its average value $\Delta\rho$ in this plane for simplicity and focus on its distribution in the y direction. The charge distribution induced by the external electric field is plotted in Fig. S2(c).Using $\partial E/\partial y = \Delta\rho(y)/\varepsilon_0$ and $\partial U/\partial y = -E$ and taking into account the vanishing field inside the bulk, $E(y = y_0) = 0$, the distribution of E and U in the y direction can be obtained; see Fig. S2(d)-(e). One can see that for an external electric field $E_0 = 0.05$ V/nm, a considerable surface potential $U \sim 0.5$ eV can be induced within the range of 0.3 nm near the surface. Such a result proves that a surface potential sufficient to drive the Lifshitz transition of FAs can be induced by the surface gate voltage, showing the feasibility of our proposal. Moreover, for the surface bands in realistic materials, some saddle points may lie naturally near the Fermi energy so that the surface potential required by the Lifshitz transition may be much smaller than 0.3 eV in our model, which further facilitates its implementation.

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