DERIVATION OF $h_1(\mathbf{q})$ USING THE LITTLE GROUP AT D_1

The full symmetry group of the thin film in the absence of applied fields is $D_{4h} \otimes T$. The little group at a Dirac point D_i is the subgroup of all operations that leave D_i invariant. The little group therefore consists of a mirror plane that passes $\bar{\Gamma}D_i$, C_{2T} and their combinations. Taking D_1 as example, the little group is generated by $M_{1\bar{1}0}$ and C_{2T}. In a general spin-1/2 system we have: $M_{1\bar{1}0}^2 = C_2^2 = T^2 = -1$ and $\{M_{1\bar{1}0}, C_2\} = [M_{1\bar{1}0}^2, T] = [C_2, T] = 0$, where C_2 is the 180-rotation about [001]-direction. Therefore the two generators satisfy (i) $M_{1\bar{1}0}^2 = -C_{2T}^2 = -1$ (ii) $\{M_{1\bar{1}0}, C_{2T}\} = 0$. There is only one 2D irreducible representation up to a basis rotation: $M_{1\bar{1}0} = i\sigma_y$ and $C_{2T} = K\sigma_x$. Physically, $M_{1\bar{1}0}$ relates the Hamiltonian $h_1(q_1, q_2)$ to $h_1(q_1, -q_2)$ and C_{2T} commutes with $h_1(\mathbf{q})$; or mathematically, $M_{1\bar{1}0}h_1(q_1, q_2)M_{1\bar{1}0}^{-1} = h_1(q_1, -q_2)$ and $[C_{2T}, h_1(\mathbf{q})] = 0$. The irreducible representation of the little group along with the symmetry constraints determine the form of $h_1(\mathbf{q})$ shown in Eq.(1).

In general, the $k \cdot p$ model is given by

$$h_1(\mathbf{q}) = d_0(\mathbf{q})I_{2\times2} + d_x(\mathbf{q})\sigma_x + d_y(\mathbf{q})\sigma_y + d_z(\mathbf{q})\sigma_z, \quad \text{(S1)}$$

which must satisfy the symmetry constraints:

$$\begin{aligned} M_{1\bar{1}0}h_1(q_1, q_2)M_{1\bar{1}0}^{-1} &= h_1(q_1, -q_2), \\ [C_{2T}, h_1(\mathbf{q})] &= 0. \end{aligned} \quad \text{(S2)}$$

These symmetry constraints give that (1) $d_{0,y}$ is even under $q_2 \to -q_2$, (2) d_x is odd under $q_2 \to -q_2$ and (3) $d_z = 0$ to arbitrary order. We expand them to the second order in $|q|$:

$$\begin{aligned} d_0(q_1, q_2) &= v_0 q_1 + \frac{q_1^2}{2m_1} + \frac{q_2^2}{2m_2}, \\ d_x(q_1, q_2) &= v_2 q_2 + \frac{q_1 q_2}{2m_3}, \\ d_y(q_1, q_2) &= v_1 q_1 + \frac{q_1^2}{2m_4} + \frac{q_2^2}{2m_5}. \end{aligned} \quad \text{(S3)}$$

These terms make the dispersion deviate from perfectly linear and may be understood as the 'warping' terms; they also make corrections to the wave functions at each $\mathbf{q}$. It should be noted that $d_z = 0$ holds up to arbitrary orders and this means there is no out-of-plain pseudo-spin component at any $\mathbf{q}$. While including higher order terms explains the shape-changing of the equal energy contours from perfect ellipsoids, the Lifshitz transition cannot be described in the framework of any two-band theory. To do so, the model must be extended a four-band one, in order to account for the hybridization between nearest cones, as discussed in Ref.[21].

RELATING THE FOUR DIRAC CONES BY C_4 SYMMETRY

In the main text, we mention that by 90-degree rotations the effective theories for the four cones can be related. This is an intuitive statement yet to be made precise. In fact, $k \cdot p$ theories are always written with respect to a chosen basis, which is our case is furnished by (the periodic part of) the two Bloch states that are degenerate at the Dirac point. Due to the degeneracy, there is a gauge degree of freedom in the choice. Here the choice is made by fixing the little group representation at D_1: $M_{1\bar{1}0} = i\sigma_y$ and $C_{2T} = K\sigma_x$. If we denote the two basis states by $|u_{1\uparrow}\rangle$ and $|u_{1\downarrow}\rangle$, we then fix the bases at $D_{2,1',2'}$ to be $\{|u_{2\uparrow}\rangle, |u_{2\downarrow}\rangle\} = \{\tilde{C}_4^2|u_{1\uparrow}\rangle, \tilde{C}_4^2|u_{1\downarrow}\rangle\}$, $\{|u_{1'\uparrow}\rangle, |u_{1'\downarrow}\rangle\} = \{\tilde{C}_4|u_{1\uparrow}\rangle, \tilde{C}_4|u_{1\downarrow}\rangle\}$ and $\{|u_{2'\uparrow}\rangle, |u_{2'\downarrow}\rangle\} = \{\tilde{C}_4^3|u_{1\uparrow}\rangle, \tilde{C}_4^3|u_{1\downarrow}\rangle\}$, respectively. Mark that here $\tilde{C}_4$ is the matrix representing the 90-degree rotation in both orbital space (including spin). Defining the Bloch wave function at $\mathbf{D}_i + \mathbf{q}$ as $|\psi_{i\uparrow/\downarrow}(\mathbf{q})\rangle = e^{i(\mathbf{D_i}+\mathbf{q})\cdot\mathbf{r}}|u_{i\uparrow/\downarrow}\rangle$, it is easy to check that $|\psi_2(\mathbf{q})\rangle = \hat{C}_4^2|\psi_1(-\mathbf{q})\rangle$, $\hat{C}_4|\psi_{1'}(\mathbf{q})\rangle = \hat{C}_4|\psi_1(-q_2, q_1)\rangle$ and $|\psi_{2'}(\mathbf{q})\rangle = \hat{C}_4^3|\psi_1(q_2, -q_1)\rangle$. Here $\hat{C}_4$ is the single particle operator acting in the Hilbert space, which is the combination of the orbital rotation $\tilde{C}_4$ plus rotation $(x, y) \to (-y, x)$, where (x, y) is a lattice point and the rotation center is also placed at a lattice point. The full single Hamiltonian, projected to the states at the vicinities of the four Dirac points, is given by

$$\hat{H} = \sum_{\mathbf{q}, i=1,2,1',2',\alpha,\beta=\uparrow,\downarrow} (h_i(\mathbf{q}))^{\alpha\beta}|\psi_{i\alpha}(\mathbf{q})\rangle\langle\psi_{i\beta}(\mathbf{q})|. \quad \text{(S4)}$$

C_4 symmetry implies $[\hat{C}_4, \hat{H}] = 0$, which immediately leads to $h_2(q_1, q_2) = h_1(-q_1, -q_2)$, $h_{1'}(q_1, q_2) = h_1(-q_2, q_1)$ and $h_{2'}(q_1, q_2) = h_1(q_2, -q_1)$, confirming the intuitive relations appearing in the main text.

CALCULATION OF THE CHERN NUMBER OF THE TOP/BOTTOM SURFACE

In the text we refer to the Chern number contributed by one massive Dirac cone, which is not mathematically well-defined. In fact, the integrated Berry's curvature of a gapped Dirac cone is non-quantized in any finite $\mathbf{k}$-space, hence possesses no well-defined Chern number. The Chern number of a whole 2D surface (top surface for example) is, however, a well-defined quantity (if periodic boundary is taken for the other two directions), which may be calculated. Suppose we are interested in the Chern number, C, at some Zeeman field $\Delta_Z = \Delta_0 > 0$. Then since time-reversal reverses the Chern number, we know for $\Delta_Z = -\Delta_0$, the Chern number must be $-C$. Consider a 3D space spanned by $q_{1,2}$ and Δ_Z, then from Gauss's law, the Chern number change from $\Delta_Z = -\Delta_0$

to Δ_0 equals the total monopole charge between these two planes in the 3D parameter space. The monopole, or gap closing point, is always at $(q_1, q_2, \Delta_Z) = 0$, around which the Hamiltonian is that of 3D Weyl fermions: $h(q_1, q_2, q_3) = \sum_{i,j=1,2,3} A_{ij}\sigma_i q_j$, where $q_3 \equiv \Delta_Z$. The charge of such a monopole is sign det(A), and since there are in total four such monopoles between $\Delta_Z = \pm\Delta_0$, we have the difference in Chern number $C - (-C) = 4\text{sign}(\det A)$, or $C = 2\text{sign}(\det A)$. All Chern numbers obtained in the text are derived using this method.

DIAGONALIZING THE HAMILTONIAN IN EQ.(4)

A Hamiltonian that describes isolated top and surface states around D_i is

$$\tilde{H}_i = \begin{pmatrix} H_i^t & 0 \\ 0 & H_i^b \end{pmatrix}, \tag{S5}$$

and hybridization is equivalent to adding an off-diagonal block term, resulting in, to the lowest order in $|q|$,

$$\tilde{H}_i = \begin{pmatrix} H_i^t & \Delta_H I_{2\times 2} \\ \Delta_H I_{2\times 2} & H_i^b \end{pmatrix}. \tag{S6}$$

Diagonalizing $\tilde{H}_1$ directly, we obtain four bands:

$$\begin{aligned}
E_1(\mathbf{q}) &= v_0 q_1 + \sqrt{{\Delta_1^t}^2 + {\Delta_1^t}^2 + 2\Delta_H^2 + 2q_1^2 v_1^2 + 2q_2^2 v_2^2 + \sqrt{(\Delta_1^t - \Delta_1^b)^2 + 4[(\Delta_1^t + \Delta_1^b)^2 + 4v_1^2 q_1^2 + 4v_2^2 q_2^2]}}, \quad \text{(S7)}\\
E_2(\mathbf{q}) &= v_0 q_1 + \sqrt{{\Delta_1^t}^2 + {\Delta_1^t}^2 + 2\Delta_H^2 + 2q_1^2 v_1^2 + 2q_2^2 v_2^2 - \sqrt{(\Delta_1^t - \Delta_1^b)^2 + 4[(\Delta_1^t + \Delta_1^b)^2 + 4v_1^2 q_1^2 + 4v_2^2 q_2^2]}},\\
E_3(\mathbf{q}) &= v_0 q_1 - \sqrt{{\Delta_1^t}^2 + {\Delta_1^t}^2 + 2\Delta_H^2 + 2q_1^2 v_1^2 + 2q_2^2 v_2^2 - \sqrt{(\Delta_1^t - \Delta_1^b)^2 + 4[(\Delta_1^t + \Delta_1^b)^2 + 4v_1^2 q_1^2 + 4v_2^2 q_2^2]}},\\
E_4(\mathbf{q}) &= v_0 q_1 - \sqrt{{\Delta_1^t}^2 + {\Delta_1^t}^2 + 2\Delta_H^2 + 2q_1^2 v_1^2 + 2q_2^2 v_2^2 + \sqrt{(\Delta_1^t - \Delta_1^b)^2 + 4[(\Delta_1^t + \Delta_1^b)^2 + 4v_1^2 q_1^2 + 4v_2^2 q_2^2]}}.
\end{aligned}$$

Straightforward algebraic work shows that the *only* solution for $E_2(\mathbf{q}) = E_3(\mathbf{q})$, i.e., a gap-closing point, exists at $q_1 = q_2 = 0$ when $|\Delta_H| = \sqrt{\Delta_1^t \Delta_1^b}$.

Parallel discussion for $D_{2,1',2'}$ proceeds and we conclude that a topological phase transition happens when

$$|\Delta_H| = \sqrt{\Delta_i^t \Delta_i^b}, \tag{S8}$$

whereas the Chern number contributed by the cone at D_i changes from ± 1, depending on the sign of $\Delta_i^{t,b}$, to zero. Mark that on the right hand side of Eq.(S8), if $\Delta_i^t \Delta_i^b < 0$, the transition cannot happen at any Δ_H.

DERIVATION OF TABLE I

Here we provide details for deriving Table I.

First we note the following two simple facts: (i) the strain tensor is a rank-2 tensor so its general transformation under $O(3)$ takes the form:

$$\epsilon_{ab} \to R_{aa'} R_{bb'} \epsilon_{a'b'}, \tag{S9}$$

where R is the three-by-three rotation matrix, and (ii) it is invariant under time-reversal. All point group operators including $C_{2,4}$ and $M_{110,1\bar{1}0}$ are elements of $O(3)$ and due to (ii), C_{2T} transforms the tensor in the same way as C_2 does. The rotation matrix for these operations are given by

$$\begin{aligned}
R_{C_2} &= \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, R_{M_{110}} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \text{(S10)}\\
R_{M_{1\bar{1}0}} &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, R_{C_4} = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}.
\end{aligned}$$

Substituting Eq.(S10) back into Eq.(S9), we have the upper part of Table I.

We then can use the upper part of Table I to determine the terms that represent spin in the effective theories for the four Dirac cones. The strain terms for the states around $D_{i=1,2,1',2'}$ are generally written as

$$\delta H_{ab,i} = m^0_{ab,i}\sigma_0 + m^x_{ab,i}\sigma_x + m^y_{ab,i}\sigma_y + m^z_{ab,i}\sigma_z + O(|q|). \tag{S11}$$

The little group of D_i gives constraints on $m^\alpha_{ab,i}$. Hereafter we ignore $m^0_{ab,i}$ because this does not change the wavefunction, thus preserving the topology, of the surface states. $\epsilon_{11,22,33}$ are unchanged under C_{2T}, M_{110} or $M_{1\bar{1}0}$, from which we know $m^x_{11/22/33,i} = m^z_{11/22/33,i} = 0$. Since C_4 relates the four Dirac points and sends $\epsilon_{11/22}$ to $\epsilon_{22/11}$, we know $m^y_{11/22,1} = m^y_{22/11,1'} = m^y_{11/22,2} = m^y_{22/11,2'}$ and $m^y_{22/11,1} = m^y_{11/22,1'} = m^y_{22/11,2} = m^y_{11/22,2'}$. So far we have derived the first three columns of the lower part of the Table.

ϵ_{12} changes sign under $M_{110,1\bar{1}0}$ and invariant under C_{2T}, from which we have $m^y_{12,i} = m^z_{12,i} = 0$. Again from C_4, we obtain $m^x_{12,1} = -m^x_{12,1'} = m^x_{12,2} = -m^x_{12,2'}$. This is the fourth column.

$\epsilon_{13/23}$ are invariant under $M_{1\bar{1}0/110}$ but changes sign under $M_{110/1\bar{1}0}$ and C_{2T}. The little group at $D_{1,2}$ is $\{M_{1\bar{1}0}, C_{2T}\}$, so we have $m^{x,z}_{13,1} = m^{x,z}_{13,2} = 0$ and $m^{x,y}_{23,1} = m^{x,y}_{23,2} = 0$. Using that C_2 maps $D_{1/2}$ to $D_{2/1}$, we have $m^y_{13,1} = -m^y_{13,2}$ and $m^z_{13,1} = -m^z_{13,2}$. Then we notice that since C_4 maps $D_{1/1'}$ to $D_{2/2'}$, and ϵ_{13} (ϵ_{23}) to ϵ_{23} ($-\epsilon_{13}$), there are $m^{x,y,z}_{23,1'/2'} = m^{x,y,z}_{13,1/2}$. This gives the last two columns.

The above relations give in total six free masses: $(m^y_{11,1}, m^y_{22,1}, m^y_{33,1}, m^x_{12,1}, m^y_{13,1}, m^z_{23})$, defined as $(\lambda_{11}, \lambda_{22}, \lambda_{33}, \lambda_{12}, \lambda_{13}, \lambda_{23})$.