Supplementary material for "Topological insulators with quaternionic analytic Landau levels"

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In this supplementary material, we present several points including the ladder algebra to explain the degeneracy of the 3D Landau level (LL) wavefunctions, the quaternionic version of the 3D lowest Landau level (LLL) states with the negative helicity, the numerical calculation on the 3D LL spectra with the open boundary, and the generalization of LLs to an arbitrary dimension.

Ladder algebra The spectra flatness of the 3D LL can be explained by constructing the ladder algebra. For example, we take the case of $qG > 0$ and consider the positive helicity Landau level states of H_+. The variable transformation for the radial eigenstates is applied as $\chi_{n_r,l}(r) = rR_{n_r,l}(r)$, and the corresponding radial Hamiltonians become

$$H_l = \hbar\omega_0 \Big\{ -\frac{d^2}{dr^{*2}} + \frac{l(l+1)}{r^{*2}} - l + \frac{1}{4} r^{*2} \Big\}, \qquad (1)$$

where the dimensionless radius is $r^* = \frac{r}{l_G}$. The ladder operators are defined as

$$\begin{aligned} A_+(l) &= \frac{d}{dr^*} - \frac{l+1}{r^*} - \frac{1}{2} r^*, \\ A_-(l) &= -\frac{d}{dr^*} - \frac{l}{r^*} - \frac{1}{2} r^*. \end{aligned} \qquad (2)$$

They satisfy the relations

$$H_{l\pm 1} A_\pm(l) = A_\pm(l) H_l. \qquad (3)$$

Consequentially, $\chi_{n_r,l\pm1} = A_\pm(l)\chi_{n_r,l}$ with the same energy independent of l. All the states in the same LL can be reached by successively applying $A_\pm$ operators.

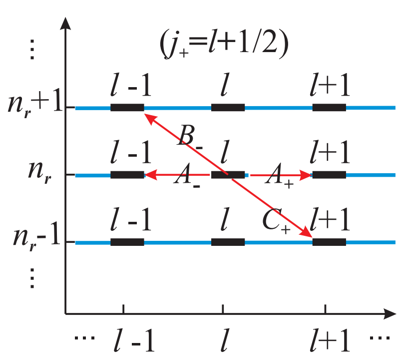

FIG. 1: The algebra structure of the 3D Landau levels in the positive helicity sector. Operators $A_\pm(l)$ connect states with different l in the same Landau level, while $B_-(l)$ and $C_+(l)$ connect those between neighboring Landau levels.

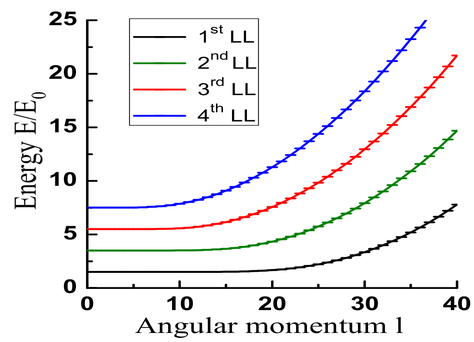

FIG. 2: The energy dispersion of the first four Landau levels *v.s.* $l = j - \frac{1}{2}$. Open boundary condition is used for a ball with the radius $R_0/l_G = 8$. The edge states correspond to those with large values of l and develop linear dispersions with l. The most probable radius of the LLL state with l is $r = l_G\sqrt{l}$.

To connect different LLs, other two ladder operators are defined as

$$\begin{aligned} B_-(l) &= -\frac{d}{dr^*} - \frac{l}{r^*} + \frac{1}{2} r^*, \\ C_+(l) &= \frac{d}{dr^*} - \frac{l+1}{r^*} + \frac{1}{2} r^*, \end{aligned} \qquad (4)$$

which satisfy

$$\begin{aligned} H_{l-1} B_-(l) &= B_-(l)(H_l + 2\hbar\omega_0), \\ H_{l+1} C_+(l) &= C_+(l)(H_l - 2\hbar\omega_0), \end{aligned} \qquad (5)$$

respectively. By applying $B_-(l)$ ($C_+(l)$) to $\chi_{n_r,l}(r)$, we arrive at

$$\begin{aligned} \chi_{n_r+1,l-1} &= B_-(l)\chi_{n_r,l}, \\ \chi_{n_r-1,l+1} &= C_+(l)\chi_{n_r,l}, \end{aligned} \qquad (6)$$

where the energy shifts $\pm 2\hbar\omega_0$, respectively, as illustrated in Fig. 1. Similar algebra can also be constructed for the case of $qG < 0$.

Gapless surface Dirac modes We have numerically calculated the spectra of the 3D LL Hamiltonian with the open boundary condition for the positive helicity states with $j_+ = l + \frac{1}{2}$ for Eq. 2 in the main text. The results for the first four LLs are plotted in Fig. 2. The radius of the boundary is $R_0/l_G = 8$. For the lowest LL (LLL) states, when the orbital angular momentum l exceeds a characteristic value $l_c \approx 30$, the spectra become dispersive indicating the onset of surface states.

Quaternionic wavefunction for the j_- sector In the main text, we have showed that the 3D LLL states with the positive helicity in the quaternion representation form a set of complete basis for the quaternionic left-analytic polynomials. For the case of the LLL with negative helicity, their quaternionic version $g^{LLL}_{j_-,j_z}(x,y,z)$ are not analytic any more. Nevertheless, they are related to the analytic one through $g^{LLL}_{j_-=(l+1)-\frac{1}{2},j_z} = (-xk - yj + zi) f^{LLL}_{j_+=l+\frac{1}{2},j_z} i$.

Generalization to N-dimensions The study in 3D and 4D LL systems can be generalized to N-D by replacing the vector and scalar potentials in Eq. 1 in the main text with the $SO(N)$ gauge field $A^a(\vec{r}) = g r^b S^{ab}$ and $V(r) = -\frac{N-2}{2} m\omega_0 r^2$, respectively, where S^{ab} are the $SO(N)$ spin operators constructed based on the Clifford algebra. The rank-k Clifford algebra contains $2k+1$ matrices with the dimension $2^k \times 2^k$ which anti-commute with each other denoted as Γ^a ($1 \leq a \leq 2k+1$). Their commutators generate

$$\Gamma^{ab} = -\frac{i}{2}[\Gamma^a, \Gamma^b], \tag{7}$$

for $1 \leq a < b \leq 2k+1$. For odd dimensions $N = 2k+1$, the $SO(N)$ spin operators in the fundamental spinor representation can be constructed by using the rank-k matrices as $S^{ab} = \frac{1}{2}\Gamma^{ab}$. For even dimensions $N = 2k+2$, we can select $2k+2$ ones among the $2k+3$ Γ-matrices of rank-$(k+1)$ to form $S^{ab} = \frac{1}{2}\Gamma^{ab}$, then all of S^{ab} commute with Γ^{2k+3}. This 2^{k+1}-D spinor representation of S^{ab} is thus reducible into the fundamental and anti-fundamental representations. Both of them are 2^k-D, which can be constructed from the rank-k Γ-matrices as $S^{a,2k+2} = \pm\frac{1}{2}\Gamma^a (1 \leq a \leq 2k+1)$ and $S^{ab} = \frac{1}{2}\Gamma^{ab} (1 \leq a < b < 2k+1)$, respectively.

As for TR properties, Γ^a's are TR even and odd at even and odd values of k, respectively. We conclude that at $N = 2k+1$, the N-D version of the LL Hamiltonian is TR invariant in the fundamental spinor representation. At $N = 4k$, it is also TR invariant in both the fundamental and anti-fundamental representations. However $N = 4k+2$, each one of the fundamental and anti-fundamental representations is not TR invariant, but transforms into each other under TR operation.

Similarly, the N-D LL Hamiltonian can be reorganized as the harmonic oscillator with SO coupling. For the case of $qG > 0$, it becomes

$$H_{N,+} = \frac{p^2}{2m} + \frac{1}{2} m\omega_0^2 r^2 - \hbar\omega_0 \Gamma_{ab} L_{ab}, \tag{8}$$

where $L_{ab} = r_a p_b - r_b p_a$ with $1 \leq a < b \leq N$. The l-th order N-D spherical harmonic functions are eigenstates of $L^2 = L_{ab} L_{ab}$ with the eigenvalue of $\hbar^2 l(l+D-2)$. The N-D harmonic oscillator has the energy spectra of $E_{n_r,l} = (2n_r + l + N/2)\hbar\omega$. When coupling to the fundamental spinors, the l-th spherical harmonics split into the positive helicity (j_+) and negative helicity (j_-) sectors, whose eigenvalues of the $\Gamma_{ab} L_{ab}$ are $\hbar l$ and $-\hbar(l+N-2)$, respectively. For the positive helicity sector, its spectra become independent of l as $E_+ = (2n_r + N/2)\hbar\omega$, with the radial wave functions are

$$R_{n_r l}(r) = r^l e^{-r^2/4l_G^2} F(-n_r, l+N/2, r^2/2l_G^2). \tag{9}$$

The highest weight states in the LLL can be written as

$$\psi^{hw}_{ab,\pm l}(\vec{r}) = [(\hat{e}_a \pm i\hat{e}_b)\cdot\vec{r}]^l e^{-r^2/4l_G^2} \otimes \alpha_{\pm,ab}, \tag{10}$$

where $\alpha_{\pm,ab}$ is the eigenstate of Γ_{ab} with eigenvalue ± 1, respectively. The magnetic translation in the ab-plane by the displacement vector $\vec{\delta}$ takes the form

$$T_{ab}(\vec{\delta}) = \exp\big[-\vec{\delta}\cdot\vec{\nabla} + \frac{i}{2l_G^2}\Gamma_{ab}(r_a\delta_b - r_b\delta_a)\big]. \tag{11}$$

Similarly to the 3D case, staring from the LLL state localized around the origin with $l = 0$, we can perform the magnetic translation and Fourier transformation with respect to the transverse spin polarization. The resultant localized Gaussian pockets are LLL states of the eigenstates of the $SO(N-1)$ symmetry with respect to the translation direction $\vec{\delta}$. Again each LL contributes to one channel of surface Dirac modes on S^{N-1} described by $H_{bd} = (v_f/R_0)\Gamma_{ab} L_{ab} - \mu$.