High-Dimensional Topological Insulators with Quaternionic Analytic Landau Levels

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We study the three-dimensional topological insulators in the continuum by coupling spin-1/2 fermions to the Aharonov-Casher SU(2) gauge field. They exhibit flat Landau levels in which orbital angular momentum and spin are coupled with a fixed helicity. The three-dimensional lowest Landau level wave functions exhibit the quaternionic analyticity as a generalization of the complex analyticity of the two-dimensional case. Each Landau level contributes one branch of gapless helical Dirac modes to the surface spectra, whose topological properties belong to the $\mathbb{Z}_2$ class. The flat Landau levels can be generalized to an arbitrary dimension. Interaction effects and experimental realizations are also studied.

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The two-dimensional (2D) quantum Hall (QH) systems [1,2] are among the earliest examples of quantum states characterized by topology [3,4] rather than symmetry in condensed matter physics. Their magnetic band structures possess topological Chern numbers defined in time-reversal (TR) symmetry breaking systems [3,5–8]. The consequential quantized charge transport originates from chiral edge modes [9,10], a result from the chirality of Landau level wave functions. Current studies of TR invariant topological insulators (TIs) have made great success in both 2D and three-dimensional (3D). They are described by a $\mathbb{Z}_2$ invariant, which is topologically stable with respect to TR invariant perturbations [11–22]. On open boundaries, they exhibit odd numbers of gapless helical edge modes in 2D systems and surface Dirac modes in 3D systems. TIs have been experimentally observed through transport experiments [23–25] and spectroscopic measurements [26–32].

The current research of 3D TIs has been focusing on the Bloch-wave band structures. Nevertheless, Landau levels (LLs) possess the advantages of the elegant analytic properties and flat spectra, both of which have played essential roles in the study of 2D integer and fractional QH effects [33–48]. As pioneered by Zhang and Hu [49], LLs and QH effects have been generalized to various high dimensional manifolds [49–54]. However, to our knowledge, TR invariant isotropic LLs have not been studied in 3D flat space before. It would be interesting to develop the LL counterpart of 3D TIs in the continuum independent of the band inversion mechanism. The analytic properties of 3D LL wave functions and the flatness of their spectra provide an opportunity for further investigation on nontrivial interaction effects in 3D topological states.

In this Letter, we construct 3D isotropic flat LLs in which spin-1/2 fermions are coupled to an $SU(2)$ Aharonov-Casher potential. When odd number LLs are fully filled, the system is a 3D $\mathbb{Z}_2$ TI with TR symmetry. Each LL state has the same helicity structure, i.e., the relative orientation between orbital angular momentum and spin. Just like that the 2D lowest LL (LLL) wave functions in the symmetric gauge are complex analytic functions, the 3D LLL ones are mapped into quaternionic analytic functions. Different from the 2D case, there is no magnetic translational symmetry for the 3D LL Hamiltonian due to the non-Abelian nature of the gauge field. Nevertheless, magnetic translations can be applied for the Gaussian pocketlike localized eigenstates in the LLL. The edge spectra exhibit gapless Dirac modes. Their stability against TR invariant perturbations indicates the $\mathbb{Z}_2$ nature. This scheme can be easily generalize to $N$ dimensions. Interaction effects and the Laughlin-like wave functions for the four-dimensional (4D) case are constructed. Realizations of the 3D LL system are discussed.

We begin with the 3D LL Hamiltonian for a spin-1/2 nonrelativistic particle as

$$H^{3D,LL} = \frac{1}{2m} \sum_a \left( -i \hbar \nabla^a - \frac{q}{c} A^a(\vec{r}) \right)^2 + V(\vec{r}), \quad (1)$$

where $A^a_{\alpha\beta} = (1/2) G e_{\alpha\beta\gamma} x^\gamma$ is a 3D isotropic $SU(2)$ gauge with Latin indices run over $x, y, z$ and Greek indices denote spin components $\uparrow, \downarrow$. $G$ is a coupling constant and $\sigma$’s are Pauli matrices; $V(\vec{r}) = -(1/2) m \omega_0^2 r^2$ is a harmonic potential with $\omega_0 = |qG|/(2mc)$ to maintain the flatness of LLs. $\vec{A}$ can be viewed as an Aharonov-Casher potential associated with a radial electric field linearly increasing with $r$ as $E(r) \times \vec{\sigma}$. $H^{3D,LL}$ preserves the TR symmetry in contrast to the 2D QH with TR symmetry broken. It also gives a 3D non-Abelian generalization of the 2D quantum spin Hall Hamiltonian based on Landau levels studied in Ref. [11]. More explicitly, $H^{3D,LL}$ can be further expanded as a harmonic oscillator with a constant spin-orbit (SO) coupling as

$$H^{3D,LL}_z = \frac{p^2}{2m} + \frac{1}{2} m \omega_0^2 r^2 + \omega_0 \vec{\sigma} \cdot \vec{L}, \quad (2)$$

where $\vec{L}$ apply to the cases of $qG > 0 (<0)$. 

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respectively. The spectra of Eq. (2) were studied in the context of the supersymmetric quantum mechanics [55]. However, its connection with Landau levels was not noticed. Equation (1) has also been proposed to describe the electrode dynamics properties of superconductors [56–58].

The spectra and eigenstates of Eq. (1) are explained as follows. We introduce the helicity number for the eigenstate of $\vec{L} \cdot \vec{\sigma}$, defined as the sign of its eigenvalue of the total angular momentum $\vec{J} = \vec{L} + \vec{S}$, which equals $\pm 1$ for the sectors of $j_z = l \pm (1/2)$, respectively. At $qG > 0$, the eigenstates are denoted as $\psi_{n_j, j_z=1/2} (\vec{r}) = R_{n_j}(r) Y_{j_z, j_z=1/2} (\vec{\Omega})$, where the radial function is $R_{n_j}(r) = r^j e^{-(r^2/4l_G^2)} F(-n_j, l + (3/2), (r^2/2l_G^2))$; $F$ is the confluent hypergeometric function and $l_G = \sqrt{\hbar / qG}$ is the analogy of the magnetic length; $Y_{j_z, j_z=1/2} (\vec{\Omega})$’s are the spin-orbit coupled spherically harmonic with $j_z = l \pm (1/2)$, respectively. Flat spectra appear with infinite degeneracy in the sector of $j_z$, where the energy dispersion $E_{n_j, l} = (2n_j + (3/2))\hbar \omega_0$ is independent of $l$, and thus $n_j$ serves as the LL index. For the sector of $j_-$, the energy disperses with $l$ as $E_{n_j, l} = (2(n_j + l) + (5/2))\hbar \omega_0$. Similar results apply to the case of $qG < 0$, where the infinite degeneracy occurs in the sector of $j_-$. These LL wave functions are the same as those of the 3D harmonic oscillator but with different organizations. As illustrated in Fig. 1(a), these eigenstates along each diagonal line with the positive (negative) helicity fall into the flat LL states for the case of $qG > 0$ ($< 0$), respectively. The ladder algebra generating the whole 3D LL states is explained in the Supplemental Material [63].

Compared to the 2D case, a marked difference is that the 3D LL Hamiltonian has no magnetic translational symmetry. The non-Abelian field strength grows quadratically with $r$ as $F_{ij}(\vec{r}) = \partial_i A_j - \partial_j A_i - (iq / \hbar c)[A_i, A_j] = e \epsilon_{ijk}(\sigma^k + (1/4\mu_G^2)r^k (\vec{\sigma} \cdot \vec{r}))$. Nevertheless, magnetic translations still apply to the highest weight states of the total angular momentum $\vec{J} = \vec{L} + \vec{S}$ in the LLL at $qG > 0$. For simplicity, we drop the normalization factors of wave functions below. For the positive helicity states with $j_z = j_+$, $\vec{L}$ and $\vec{S}$ are parallel to each other. Their wave functions are denoted by $\psi_{j_z, \vec{L}}(\vec{r}) = (x + iy)^{j_z} e^{-(r^2/4l_G^2)} \otimes \alpha_{j_z}$, where $\alpha_{j_z}$ is the spin eigenstate of $\vec{\Omega} \cdot \vec{\sigma}$ with eigenvalue $j_z$. For these states, the magnetic translation is defined as usual $T_{\vec{z}}(\vec{r}) = \exp[-\vec{r} \cdot \vec{\nabla} + ((i/4l_G^2) \vec{r}\times (\vec{r} \times \vec{\nabla}))]$, where $\vec{\nabla}$ is the displacement vector in the xy plane and $\vec{r}\times \vec{\nabla}$ is the projection of $\vec{r}$ in the xy plane. The resultant state, $T_{\vec{z}}(\vec{r}) \psi_{j_z, \vec{L}}(\vec{r}) = e^{i(\vec{r} \cdot \vec{\nabla} + (i/4\mu_G^2) \vec{r}\times \vec{\nabla})} \psi_{j_z, \vec{L}}(\vec{r} + \vec{z})$, remains in the LLL. Generally speaking, the highest weight states can be defined in a plane spanned by two orthogonal unit vectors $\hat{\vec{e}}_1, 2$ as $\psi_{j_z, \vec{L}}(\vec{r}) = [(\hat{e}_1 + i\hat{e}_2) \cdot \vec{r}] e^{-(r^2/4l_G^2)} \otimes \alpha_{j_z}$, with $\hat{e}_3 = \hat{e}_1 + \hat{e}_2$. The magnetic translation for such states is defined as $T_{\vec{z}}(\vec{r}) = \exp[-\vec{r} \cdot \vec{\nabla} + ((i/4\mu_G^2) \vec{r}\times (\vec{r} \times \vec{\nabla}))]$, where $\vec{\nabla}$ lies in the $\hat{e}_1, 2$ plane and $\vec{\nabla} \rightarrow \vec{\nabla} - \vec{z} \times \hat{e}_3$. As an example, let us translate the LLL state localized at the origin as illustrated in Fig. 1(b). We set the spin direction of $\psi_{j_z, \vec{L}}|\vec{r}=0\rangle$ in the xy plane parametrized by $\vec{e}_3(\gamma) = \hat{z} \cos \gamma + \hat{y} \sin \gamma$, i.e., $\alpha_{j_z}(\gamma) = (1/2\sqrt{2})(|0\rangle + e^{i\gamma}|1\rangle)$, and translate it along $\hat{e}_1 = \hat{z}$ at the distance $R$. The resultant states read as

$$\psi_{j_z, \vec{L}}(\rho, \phi, z) = e^{i(\rho/2)R \rho \sin(\phi - \gamma)} e^{-(r^2/4l_G^2)} \otimes \alpha_{j_z}(\gamma),$$

where $\rho = \sqrt{x^2 + y^2}$ and $\phi$ is the azimuthal angular of $\vec{r}$ in the xy plane. Such a state remains in the LLL as an off-centered Gaussian wave packet.

The highest weight states and their descendent states from magnetic translations defined above have a clear classical picture. The classic equations of motion are derived as

$$\dot{\vec{r}} = \frac{1}{m} \vec{p} + 2\omega_0 \vec{z} \times \frac{1}{\hbar} \hat{S},$$

$$\dot{\vec{p}} = 2\omega_0 \vec{p} \times \frac{1}{\hbar} \hat{S} - m\omega_0^2 \vec{\Omega}, \quad \dot{\hat{S}} = \frac{2\omega_0}{\hbar} \hat{S} \times \hat{L},$$

where $\vec{p}$ is the canonical momentum, $\vec{L} = \vec{r} \times \vec{p}$ is the canonical orbital angular momentum, and $\hat{S}$ here is the expectation value of $(\hbar / 2)\vec{\sigma}$. The first two describe the motion in a noninertial frame subject to the angular velocity $(2\omega_0 / \hbar)\hat{S}$, and the third equation is the Larmor precession. $\vec{L} \cdot \hat{S}$ is a constant of motion of Eq. (4). In the case of $\hat{S} \parallel \hat{L}$, it is easy to prove that both $\hat{S}$ and $\vec{L}$ are conserved. Then the cyclotron motions become coplanar within the equatorial plane perpendicular to $\hat{S}$. Centers of the circular orbits can be located at any points in the plane.

The above off-centered LLL states break all the rotational symmetries. Nevertheless, we can recover the rotational symmetry around the axis determined by the origin and the packet center. Let us perform the Fourier transform of $\psi_{j_z, \vec{L}}(\rho, \phi, z)$ in Eq. (3) with respect to the azimuthal angle $\gamma$ of spin polarization. The resultant
state, $\psi_{j,-m+(1/2),R}(\rho, \phi, z) = \int_0^{2\pi} (d\gamma / 2\pi) e^{im\gamma} \psi_{j,R}$, is a $\mathbf{j}_z$ eigenstate as

$$e^{(i\beta R^2/2)4\rho} e^{im\phi} \{ J_m(x) \mid l \} + J_{m+1}(x) e^{i\phi} \mid l \} \right), \tag{5}$$

with $x = R\rho / (2l_G^2)$. At large distance of $R$, the spatial extension of $\psi_{j,-m+(1/2),R}$ in the xy plane is at the order of $m l_G^2 / R$, which is suppressed at large values of $R$ and scales linear with $m$. In particular, the narrowest states $\psi_{\pm(1/2),R}$ exhibit an ellipsoid shape with an aspect ratio decaying as $l_G / R$ when $R$ goes large.

In analogy to the fact that the 2D LLL states are complex analytic functions due to chirality, we have found an impressive result that the helicity in 3D LL systems leads to the quaternionic analyticity. Quaternion is the first impressive result that the helicity in 3D LL systems leads to analytic functions due to chirality. We have found an extended basis for the angular momentum representations, connected through SU(2) rotations, and they form an over-complete basis for the angular momentum representations. We conclude that all the 3D LLL states with the positive helicity are quaternionic analytic.

Essentially, we have proved that Fueter condition is rotationally invariant. Since all the highest weight states are connected through SU(2) rotations, and they form an over-complete basis for the angular momentum representations, we conclude that all the 3D LLL states with the positive helicity are quaternionic analytic.

Next we prove that the set of quaternionic LLL states $f_{j,+l-(1/2),j}$ form the complete basis for quaternionic valued analytic polynomials in 3D. Any linear superposition of the LLL states with $j_+ = 1$ can be represented as

$$f_{j_+,l_+} = \sum_{j_-,l_-} f_{j_+,l_+} c_{j_-,l_-},$$

where $c_{j_-,l_-}$ is a complex coefficient. Because of the TR relation $f_{j_+,l_+} = -f_{j_-,l_-}^*$, $f_{j_+,l_+}$ can be expressed in terms of $l + 1$ linearly independent basis as

$$f_{j_+,l_+} = \sum_{m=0}^{l} f_{j_+,l_+,m+1/(2),m} q_m^m.$$

The topological nature of the 3D LL problem exhibits clearly in the gapless surface states. A numeric calculation of the gapless surface spectra is presented in the Supplemental Material [63]. At $qG > 0$, inside the bulk, LL spectra are flat with respect to $j_+ = l + 1/2$. As $l$ goes large, the classical orbital radius $r_c$ approaches the open boundary with the radius $R_0$. For example, for a LLL state, $r_c = \sqrt{2l_G}$. States with $l > l_+ = 1/(2R_0/l_G)$ become surface states. Their spectra become $E(l) = l(l+1) + \hbar^2/(2m r_c^2) - \hbar \omega_0$. When the chemical potential $\mu$ lies inside the gap, it cuts the surface states with the Fermi angular momentum denoted by $l_f$. These surface states satisfy $\tilde{\sigma} \cdot \tilde{L} = \hbar l_f$; thus, their spectra can be linearized around $l_f$ as $H_{bd} = (v_f / R_0) \tilde{\sigma} \cdot \tilde{L} - \mu$. This is the Dirac equation defined on a sphere with the radius $R_0$. It can be expanded around $\tilde{r} = R_0 \tilde{\rho}$ as $H_{bd} = h x_f (\tilde{k} \times \tilde{\sigma}) \cdot \tilde{e}_z - \mu$. Similar reasoning applies to other Landau levels which also give rise to Dirac spectra. Because of the lack of Bloch wave band structure, it remains a challenging problem to directly calculate the bulk topological index. Nevertheless, the $\mathbb{Z}_2$ structure manifests through the surface Dirac spectra. Since each fully occupied LL contributes one helical Dirac Fermi surface, the bulk is $\mathbb{Z}_2$ nontrivial (trivial) if odd (even) number of LLs are occupied. In the $\mathbb{Z}_2$-nontrivial case, the gapless helical surface states are protected by TR symmetry and are robust under TR invariant perturbations.

$$e^{i(\alpha/2) \beta (\beta/2) e^{i(\gamma/2) \beta f_{j_+,l_+} (x', y', z') \right), \tag{7}$$

where $(x', y', z')$ are the coordinates by applying the inverse of $g$ on $(x, y, z)$. We check that
In Eq. (2), the harmonic frequency \( \omega_T \) is set to be equal with the SO frequency \( \omega_0 \) to maintain the flatness of LL spectra. However, the \( Z_2 \) topology of the 3D LLs does not rely on this. Define \( \Delta \omega = \omega_T - \omega_0 \), and we set \( \Delta \omega \approx 0 \) to maintain the spectra bounded from below. \( \Delta \omega > 0 \) corresponds to imposing an external potential \( \Delta V(r) = 1/2m(\omega_T^2 - \omega_0^2) r^2 \) to the bulk Hamiltonian of Eq. (2). If \( \Delta \omega \ll \omega_0 \), \( \Delta V(r) \) is soft. It results in energy dispersions of 3D LLs but does not affect their topology. For simplicity, let us check the case of \( \Delta G > 0 \). The \( \sigma \cdot \hat{L} \) term commutes with the overall harmonic potential; thus, the LL wave functions remain the same as those of Eq. (2) by replacing \( \omega_0 \) with \( \omega_T \). Their dispersions become \( E_{n,j} = (2n_r + 1)\hbar \omega_T + (1/2)\hbar \omega_0 + j_s \hbar \Delta \omega \) which are very slow. In other words, \( \Delta V(r) \) imposes a finite sample size with the radius of \( R^2 < \hbar/(m\Delta \omega) = 2l_G(\omega_0/\Delta \omega) \) even without an explicit boundary. Inside this region, \( \Delta V \) is smaller than the LL gap, and the LL states are bulk states. Their energies are within the LL gap and the angular momentum numbers \( j_s < (2\omega_T/\Delta \omega) \). LL states outside this region can be viewed as surface states with positive helicity. For a given Fermi energy, it also cuts a helical Fermi surface with the same form of effective surface Hamiltonian. The above scheme can be easily generalized to arbitrary dimensions [63] by combining the \( N \)-D harmonic oscillator potential and SO coupling. For example, in 4D, we have \( H^{1D,LL} = (p^2_3/2m) + (1/2)ma_0^2 \hbar^2 - \omega_0 \sum_{l,s,\alpha=\pm}\psi_{l,s}^{\alpha}L_{l,s} \), where \( L_{l,s} = R_a P_b - R_b P_a \) and the 4D spin operators are defined as \( \Gamma^{\alpha \beta} = -i(1/2)[\sigma^i, \sigma^j] \), \( \Gamma^{\alpha \beta} = \pm \sigma^i \) with \( 1 \leq i < j \leq 3 \). The signs of \( \Gamma^{\alpha \beta} \) correspond to two complex conjugate irreducible fundamental spinor representations of \( SO(4) \), and the \( + \) sign will be taken below. The spectra of the positive helicity states are flat as \( E_{n,m} = (2n_r + 2)\hbar \omega \). Following a similar method in 3D, we prove that the quaternionic version of the 4D LLL wave functions satisfy the full equation of Eq. (6). They form the complete basis for quaternionic left-analytic polynomials in 4D.

We consider the interaction effects in the LLLs. For simplicity, let us consider the 4D system and the short-range interactions. Fermions can develop spontaneous spin polarization to minimize the interaction energy in the LLL flat band. Without loss of generality, we assume that spin takes the eigenstate of \( \Gamma^{12} = \Gamma^{34} = \sigma^3 \) with the eigenvalue 1. The LLL wave functions satisfying this spin polarization can be expressed as \( \Psi_{m,n}^{LL,4D} = (x + iy)^m(z + iu)^n e^{-i(\alpha \cdot \mathbf{k})^2/2m} | \alpha \rangle \) with \( | \alpha \rangle = (1, 0)^T \). The 4D orbital angular momentum number for the orbital wave function is \( l = m + n \) with \( m \geq 0 \) and \( n \geq 0 \). It is easy to check that \( \Psi_{m,n}^{LL,4D} \) is the eigenstate of \( \sum_{a,b} L_{ab} \Gamma_{ab} \) with the eigenvalue \( (m + n)\hbar \). If all the \( \Psi_{m,n}^{LL,4D} \)'s are filled with \( 0 \leq m < N_m \) and \( 0 \leq n < N_n \), we write down a Slater-determinant wave function as

\[
\Psi(v_1, v_1; \ldots; v_N, w_N) = \det[v_\alpha^\alpha w_\beta^\beta],
\]

where the coordinates of the \( i \)th particle form two pairs of complex numbers abbreviated as \( v_i = x_i + iy_i \) and \( w_i = z_i + iw_i \); \( \alpha, \beta \), and \( i \) satisfy \( 0 \leq \alpha < N_m, 0 \leq \beta < N_n \), and \( 1 \leq i \leq N = N_m N_n \). Such a state has a 4D uniform density as \( \rho = \frac{1}{4\pi \hbar^2} \). We can write down a Laughlin-like wave function as the \( k \)th power of Eq. (9) whose filling relative to \( \rho \) should be \( 1/k^2 \). For the 3D case, we also consider the spin polarized interacting wave functions. However, it corresponds to that fermions concentrate to the highest weight states in the equatorial plane perpendicular to the spin polarization, and thus reduces to the 2D Laughlin states. In both 3D and 4D cases, fermion spin polarizations are spontaneous; thus, low energy spin waves should appear as low energy excitations. Because of the SO coupled nature, spin fluctuations couple to orbital motions, which leads to SO coupled excitations and will be studied in a later publication.

One possible experimental realization for the 3D LL system is the strained semiconductors. The strain tensor \( e_{ab} = 1/(2)(\delta_{ai}u_a + \delta_{ai}u_i) \) generates SO coupling as \( H_{SO} = \hbar \alpha[(\epsilon_{zi} k_i - \epsilon_{zi} k_j) \sigma_i + (\epsilon_{zi} k_i - \epsilon_{zi} k_j) \sigma_j + (\epsilon_{zi} k_i - \epsilon_{zi} k_j) \sigma_z] \) where \( \alpha = 8 \times 10^5 \text{ m/s} \) for GaAs. The 3D strain configuration with \( \tilde{u} = f/(yz, zx, xy) \) combined with a suitable scalar potential gives rise to Eq. (1) with the correspondence \( \omega_0 = (1/2)\alpha f \). A similar method was proposed in Ref. [11] to realize 2D quantum spin Hall LLs. A LL gap of 1 mK corresponds to a strain gradient of the order of 1% over 60 \( \mu \text{m} \), which is accessible in experiments. Another possible system is the ultracold atom system. For example, recently evidence of fractionally filled 2D LLs with bosons has been reported in rotating systems [64].

Furthermore, synthetic SO coupling generated through atom-light interactions has become a major research direction in ultracold atom system [65,66]. The SO coupling term in the 3D LL Hamiltonian \( \omega_T \sigma \cdot \hat{L} \) is equivalent to the spin-dependent Coriolis forces from spin-dependent rotations; i.e., different spin eigenstates along \( \pm x, \pm y, \) and \( \pm z \) axes feel angular velocities parallel to these axes, respectively. An experimental proposal to realize such an SO coupling has been designed and will be reported in a later publication [67].

In conclusion, we have generalized the flat LLs to 3D and 4D flat spaces, which are high dimensional topological insulators in the continuum without Bloch wave band structures. The 3D and 4D LLL wave functions in the quaternionic version form the complete bases of the quaternionic analytic polynomials. Each filled LL contributes one helical Dirac Fermi surface on the open boundary. The spin polarized Laughlin-like wave function is constructed for the 4D case. Interaction effects and topological excitations inside the LLLs in high dimensions would be interesting for further investigation. In particular, we expect that the quaternionic analyticity would greatly facilitate this study.

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