Low-energy electronic properties of Weyl semimetal quantum dot

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It is necessary to study the properties of Weyl semimetal nanostructures for potential applications in nanoelectronics. Here we study the Weyl semimetal quantum dot with a most simple model Hamiltonian with only two Weyl points. We focus on the low-energy electronic structure and show the correspondence to that of three-dimensional Weyl semimetal, such as Weyl point and Fermi arc. We find that there exist both surface and bulk states near Fermi level. The direct gap of bulk states reaches the minimum with the location determined by Weyl point. There exists a quantum number with only several values supporting surface states, which is the projection of Fermi arc. The property of surface state is studied in detail, including circular persistent current, orbital magnetic moment, and chiral spin polarization. Surface states will be broken by a strong magnetic field and evolve into Landau levels gradually. Simple expressions are derived to describe the energy spectra and electronic properties of surface states both in the presence and absence of magnetic field. In addition, this study may help design a method to verify Weyl semimetal by separating out the signal of surface states since quantum dot has the largest surface-to-volume ratio.

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I. INTRODUCTION

Topological materials have been one of the frontiers of condensed matter physics over the past decade, with the focus shifting from topological insulators1,2 to topological semimetals, one of which is Weyl semimetal proposed in 2011.3 Its conduction and valence bands touch at some crystal momentums, the Weyl points, in the first Brillouin zone near the Fermi level. The low-energy excitations behave like Weyl fermions described by Weyl equation4 suggesting a platform to study and verify the properties of Weyl fermions. Due to the “no-go” theorem2 Weyl points emerge in pairs in the crystal system, being the singular points of Berry curvature with opposite topological charge or chirality. There will be Fermi-arc surface states terminated at the projection of Weyl points due to the bulk-boundary correspondence. Recently, both Weyl points and Fermi arc have been discovered by ARPES measurements in TaAs6,7 soon after the prediction5,9 and then in some other materials10–18.

Plenty of attentions have been paid to Weyl semimetal15,18 including predicting new materials (especially those with less Weyl points locating near Fermi level or magnetic Weyl semimetal)3,19–22 verifying novel behaviors of Weyl fermions21,22 tuning these unique properties for real applications by magnetic or optical methods24,25. However, we notice that: (1) The measurement of magnetic Weyl semimetal is still challenging. All Weyl semimetal materials verified directly are time-reversal invariant6,7,19–16 though magnetic Weyl semimetal is predicted earlier2. Due to the formation of magnetic domains, the direct ARPES measurement is still unavailable in the magnetic Weyl semimetal. It is still in need to design an effective method to verify the magnetic Weyl semimetal. The observation of Fermi arc provides a method to verify the Weyl physics, which may be realised in a nanostructure with high surface-to-volume ratio. (2) So far, only a few reports pay attention to the low-dimensional system of Weyl semimetal26,27. Due to the high mobility28–30 dissipationless surface channels and exotic chirality anomaly, Weyl semimetal may play an important role in nanoelectronics and other fields. The study of Weyl semimetal nanostructures, including the electronic and transport properties, may be helpful and necessary for promoting the potential applications. And it’s also a wonder what’s the correspondence of those exotic behaviors of three-dimensional (3D) Weyl semimetal in low-dimensional systems and whether new phenomena would emerge.

Quantum dot (QD) is a zero-dimensional nanostructure with the largest surface-to-volume ratio30,31. It has been used widely with mature technology for conventional semiconductors. We believe that the study of Weyl semimetal QD will help reveal the evolution of properties of 3D Weyl semimetal in low-dimensional system, provide a new method of verifying Weyl semimetal by separating signal of surface states especially in transport measurements and promote the potential applications in nanoelectronics. As far as we know rare works focus on Weyl semimetal QD. At the same time we notice that there have been lots of works on the topological insulator QD32–48 focusing on the electronic structure36,49 orbital magnetic moment41 transport behavior42,44 applications in quantum computing45 and so on. Topological insulator QD has been fabricated successfully in experiments49,50. These works on topological insulator QD not only offer valuable lessons on the study of Weyl semimetal QD but also suggest that Weyl semimetal QD will be a fruitful field and deserves more attentions.

The first step in the study of Weyl semimetal QD is to understand the electronic structure and property. Generally, the confinement in the spatial distribution of ele-
trons result in the discrete quantization of energy levels and Coulomb interaction if there is several electrons in the QD. In this paper we focus on the first effect only. For simplicity, but still universal, we have chosen the model with only two Weyl points located on the z-axis which breaks the time reversal symmetry. The geometry is chosen to be a cylinder to simplify the numerical calculation without losing the universality for properties being protected topologically. The confinement in the z (axial) direction and rotation invariance around the axial direction result in good quantum numbers \( n_z \) and \( j_z \), which are the projections of quantized momentum and total angular momentum along z-direction, respectively. The direct energy gap of bulk states meets the minimum at certain \( n_z \) and \( j_z \), which is determined by the location of Weyl point. There will be both surface and bulk states near Fermi level. The surface state distributes on the side surface but absent on the top and bottom surfaces of the QD. It emerges only for several values of \( n_z \) which are determined by the spacing between the two Weyl points. The surface states are similar with Fermi-arc surface states and can be taken as its correspondence in QD system. We have analyzed the properties of the surface state in detail. The band of surface states depends linearly on \( j_z \), leading to chiral persistent currents and orbital magnetic moments. Its local spin direction is approximately parallel to the current indicating a correspondence of spin-momentum locking in 3D case. Besides we also study the size effect. There will be no surface state in an ultra thin Weyl semimetal QD, which suggests that it’s possible to control surface states by tuning its thickness. Magnetic field will break the surface state and lead to Landau quantization gradually. Energy bands in these two regimes, the surface state regime and Landau level regime, are fitted well with the derived expressions approximately. The location of the crossover of the two regimes is also fitted which provides a criterion to determine whether the magnetic filed or the system size is large enough to realize Landau quantization.

The rest of the paper is organized as follows. In Sec. II, we give the model Hamiltonian and describes the method to solve the electron structure of the cylinder Weyl semimetal QD. In Sec. III, we show the numerical results and analyses in the absence of the magnetic field. The effect of the magnetic field is discussed in Sec. IV. Finally, we provide a brief discussion and conclusion in Sec. V.

II. THE MODEL HAMILTONIAN AND FORMALISM

A. The Model Hamiltonian

In this paper, we study a model of Weyl semimetal with only two Weyl points, protected by inversion symmetry while with time reversal symmetry broken. The Hamiltonian in momentum space can be written as

\[
H = \tilde{\Delta}_z \sigma_z + A(k_x \sigma_x + k_y \sigma_y), \tag{1}
\]

in which the Zeeman term \( \tilde{\Delta}_z \) is given as

\[
\tilde{\Delta}_z = M - \frac{m_0}{2}(k_x^2 + k_y^2 + k_z^2). \tag{2}
\]

\( \sigma_{x,y,z} \) are the spin Pauli matrices. \( A, M \) and \( m_0 \) are model parameters. There are two energy bands which are obtained as

\[
E_{\pm}(k) = \pm \sqrt{\tilde{\Delta}_z^2 + A^2(k_x^2 + k_y^2)}. \tag{3}
\]

There is an energy gap if \( M/m_0 < 0 \), and it lies in a normal insulator phase. However, if \( M/m_0 > 0 \), these two bands will touch at two isolated points on z-axis, \( k_0 = (0, 0, \pm k_0)^T \), with \( k_0 = \sqrt{2M/m_0} \). This two-fold degenerate point is named Weyl point since low-energy excitations near \( k_0 \) can be described by Weyl equation approximately which is derived to be \( H_k = \mp i m_0 \delta_k \delta_z \sigma_z + A(\sigma_x \delta_k + \sigma_y \delta_{k_y}) \) in our model, with the new wave vector \( (\delta_k x, \delta_k y, \delta_{k_z}) = k - k_0 \) measured from the corresponding Weyl point. Weyl point is the singular point of Berry curvature in momentum space and has a topological charge determined by the flux of Berry curvature, \( \mp \text{sign}(m_0) \) at \((0, 0, \pm k_0)^T \) which also describes the chirality or helicity of the excitations. Weyl points always appear in pairs of opposite topological charge in bulk lattice. The two Weyl points in our model are related by spatial inversion.

It is obvious that the Hamiltonian in Eq.(1) is invariant with rotation around the axial direction, as is also presented clearly in the energy dispersion since it depends on \( k_z^2 + k_y^2 \) and \( k_x^2 \). Besides, we find that there is also another antiunitary symmetry described by

\[
P = \sigma_x K, \tag{4}
\]

where \( K \) is the complex conjugate operator. By replacing \( k \) with \( -i \partial_k \), it is straightforward to prove that \( P \) anti-commutes with the Hamiltonian in Eq. (1), which means \( \{P, H\} = 0 \) in coordinate representation. This symmetry leads to a constrain on the energy band, \( E_-(k) = -E_+(k) \), consistent with the energy band given above.

Hamiltonians with the opposite Zeeman term are related by time reversal transformation \( T \), which indicates \( H(-M, -m_0) = TH(M, m_0)T^{-1} \). On the other hand, Hamiltonians with the opposite \( A \) are related by rotating the spin space, which means \( H(-A) = \sigma_z H(A) \sigma_z \). Therefore, we take both \( A \) and \( m_0 \) to be real and consider both positive and negative \( M \) cases.

B. Formalism

In this paper, we consider a cylinder QD with height \( L \) and radius \( R \). We simulate this system by applying an infinite potential \( V = \infty \) outside the dot region. Therefore,
it will be convenient to solve the Schrödinger equation in the cylindrical coordinate system. The boundary condition becomes \( \Psi(r, \varphi, 0) = \Psi(r, \varphi, L) = \Psi(R, \varphi, z) = 0 \) and \( \Psi(r, \varphi, z) = \Psi(r, \varphi + 2\pi, z) \), with \( r, \varphi \) and \( z \) being the coordinates in the radial, tangential and axial direction, respectively.

In the absence of the translation invariance, momentum is not a good quantum number any more and it should be replaced with \( K = -i\partial_x \) in the Hamiltonian in Eq.(1). However, it will be enlightening to consider the case with only the confining potential along \( z \)-direction. We will get a two-dimensional film with \( k_{x,y} \) being good quantum numbers. Then, we arrive at the problem of standard one-dimensional infinite potential well for fixed \( k_z \) and \( k_y \), which has standing wave eigenvectors denoted by \( k_z = \frac{n\pi}{L} \) with \( n_z = 1, 2, 3, \ldots \). It indicates that the \( z \)-component can be separated. Besides, the projection of total angular momentum along \( z \)-axis, \( j_z \), is also a good quantum number since the Hamiltonian and geometry are rotation invariant around the \( z \)-axis. And these two good quantum numbers \( n_z \) and \( j_z \) ensure that variables \( \varphi \) and \( r \) can be separated from each other. A careful analysis suggests that the eigenvector can be written as

\[
\Psi_{n_z,j_z}(r, \varphi, z) = \phi_{n_z}(z) \psi_{j_z}(r, \varphi),
\]

\[
\phi_{n_z}(z) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L} z\right),
\]

\[
\psi_{j_z}(r, \varphi) = \frac{1}{\sqrt{2\pi}} e^{-i\frac{m\varphi}{L}} e^{ij_z\varphi} \left( A^{(n_z,j_z)}(r) B^{(n_z,j_z)}(r) \right).
\]

The \( z \)-component of total angular momentum is \( j_z = L_z + \hat{s}_z \), with \( L_z = -i\partial_z \) and \( \hat{s}_z = \sigma_z/2 \) being the orbital and spin operators respectively. The eigenvector of \( L_z \) is \( e^{im\varphi}/\sqrt{2\pi} \) with eigenvalue \( m \). It’s straightforward to verify that \( j_z \psi_{j_z}(r, \varphi) = j_z \psi_{j_z}(r, \varphi) \). For a more intuitive understanding, we rewrite the eigenvector as

\[
\psi_{j_z}(r, \varphi) = \left( A^{(n_z,j_z)}(r) \right) \frac{e^{(m-1)\varphi}}{\sqrt{2\pi}} e^{im\varphi} \left( B^{(n_z,j_z)}(r) \right).
\]

For the spin-up component, \( L_z = m - 1, \ s_z = 1/2 \), while for the spin-down component \( L_z = m, \ s_z = -1/2 \). Therefore, for the both components, we have the total angular momentum \( j_z \) related to the parameter \( m \) by

\[
j_z = m - \frac{1}{2}.
\]

The Hamiltonian in cylindrical coordinate, \( H(r, \varphi, z) \), can be obtained by substituting the momentum operator in the form of

\[
k_+ = e^{i\varphi} \left( -i\partial_r + \frac{1}{r}\partial_\varphi \right),
\]

\[
k_- = e^{-i\varphi} \left( -i\partial_r - \frac{1}{r}\partial_\varphi \right),
\]

\[
k_z^2 + k_y^2 = \frac{1}{r^2} \partial_r^2 + \frac{1}{r}\partial_\varphi + \partial_\varphi^2.
\]

With the wave function of fixed quantum numbers \( n_z \) and \( j_z \), Eqs. (5a) and (5b) substituted, the Schrédinger equation can be reduced with only the radial component left. Then we have the radial Schrödinger equation in the form of

\[
H_{n_z,j_z}(r) \begin{pmatrix} A_{m-1}(r) \\ B_m(r) \end{pmatrix} = E \begin{pmatrix} A_{m-1}(r) \\ B_m(r) \end{pmatrix}.
\]

The quantum number \( n_z \) in the eigenvectors \( A_{m-1}^{(n_z)}(r) \) and \( B_m^{(n_z)}(r) \) is not marked explicitly in the above equation and it will also be the case in the following unless it causes confusion. Then replacing \( k_z \) with \( n_z\pi/L \) and taking a unitary transformation \( H = UH(r, \varphi, z)U^\dagger \) with the unitary matrix \( U = e^{i\frac{m\varphi}{L}} e^{-ij_z\varphi} \), the radial Hamiltonian in Eq.(10) can be obtained as

\[
H_{n_z,j_z}(r) = \begin{pmatrix} M_{n_z} + \frac{m^2}{r^2} & iA \hat{j}^{(m-1)}(r) \\ iA \hat{j}^{(m-1)}(r) & -[M_{n_z} + \frac{m^2}{r^2}] \end{pmatrix},
\]

in which we have denoted the effective mass term

\[
M_{n_z} = M - \frac{1}{2} m_0 \left( \frac{n_z\pi}{L} \right)^2
\]

and several new operators

\[
\hat{j}^{(m)}(r) = -\frac{m^2}{r^2} + \frac{1}{r}\partial_r + \partial_\varphi,
\]

\[
\hat{j}^{(m)}(r) = \partial_r + \frac{m}{r},
\]

\[
\hat{j}^{(m)}(r) = -\partial_r + \frac{m}{r}.
\]

The axial and angular components of the eigenvector given in Eqs.(6) and (5b) satisfy the boundary and normalization conditions. For the radial component, these two conditions demand

\[
\int_0^R |A_{m-1}(r)|^2 + |B_m(r)|^2 dr = 1.
\]

The radial Schrödinger equation, Eq.(11), can be solved by expanding the wave function with an appropriate basis. We notice that the first kind Bessel function of \( m \)-th order, \( J_m(r) \), is the eigenvector of the operator \( \hat{j}^{(m)}(r) \), while \( \hat{j}^{(m)}(r) \) and \( \hat{j}^{(m)}(r) \) are the raising and lowering operators of \( J_m(r) \) respectively, which means

\[
\hat{j}^{(m)}(r) \hat{J}_m(r) = -J_m(r),
\]

\[
\hat{j}^{(m)}(r) \hat{J}_m(r) = \hat{J}_{m+1}(r),
\]

\[
\hat{j}^{(m)}(r) \hat{J}_m(r) = \hat{J}_{m-1}(r).
\]

It suggests that an appropriate basis to expand the radial eigenvector can be constructed with the first kind Bessel function and

\[
\hat{j}^{(m)}(r) = \frac{J_m(x_n^{(m)} \frac{r}{L})}{N_n^{(m)}},
\]
where $x^{(m)}_n$ is the $n$-th node of the first kind Bessel function of $m$-th order, i.e. $J_m(x^{(m)}_n) = 0$. And $N^{(m)}_n = \frac{R J_{m+1}(x^{(m)}_n)}{\sqrt{2}}$ is the normalization factor. The orthonormal constraint is satisfied $\int_0^R J^{(m)}_n(r) J^{(m)}_{n'}(r) r dr = \delta_{n,n'}$.

Then we can expand the radial eigenvector as

$$A_{m-1}(r) = \sum_n A^{(m-1)}_n J^{(m-1)}_n(r),$$

$$B_m(r) = \sum_n B^{(m)}_n J^{(m)}_n(r),$$

(16)

where $A^{(m-1)}_n$ and $B^{(m)}_n$ are expansion coefficients satisfying the normalization condition $\sum_n |A^{(m-1)}_n|^2 + \sum_n |B^{(m)}_n|^2 = 1$. The boundary condition of Eq. (16) is satisfied automatically by using the basis $\tilde{J}_n^{(m)}(r)$. The coefficients $A^{(m-1)}_n$ and $B^{(m)}_n$ can be obtained by substituting the expanded eigenvector Eq. (16) into the radial Schrödinger equation, Eq. (15) and then solving the eigenvalue problem. In the new basis of Bessel functions, the radial Schrödinger equation becomes

$$\sum_{n'} [(\tilde{J}^{(m-1)}_n | H_{11} | \tilde{J}^{(m-1)}_{n'}) A^{(m-1)}_{n'} + (\tilde{J}^{(m-1)}_n | H_{12} | \tilde{J}^{(m)}_{n'}) B^{(m)}_{n'}]$$

$$= EA^{(m-1)}_n,$$

$$\sum_{n'} [(\tilde{J}^{(m)}_n | H_{21} | \tilde{J}^{(m-1)}_{n'}) A^{(m-1)}_{n'} + (\tilde{J}^{(m)}_n | H_{22} | \tilde{J}^{(m)}_{n'}) B^{(m)}_{n'}]$$

$$= E B^{(m)}_n,$$

(17)

where $H_{ij}$ is the $(i,j)$ element of the Hamiltonian operator matrix $H_{njz,jz}(r)$ and we have used the Dirac bracket to represent the wave function for convenience. In this discrete representation, each element of Hamiltonian matrix can be obtained as

$$\langle \tilde{J}^{(m-1)}_n | H_{11} | \tilde{J}^{(m-1)}_{n'} \rangle = [M_{n_z} - \frac{m_0}{2} (x^{(m-1)}_n / R)^2] \delta_{nn'},$$

$$\langle \tilde{J}^{(m)}_n | H_{22} | \tilde{J}^{(m)}_{n'} \rangle = -[M_{n_z} - \frac{m_0}{2} (x^{(m)}_n / R)^2] \delta_{nn'},$$

$$\langle \tilde{J}^{(m)}_n | H_{21} | \tilde{J}^{(m-1)}_{n'} \rangle = (\tilde{J}^{(m-1)}_n | H_{12} | \tilde{J}^{(m)}_{n'}),$$

$$= i A^{(m-1)}_n \frac{J_m(x^{(m)}_n)}{R} J_m(x^{(m)}_n/r/R)J_m(x^{(m-1)}_n/r/R) r dr. \quad (18)$$

The number of basis functions used in the expansion is chosen to ensure the convergence of the energy levels near the Fermi level. It is adequate to take 800 basis functions in our calculation.

Finally, we point out that the phase of the eigenvector can be thus chosen, $A_{m-1}(r)$ is real while $B_m(r)$ is imaginary. This point can be seen clearly by rotating the spin space with a unitary matrix

$$S = \begin{pmatrix} 1 & i \\ i & 1 \end{pmatrix}. \quad (19)$$

After this transformation, we can obtain a real radial Hamiltonian $H'_{njz,jz}(r) = S H_{njz,jz}(r) S^T$ and therefore a real eigenvector $(A^{(m-1)}_n, B'_m)^T = S (A_{m-1}, B_m)^T$. Then, we can set $A_{m-1}(r)$ real while $B_m(r)$ imaginary.

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**III. ELECTRONIC STRUCTURE AND PROPERTIES OF WEYL SEMIMETAL QD**

This section gives the numerical results and analyses in the absence of external magnetic field. Firstly, we study the energy spectra as a function of the total angular momentum $j_z$. There will be a linear band in the energy gap regime if the system lies in the Weyl semimetal phase. It is verified to be the band of surface states by plotting the electron density distribution and calculating the dependence of energy on QD size. Then, we further calculate the corresponding current density distribution, orbital magnetic moment and the spin orientation to show the property of these surface states. Finally, we show the projection of Fermi arc and Weyl point of 3D Weyl semimetal in the QD system. Besides, we study the size effect as well. In the numerical calculations, unless otherwise stated, we take the cylinder QD with height $L = 100$ nm and radius $R = 75$ nm, and the systemic parameters are set $A = 500$ meVnm, $m_0 = 1000$ meVnm^2, $M = 50$ meV and $-50$ meV for the Weyl semimetal phase and the normal insulator phase, respectively.

**A. Energy spectra**

The confinement in axial, tangential and radial direction leads to energy quantization denoted by $n_z$, $j_z$ and $n_r$, respectively. At first we consider the $n_z = 1$ subband. In Fig. 1(a) we plot the energy spectra as a function of the total angular momentum $j_z$. Fig. 1(a) and Fig. 1(b) correspond to the normal insulator and Weyl semimetal cases respectively. It’s clear that the energy spectra is not symmetric about $j_z$, which means $E_{n_z,-j_z} \neq E_{n_z,j_z}$.
However, with a detailed analysis we find that there exists an alternative relation written as

\[ E_{n_z, -j_z} = -E_{n_z, j_z}. \]  

(20)

We have pointed out that the Hamiltonian in Eq. (11) satisfies a certain symmetry determined by an antiunitary transformation \( P = \sigma_x K \). For the radial Hamiltonian \( H_{n_z, j_z} \) as shown in Eq. (11), it results in

\[ PH_{n_z, j_z}(r)P^\dagger = -H_{n_z, -j_z}(r), \]

(21)

which leads to the constrain on energy spectra shown in Eq. (20) and constrain on corresponding eigenstates,

\[ \psi^{(n_z)}(r) = \sigma_x[\psi^{(n_z)}(r)]^*. \]  

(22)

Considering this relation, we are able to focus only on eigenstates with the positive angular momentum.

Another and the most significant feature is that the energy spectra is gapped for the normal insulator QD, shown in Fig. (1a), while there is a linear band (red dots) emerging even in the gap regime for the Weyl semimetal QD, shown in Fig. (1b). As is well known, the energy band due to edge or surface states of topological insulators is a linear Dirac cone. Therefore, it is natural to expect that the linear band here may correspond to surface states as well. To test this point, we plot the distribution of electrons in this linear band and study the dependence of these energy levels on QD radius \( R \).

For an electron in the eigenstate described by Eq. (5), the density distribution \( \rho(r, \varphi, z) = \Psi^\dagger(r, \varphi, z)\Psi(r, \varphi, z) \) is given as,

\[ \rho(r, \varphi, z) = \frac{2\sin^2(n_z\pi z/L)}{L}(|A_{n_z-1}^2(r)| + |B_{n_z}^2(r)|). \]

(23)

It is independent of \( \varphi \) because of the rotation invariance around the axial direction. The distribution in the axial direction is described by a sinusoidal function. Then the unknown is only the radial distribution which is determined numerically and plotted in Fig. 2 (b) for an electron in the linear band \( (n_r = 0) \) and two neighbouring bands \( (n_r = \pm 1) \) with angular momentum \( j_z = 1/2 \).

It’s obvious that the red line, eigenvector from the linear Dirac cone, is a linear Dirac cone.

\[ \rho^{(n_z)}(r) = \sigma_x[\rho^{(n_z)}(r)]^*. \]

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It’s obvious that the red line, eigenvector from the linear band, locates near the side surface of the QD, which is consistent with the feature of surface wave states. But the other eigenvectors spread over the whole QD region, which is the feature of bulk states. Fig. 2 (a) plots the corresponding electron density distributions of the first conduction band \( (n_r = 1) \) and the first two valence bands \( (n_r = 0, -1) \) of the normal insulator QD with \( j_z = 1/2 \).

All three states spread over the whole QD displaying bulk state behavior as expected.

The dependence of the energy levels on the radius of Weyl semimetal QD is calculated and shown in Fig. 3. Fig. 3(a) focuses on the linear band \( (n_r = 0) \). The energy level \( E_{j_z=1/2, n_r=0} \) and energy spacing \( \delta E_L = E_{j_z=1/2, n_r=0} - E_{j_z=3/2, n_r=0} \) depend linearly on the inverse of the radius, \( 1/R \), as expected for surface states on the side surface. However, the direct gap \( E_g = E_{j_z=1/2, n_r=1} - E_{j_z=1/2, n_r=-1} \) of the normal insulator QD, shown in Fig. 3(b), which is the bulk state behavior.

From the electron density distribution and energy dependence on QD radius, it concludes that the linear band corresponds to the surface state. It emerges since the topology of the Weyl semimetal QD and the vacuum is determined numerically and plotted in Fig. 2 (b) for the normal insulator phase (a) and Weyl semimetal phase (b). For the normal insulator phase, the three bands are the first conduction band \( (n_r = 1) \) and the first two valence bands \( (n_r = 0, -1) \). For the Weyl semimetal phase, the bands with \( n_r = 1, 0, \) and \(-1\) are the first conduction band, linear band, and the first valence band, respectively. The other quantum numbers of the eigenstates are \( j_z = 1/2 \) and \( n_z = 1 \).

\[ \psi'(r) = \frac{1}{\sqrt{2}} \left( -i \cdot \text{sign}(A) \right) \hat{\psi}(r). \]

(24)

The phase is chosen according to numerical results and the unitary transformation \( S \) given in Eq. (19). We as-
We have replaced the coefficient $c_L$ in the approximate expression of the linear band Schrödinger equation, Eq. (9), then we can derive

$$ E = -j_z \frac{|A|}{\tilde{c}_L R} + j_z \frac{m_0}{2c_L^2 R^2}. $$  

Substituting this trial function into the radial Schrödinger equation, Eq. (9), then we can derive an approximate expression of the linear band

$$ E = -j_z \frac{|A|}{\tilde{c}_L R} + j_z \frac{m_0}{2c_L^2 R^2}. $$  

We have replaced the coefficient $c_L$ with $\tilde{c}_L$ manually to phenomenally describe the effect not included in the trial wave function, such as the extension of wave function in the QD and the unequal weight of spin components. It's clear that it depends linearly on angular momentum $j_z$. The second term is proportional to $1/R^2$ but with a much little weight factor, therefore it depends linearly on QD radius $R$ approximately. With the second term, Eq. (26) also describes the interplay of bulk and surface characteristics. The fitting line due to Eq. (26) is plotted in Fig. 1(b) (see the black solid line). We can see that a good fitting is realized with coefficient $\tilde{c}_L \approx 0.9$. However, we determine that $c_L \approx 0.96$ or 0.93 from the maximum and median of the electron density plotted in Fig. 2(b), respectively. It indicates that the extension of wave function decreases the effective radius of the surface state just as expected.

### B. Properties of the surface state

In this subsection, we study the electronic properties of the surface state. We focus on the current density distribution, orbital magnetic moment and the spin polarization. The surface state with $j_z = \frac{1}{2}$ is taken as an example.

#### 1. Current and magnetic moment

Here we show that there is a persistent vortex current due to the surface state. The local probability current density $\vec{J} (\vec{r})$ can be derived via the equation of continuity

$$ \frac{\partial \rho}{\partial t} + \nabla \cdot \vec{J} = 0, $$  

in which $\rho(\vec{r}) = \Psi^\dagger (\vec{r}, \varphi, z) \Psi (\vec{r}, \varphi, z)$ is the probability density of electrons. Here $\vec{r} = (x, y, z) = (r \sin \varphi, r \cos \varphi, z)$ is the 3D vector. With a straightforward process, we arrive at

$$ \vec{J} = -\frac{2}{\hbar} \text{Im} \left[ \frac{m_0}{2} \Psi^\dagger \sigma_z \nabla \Psi \right] + \frac{A}{\hbar} \text{Re} \left[ \Psi^\dagger (\vec{e}_z \sigma_z + \vec{e}_y \sigma_y) \Psi \right]. $$  

Due to the cylindrical geometry and rotation invariance, only the tangential current $J_\varphi$ does not vanish and it is independent of $\varphi$. For the eigenvector given in Eqs. (5) and (6), the tangential current $J_\varphi (r, z)$ becomes

$$ J_\varphi = \left[ -\frac{m_0}{2\pi \hbar} \psi_{j_z, n_z}^{(n_z)} (r) \left( \begin{array}{c} m - 1 \ 0 \ -m \end{array} \right) \frac{1}{r} \psi_{j_z, n_z}^{(n_z)} (r) + \frac{A}{2\pi \hbar} \psi_{j_z, n_z}^{(n_z)} (r) \sigma_y \psi_{j_z, n_z}^{(n_z)} (r) \right] \frac{2 \sin^2 (n_z \pi z / L)}{L}. $$  

The eigenvector will vanish on the axis of the cylinder QD, $\psi_{j_z, n_z}^{(n_z)} (r = 0) = 0$, except for the spin-up (spin-down) component of the state with $j_z = \frac{1}{2}$ ($j_z = -\frac{1}{2}$). Then it is evident from Eq. (29) that the current density $J_\varphi$ on the axis vanishes, which is consistent with the physical intuition. The distribution of $J_\varphi (r, z)$ in the axial direction is described by a sinusoidal function explicitly as seen in Eq. (29). Therefore we calculate and plot only the current density distribution in the horizontal plane in Fig. 4. The current locates around the side which is consistent with the density distribution of surface state. We find that there will always be $J_\varphi (r, z) < 0$ in the whole QD region which corresponds to a clockwise probability current and an anticlockwise electric current.

The probability current $I_\varphi$ can be calculated by integrating over the cross-section

$$ I_\varphi = \int_0^R \int_0^L J_\varphi (r, z) dr dz. $$  

And then we have the electric current $I_e = -e I_\varphi$ with $e$ being the magnitude of the electron charge. On the other
hand with the Hellmann-Feynman theorem, we can calculate the derivative of eigen-energy with respect to angular momentum \( j_z \). We derive that these two quantities are related by\(^{24}\)

\[ I_e = -\frac{e}{\hbar} \frac{dE_{n_z j_z n_x}}{dj_z} \]  

(31)
in which \( \hbar = 2\pi \hbar \) is the Plank constant. Similar expressions also apply for the current of the Bloch state and Andreev bound state in a Josephson junction. It indicates that the directions of currents due to all surface states are identical regardless of positive or negative angular momentums \( j_z \) because of the negative slope of the linear surface band shown in Fig. 1(b). In fact the flow directions are identical for the current of the Bloch state and\(^{24}\) 

\[ \text{Fig. 4: (Color online) The probability current density distribution of the surface state } n_r = 0, j_z = \frac{1}{2}, n_z = 1 \text{ in the horizontal plane. Red arrows show directions of both current and spin orientation.} \]

Particle in the ring, where the moment is independent of the ring size.\(^{25}\) It indicates that the surface state in Weyl semimetal QD can be seen as Weyl fermions confined in the side surface. On the other hand, we find that the current depends linearly on the inverse of QD radius \( 1/R \) as shown in Fig. 5. It suggests that the product of current and magnetic moment may be a constant. The numerical result in Fig. 4 indicates that

\[ \frac{M_z I_e}{\pi A^2} \approx \frac{e^2}{h^2}. \]  

(33)

By supposing a perfect surface state, we can derive an analytical current formula and explain the dependence of current and magnetic moment on QD radius approximately. Here the perfect surface state means that the radial component of the wave function located at a certain \( R_L \) and it can be written as

\[ \psi(r) = \begin{pmatrix} A_L \\ B_L \end{pmatrix} \tilde{\psi}(r), \]  

(34)

where \( \tilde{\psi}(r) \) is given in Eq. 25. This wave function is similar with that defined in Eq. 24 but with no constrain on the weight on two spin components. The normalization condition is realized by setting \( |A_L|^2 + |B_L|^2 = 1 \). Substituting the trial wave function given in Eq. 34 into the current formula in Eqs. 24 and 25, we derive

\[ hI_\varphi = -\frac{|A|}{R_L} \sqrt{1 - 4\langle s_z \rangle^2} + \frac{m_0}{2R_L^2} - \frac{2m_0}{R_L^2} j_z \langle s_z \rangle, \]  

(35)

where \( \langle s_z \rangle = (|A_L|^2 - |B_L|^2)/2 \) is the mean value of z-component of spin. The numerical calculation suggests...
that \( \langle s_z \rangle \) is small, shown in Fig.13 at \( B = 0 \), which indicates that the current is nearly independent of angular momentum \( j_z \). With \( \langle s_z \rangle \) neglected, the current formula becomes

\[
hI = -\frac{|A|}{R_L} + \frac{m_0}{2R_L^2}. \tag{36}
\]

The first term is dominate and it depends on QD radius linearly, which explains the numerical results in Fig. 5.

With the help of Eq. (34), we can derive the energy dispersion of the perfect surface state with the derived current expression in Eq. (36). In fact, we are able to arrive at an identical expression as is given in Eq. (26). This consistency indicates the reliability of our analytical derivation.

According to Eq. (32), the magnetic moment and current are related by \( M_z = \pi R_L |A| - \frac{\pi}{2} m_0 \).

The second term is much smaller than the first term in our parameter regime and then it explains the linear dependence of the magnetic moment on QD radius. Eqs. (30) and (37) combine to lead to \( \frac{M_z}{e/h} = \pi R_L |A| - \frac{\pi}{2} m_0 \).

2. Spin orientation

As is well known that the spin and momentum will be locked for the edge or surface state of topological materials. Recently, the spin texture of Fermi arc in Weyl semimetal is also observed directly by ARPES measurements. Here we show that there is also a corresponding relation in our Weyl semimetal QD system. Considering that momentum is not a good quantum number now in the absence of translation invariance, we replace momentum with current and study the relation between spin orientation and the flow direction of current.

The density distribution of spin can be calculated by \( \langle s_i \rangle = \frac{1}{2} \Psi \dagger \sigma_i \Psi \). For the surface state, the radial (\( \langle s_r \rangle \)), tangential (\( \langle s_\phi \rangle \)) and axial (\( \langle s_z \rangle \)) components can be derived as

\[
\langle s_r \rangle = \frac{2\sin^2(n_z \pi z/L)}{L} |A_{m-1}(r)B_m(r)| \cos \delta \theta,
\]

\[
\langle s_\phi \rangle = \frac{2\sin^2(n_z \pi z/L)}{L} |A_{m-1}(r)B_m(r)| \sin \delta \theta,
\]

\[
\langle s_z \rangle = \frac{2\sin^2(n_z \pi z/L)}{L} \left( |A_{m-1}(r)|^2 - |B_m(r)|^2 \right) / 2. \tag{38}
\]

where \( \delta \theta = \theta_B - \theta_A \) determines the phase difference between the radial wave function \( A_{m-1}(r) \) and \( B_m(r) \). Fortunately, \( \delta \theta \) is a constant and can be taken to be \(-\pi/2\) according to our numerical calculation and discussions above. It vanishes the radial component, \( \langle s_r \rangle = 0 \), and indicates that the spin lies in the plane of surface states. The projection of spin in the horizontal plane is antiparallel to the azimuthal direction, which suggests a clockwise distribution. As we have shown, it is also clockwise for the probability current density, \( J = -|\mathbf{J}| e \phi \). Therefore the projection of spin on the horizontal plane will be parallel with the current. Our numerical calculation suggests that \( \langle s_z \rangle \) is small enough to be neglected (see Fig.13 at \( B = 0 \)). Then we arrive at

\[
\frac{\mathbf{J} \cdot \hat{z}}{|\mathbf{J}| |\hat{z}|} \approx 1. \tag{39}
\]

It is similar with the definition of helicity which is the projection of spin on the moving direction. Eq. (39) suggests that an electron in the surface state has a positive helicity or chirality. In fact, the value of \( \frac{\mathbf{J} \cdot \hat{z}}{|\mathbf{J}| |\hat{z}|} \) is mainly determined by the topological properties of the system. It corresponds to the spin-momentum locking in 3D case.

C. Quantization in the axial direction

In this subsection we reveal the effect of quantization in the axial direction which is denoted by \( n_z \). We construct the relation between properties of Weyl semimetal QD and Weyl semimetal. Besides, we also study the size effect.

In Fig. 6 we plot the energy spectra for \( n_z = 1, 4, 7, 8, 9, 10, 13, \) and 16. We find that there is a linear band in the gap regime for \( n_z = 1, 4, 7, \) and 8, which is fitted well by the black line due to Eq. (26). The linear band.
disappears for \( n_z = 10, 13, 16 \) leaving a bare energy gap. The case of \( n_z = 9 \) lies in the crossover regime, though we also use Eq. (28) to fit the band. The direct energy gap decreases gradually with raising \( n_z \) at first for \( n_z \leq 10 \), reaches the minimum at \( n_z = 10 \) and then increases with raising \( n_z \) any more. It indicates that the linear band, which has been proved to be the band of surface states in the discussion above, approaches the bulk band gradually as the direct gap decreases and merges into the bulk band at the minimum of the bulk gap.

The linear band for small \( n_z \) (\( n_z \leq 8 \)) is expected naturally to be surface states as is shown in Fig. 7 where we plot and study the evolution of the radial electron density distributions for eigenstates with \( j_z = 1/2, n_r = 0 \) and several \( n_z \). The \( n_r = 0 \) band corresponds to the linear band for \( n_z < 9 \) while the first conduction band for \( n_z \geq 9 \), respectively. We have a surface state for \( n_z = 1, 4, 7, 8 \), while the weight of distribution shifts from the side surface to the bulk of the QD with increasing \( n_z \). The density distribution of \( n_z = 9 \) lies in the crossover regime with a considerable weight both around the side surface and spreading in the bulk. For \( n_z = 10, 13 \) and 16, the weight has shifted mostly into the bulk. It indicates that the eigenstate denoted by \( j_z = 1/2 \) and \( n_r = 0 \) evolves from the surface state into the bulk state gradually with increasing \( n_z \).

Our numerical results indicate that there will be both surface and bulk states near the Fermi level due to sub-bands corresponding to different \( n_z \), which makes the Weyl semimetal QD distinguished from the topological insulator QD and conventional semiconductor QD. It is consistent with the coexistence of Weyl point (bulk states) and Fermi arc (surface states) in 3D Weyl semimetal and may be taken as its projection in zero-dimensional QD system. The minimum of the bulk energy gap corresponds to the Weyl point which is the touch point of valence and conduction bands. The chirality of Weyl points determines the flow direction of the vortex current of surface states. Surface states of the Weyl semimetal QD emerge for several \( n_z \) only, which is the correspondence that surface states of 3D Weyl semimetal exist only for several momentum to form the Fermi arc. It is fortunate that these correspondences exist and it allows the study of Weyl semimetal in the QD system.

The location of the minimum of direct bulk gap borders on the region with surface states and it is determined by the spacing of two Weyl points of 3D Weyl semimetal. If we take \( k_z = n_z \pi / L \) as a constant, then the Hamiltonian in Eq. (1) becomes a two-dimensional system, with \( M_{n_z} \) acting as the mass term. A negative \( M_{n_z} \) leads to a normal insulator phase, while a positive one leads to a quantum anomalous Hall phase with edge states which are just the surface states in our QD system. The criterion \( M_{n_z} > 0 \) demands \( k_z = n_z \pi / L < k_0 \) for the emergence of surface states, where \( k_0 \) is half of the spacing between two Weyl points. It explains why surface states emerge for small \( n_z \) while disappear for large \( n_z \).

This criterion predicts that there will be surface states in the regime \( n_z = 1 \sim 10 \) for parameters we have chosen. However, our numerical results show that the \( n_z = 9 \) case lies in the crossover regime and there is no surface state for \( n_z = 10 \) case. This inconsistency is due to the size effect. To show this point, we plot the radial electron density distribution \( \rho(r) \) of the eigenstate with \( j_z = 1/2, n_r = 0, n_z = 9 \) for several QD radius \( R \). The result is shown in Fig. 8(a), and it’s clear that the weight shifts from the bulk to the side surface as we increase the QD radius. Once the radius is large enough it turns out to be a surface state. Therefore, it is the size effect that...
breaks the surface state for \( n_z \) neighbouring the critical value and results in the crossover regime.

Fig. 8(b) plots the radial electron density distribution \( \rho(r) \) to show the effect of QD height \( L \). It’s clear that \( \rho(r) \) locates around the side surface for a large \( L \) for the chosen two eigenstates. Decreasing \( L \) will shift the weight to the bulk. The \( n_z = 7 \) eigenstate becomes a bulk state already for \( L = 50 \) nm while it is still a surface state even for \( L = 25 \) nm in the case of \( n_z = 1 \) eigenstate. It indicates that a large QD height is in favor of the emergence of surface states and the eigenstates with large \( n_z \) will be effected more significantly by QD height, which can be inferred from the criterion \( M_{n_z} = M - \frac{3}{2}m_0(c^2/2) < 0 \). An extreme case is that if \( L \) is small enough to make \( M_{n_z} < 0 \) for any \( n_z \), then there will be no surface states any more. This effect provides a feasible method to control the surface state.

IV. THE EFFECT OF MAGNETIC FIELD ON SURFACE STATES

In this section we study the property of surface states in the presence of a uniform magnetic field \( \mathbf{B} = (0, 0, B) \) along axial direction. By studying the evolutions of energy levels and radial electron density distribution, we show that magnetic fields will break topological surface states gradually to form Landau levels. The location of the crossover regime separating these two phases is determined with a approximate derivation. Besides, we also study the spin polarization. Without loss of generality, we focus on the \( n_z = 1 \) case to show these interesting properties.

Magnetic fields will induce two types of contributions, the orbital and Zeeman effects. The Zeeman term takes the same form as \( \Delta_z \sigma_z \) in the Hamiltonian given in Eq. (1), but with a smaller magnitude. Therefore it is neglected in the following discussion. The orbital effect can be included by a Peierls substitution \( k \rightarrow \pi = k + \frac{\pi}{2} \mathbf{A} \), where \( \mathbf{A} \) is the vector potential and \( e \) is the magnitude of the elementary charge. Then the Hamiltonian in Eq. (11) becomes

\[
H = \left( M - \frac{m_0}{2}(\pi_x^2 + \pi_y^2 + k_z^2) \right) - \frac{A\pi_z}{A\pi_+} \left[ M - \frac{m_0}{2}(\pi_x^2 + \pi_y^2 + k_z^2) \right] \tag{40}
\]

in which \( \pi_\pm = \pi_x \pm \pi_y \). For a cylinder geometry, we take the gauge as \( \mathbf{A} = \mathbf{B} \times \hat{r}/2 \), which becomes \( \mathbf{A} = \frac{\mathbf{B}_z}{2} \mathbf{r} \) in the cylindrical coordinate system. It is clear that the rotation invariance survives and there is no \( z \)- and \( \varphi \)- dependent terms in the vector potential. Therefore, the two variables \( z \) and \( \varphi \) can be separated the same as we have done in the absence of magnetic field, making \( n_z \) and \( j_z \) still good quantum numbers. And the eigenvector shares the identical form as is given in Eqs. (15) and (32), then it’s enough to modify the radial Hamiltonian by adding an extra term

\[
\delta H = \frac{m_0}{2} \mathbf{B}_z \sigma_0 + \mathbf{A} \mathbf{B}_z \sigma_y - m_0 \mathbf{B}_z j_z \sigma_z - \frac{m_0}{2} \mathbf{B}_z^2 r^2 \sigma_z \tag{41}
\]

in which \( \sigma_0 \) is a \( 2 \times 2 \) identity matrix and \( \mathbf{B}_z = \frac{\mathbf{e}_z}{2} \mathbf{B} \) proportional to the magnetic field with magnitude \( 7.583 \times 10^{-4}/(\text{nm})^2 \) for \( B = 1 \text{T} \). The first term is a trivial constant to shift the energy spectra as a whole. The second and last two terms are to revise the spin-orbit coupling and Zeeman terms respectively.

The evolution of energy levels against the magnetic field is plotted in Fig. 9. A detailed analysis indicates that the energy spectra displays a symmetry

\[
E_{-j_z}(-B) = -E_{j_z}(B). \tag{42}
\]

In absence of magnetic field it reduces to Eq. (20), which suggests that this relation is also due to the antunitary transformation \( \mathbf{P} \) given in Eq. (11). It’s straightforward to prove that \( \mathbf{P} \mathbf{H}_{-j_z,-B} \mathbf{P}^\dagger = -\mathbf{H}_{j_z,B} \) which leads to the symmetry of energy spectra given in Eq. (12) and a constrain on corresponding eigenvectors

\[
\psi_{j_z,B} = \mathbf{P}\psi_{-j_z,-B}. \tag{43}
\]

The energy level of the specific eigenstate with \( j_z = \frac{1}{2} \) and \( n_r = 0 \) is plotted as the black line in Fig. 9. It can be divided into three linear regimes with different slopes. The lines corresponding to eigenstates of \( n_r = 0 \) but with different \( j_z \) are nearly parallel in the weak field regime but degenerate in both positive and negative strong field regimes. There is a crossover regime separating the weak and strong regimes and its location \( B_c \) varies between eigenstates labeled with \( j_z \).

To further understand the weak and strong field regimes, we plot the radial electron density distributions of eigenstates for several magnetic fields with fixed angular momentum \( j_z = \frac{1}{2} \) in Fig. 10(a) and for different \( j_z \) with fixed magnetic field \( B = 5 \text{T} \) in Fig. 10(b). It’s clear that the eigenvector is a surface state in the weak field regime for curves with \( B = 0, 1 \text{T} \) in Fig. 10(a)
and \( j_z = -\frac{3}{2}, \frac{7}{2} \) in Fig. 10(b). However, eigenvectors distribute in the bulk in the QD in the strong field regime for curves with \( B = -3 \) T and 5 T in Fig. 10(a) and \( j_z = -\frac{3}{2} \) and \(-\frac{11}{2} \) in Fig. 10(b). Eigenstates with \( B = -2 \) T and 2.2 T in Fig. 10(a) and \( j_z = -\frac{19}{2} \) and \(-\frac{21}{2} \) in Fig. 10(b) lie in the crossover regime, and we find that the electron density distribution is a mixing of states in the bulk and on the side surface.

Figure 11 displays the energy spectra for several magnetic fields \( B = 0, 1, 2.2, \) and \(\pm 5\) T. The \( n_r = 0 \) band is linear in Fig. 11(b,c) with \( B = 0 \) and 1 T lying in the weak magnetic field regime. As studied above, the linear band in the gap regime corresponds to surface states. It moves downward with rising magnetic field, partly merges with the bulk bands for \( B = 2.2 \) T. It becomes complex for \( B = 5 \) T. There is a linear band for \( j_z < -\frac{17}{2} \) but a flat band with high degeneracy for \(-\frac{17}{2} < j_z < 0 \), lying in the weak and strong field regimes respectively, concluded from Fig. 9. The case of \( B = -5 \) T is similar with the \( B = 5 \) T case, with eigenenergy and \( j_z \) reversed due to the \( P \) symmetry given in Eq. (12). Besides, we also notice that there is a dip and hump structure connected to the flat energy band in Fig. 11(a) and (e) respectively, which is similar to the structure predicted in the nanoribbon of quantum spin Hall and quantum anomalous Hall insulators. It suggests that the dip and hump structures may be universal in topological nontrivial materials in presence of strong magnetic field.

By assuming a perfect surface state the same as that in Eq. (24), we can derive a simple expression of the energy spectra of the surface band,

\[
E_{j_z}(B) = -j_z\left(\frac{|A|}{R_L} - \frac{m_0}{2R_L^2}\right) - A|\vec{B}R_L + \frac{1}{2}m_0\vec{B},
\]

which reduces to Eq. (26) in the absence of magnetic field. It depends linearly on magnetic field and angular momentum, consistent with numerical results in the weak magnetic field regime. The linear bands in the weak field regime are fitted well with this expression as red circles in Fig. 9 and red lines in Fig. 11 respectively. In the strong field regime, magnetic field makes the weight of distribution shifts from the surface to the bulk to break the surface state as is shown in Fig. 10(a) for eigenstate with \( j_z = \frac{1}{2} \). Resultantly, Eq. (44) lacks the high degeneracy of eigenstates with different \( j_z \) and fails to describe the degenerate band in the strong field regime. The critical magnetic field depends on \( j_z \). Therefore, there will be states with higher \( j_z \) still distributing near the surface for a large magnetic field, which originate from both the nontrivial topology and magnetic field, as is shown by the states fitted with red lines in Fig. 11(a) and (e).

In general, a strong magnetic field will lead to Landau quantization. Therefore it’s also expected that Landau quantization occurs in the Weyl semimetal QD system in the strong magnetic field regime. Landau levels of a infinite system can be derived to be

\[
E_N^{(c)} = m_0\vec{B} + \sqrt{(M_{n_z} - 2m_0\vec{B}|N)^2 + 4A^2|\vec{B}|N}, \quad E_0 = m_0\vec{B} - \text{sign}(\vec{B})M_{n_z},
\]

\[
E_N^{(h)} = m_0\vec{B} - \sqrt{(M_{n_z} - 2m_0\vec{B}|N)^2 + 4A^2|\vec{B}|N},
\]

in which \( N = 1, 2, ..., \) \( E_0 \) is the zeroth mode, and \( E_N^{(c)} \) (\( E_N^{(h)} \)) describes the electron-like (hole-like) Landau levels. Degenerate magnetic levels in Fig. 9 and flat bands...
In Fig. 11(e) are well fitted by the zeroth and $N = 1$ Landau levels, which indicates the well formation of Landau levels in the strong magnetic field regime. The eigenvectors belonging to the same Landau level are expected to share the similar form but located in different positions in the bulk of QD as shown in Fig. 10(b). Based on these results, it concludes that the strong filed regime lies in the Landau quantization phase.

Combining Eqs. (44) and (45), it’s able to determine the location of the crossover regime between the weak and strong field phases. The transition from the surface state to the zeroth mode occurs at

$$\tilde{B}_c = \frac{-j_z \left( A \frac{\hbar}{R_L} - \frac{m_n}{2R^2} \right) + \text{sign}(\tilde{B}) M_{n_z}}{A R_L + \frac{m}{2}},$$

which also determines the beginning of Landau quantization. The analytical expression of the critical magnetic field $\tilde{B}_c$ transiting from the surface state to the $N = 1$ Landau level can also be derived by setting $E_1^{(r/h)} = E_{j_z}(B)$, in which $E_{j_z}(B)$ is the dispersion of surface states given in Eq. (14). But the expression of $\tilde{B}_c$ is in a tediously long form which is not given here. The calculated values lie approximately in the crossover regime in Figs. 9 and 11.

In Fig. 12 we plot the energy level as a function of QD radius $R$ for magnetic fields $B = 1, 1.5, 2, 2.5, 3$ T. The energy level decreases with raising $R$ at first and then saturates for $R$ larger than a critical value $l_B$. It’s as expected that $l_B$ will decrease with raising magnetic field. In the inset, we plot the radial electron density distribution $\rho(r)$ for $R = 75, 80, 85, 90$ nm at fixed $B = 2$ T. We find that it is a surface state for $R = 75$ nm, an eigenvector of Landau level for $R = 90$ nm similar with that in Fig. 9 and a mixing of those two states for $R = 80$ and 85 nm. The curves of the levels versus the magnetic field before and with the saturation value can be fitted by the red and dark yellow lines due to Eq. (44) and Landau level $E_{1}^{(h)}$, respectively. The position of the crossover regime, $l_B$, is well fitted by the black dash line derived by combining Eq. (14) and Landau level $E_{1}^{(h)}$. It indicates that Landau quantization phase occurs for large enough QD radius, while the phase with only surface states appear at a moderate regime of QD radius. Here we point out that a more precise magnetic length $l_B$ and criterion $R > l_B$ is given instead of the usual one $\hbar \omega_{c} R \gg l_B = \frac{\hbar}{|\mu_B|}$ to judge whether the magnetic field and QD size are large enough to realize Landau quantization. Besides, we notice that increasing magnetic field makes the level depend on $R$ more linearly before saturation. It is consistent with Eq. (43) since the second term of Eq. (41) is proportional to magnetic filed and will be dominate for a large magnetic field.

In Fig. 13 we plot the spin polarization of the eigenstate $j_z = \frac{1}{2}$ and $n_r = 0$, the one denoted as a black line in Fig. 9. The radial component $\langle s_r \rangle$ vanishes exactly since the unitary matrix given in Eq. (15) makes the Hamiltonian in Eq. (41) real to lead to the phase difference $\delta \theta = -\pi/2$, as is discussed in absence of magnetic field. The angular and axial components $\langle s_\varphi \rangle$ and $\langle s_z \rangle$ can be divided into three regions which corresponds to Landau level $E_0$, the nontrivial surface state, Landau level $E_{1}^{(h)}$, successively from left to right. In the regime of zeroth Landau level $E_0$, spin is polarized in the axial direction with $\langle s_z \rangle = \frac{1}{2}$ and the other components vanished. In the surface state regime, we have $\langle s_\varphi \rangle \approx \frac{1}{2}$ while $s_z$ is small, suggesting that spin aligns antiparallel to the tangential direction approximately. And the spin density distributes around the side surface in this regime. In the $E_{1}^{(h)}$ regime, $s_z$ (or $s_\varphi$) increases (decreases)
with raising magnetic field and spin is not locked into a specific direction any more.

V. DISCUSSION AND CONCLUSION

We have proposed and studied the Weyl semimetal QD. Our results reveal that there will be both surface and bulk states coexisting near the Fermi level. We focus on properties of the surface state, which locates only on the side surface of the cylinder QD studied here. Its energy dispersion depends linearly on total angular momentum leading to a chiral current and orbital magnetic moment with their product being a constant. The spin orients clockwisely in the horizontal plane near the side surface. A strong magnetic field along the axial direction will destroy the surface state and result in the Landau quantization. The spin will deviate away from the horizontal plane and become completely polarized in the axial direction for the zeroth Landau level.

Our results show the projection of properties of 3D Weyl semimetal in the zero-dimensional QD system. Surface states will emerge only for some certain quantum numbers determined by the spacing of Weyl points, which act as the correspondence of the Fermi arc. There is a minimum of direct energy gap with its location related to the projection of the Weyl point. It provides the possibility of study the Weyl physics in the Weyl semimetal QD system which may be fabricated and tuned more easily. Due to the large surface-to-volume ratio, the contribution of surface-state carriers are amplified and it suggests a new method to verify the topological nontrivial property of surface-state carriers. These new terms will give rise to new phenomena absent in the topological insulator QDs and conventional semiconductor QDs. In a few words, the further study of Weyl semimetal QD will pave a new way for the investigation of Weyl semimetal.

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9 S.-M. Huang, S.-Y. Xu, I. Belopolski, C.-C. Lee, G. Chang, B. Wang, N. Alidoust, G. Bian, M. Neupane, C. Zhang, S. Jia, A. Bansil, H. Lin, and M. Z. Hasan, Nat. Commun. 6, 7373 (2015).
10 S. Y. Xu, N. Alidoust, I. Belopolski, Z. Yuan, G. Bian, T. R. Chang, H. Zheng, V. N. Strocov, D. S. Sanchez, G. Chang, C. Zhang, D. Mou, Y. Wu, L. Huang, C. C. Lee, S.M. Huang, B. Wang, A. Bansil, H. T. Jeng, T. Neupert, A. Kaminski, H. Lin, S. Jia and M. Z. Hasan, Nat. Phys. 11, 748 (2015).
11 Z. K. Liu, L. X. Yang, Y. Sun, T. Zhang, H. Peng, H. F. Yang, C. Chen, Y. Zhang, Y. F. Guo, D. Prabhakaran, M. Schmidt, Z. Hussain, S.-K. Mo, C. Felser, B. Yan, and Y. L. Chen, Nat. Mater. 15, 27 (2015).
12 D.-F. Xu, Y.-P. Du, Z. Wang, Y.-P. Li, X.-H. Niu, Q. Yao, D. Pavel, Z.-A. Xu, X.-G. Wan and D.-L. Feng, Chin. Phys. Lett. 32, 107101 (2015).
13 K. Deng, G. Wan, P. Deng, K. Zhang, S. Ding, E. Wang, M. Yan, H. Huang, H. Zhang, Z. Xu, J. Denlinger, A. Fedorov, H. Yang, W. Duan, H. Yao, Y. Wu, S. Fan, H. Zhang, X. Chen and S. Zhou, Nat. Phys. 12, 1105 (2016).
14 I. Belopolski, D.S. Sanchez, Y. Ishida, X. Pan, P. Yu, S.-
