Unprotected quadratic band crossing points and quantum anomalous Hall effect in FeB$_2$ monolayer

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Quadratic band crossing points (QBCPs) and quantum anomalous Hall effect (QAHE) have attracted the attention of both theoretical and experimental researchers in recent years. Based on first-principle calculations, we find that the FeB$_2$ monolayer is a nonmagnetic semimetal with QBCPs at K. Through symmetry analysis and $\mathbf{k} \cdot \mathbf{p}$ invariant theory, we find that the QBCP is not protected by rotation symmetry and consists of two Dirac points with the same chirality (Berry phase of 2π). Once introducing Coulomb interactions, we find that there is a spontaneous-time-reversal-breaking instability of the spinful QBCPs, which gives rise to a $C = 2$ QAHE insulator with orbital moment ordering.

two dimension, topological phase, quantum anomalous Hall effect

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1 Introduction

In a two-dimensional (2D) system, the finite density of states associated with the parabolic dispersion could lead to instability for arbitrarily weak interactions [1-5]. For a quadratic band crossing point (QBCP) being stable without fine-tuning, the system must be time-reversal invariant and the QBCP must have $C_4$ or $C_5$ rotational symmetry [1]. An interaction would lead to the possibility of spontaneous breaking of rotational symmetry (nematic phase) or time-reversal invariance. However, the QBCPs at the threefold-invariant

*momentum on the honeycomb lattice and relatives are unprotected. The introduction of interactions leads to qualitatively different low-energy behavior, without breaking the underlying symmetries [2]. Although there are many theoretical studies of spinless QBCPs on many tailored 2D systems, such as single-layer graphene [2, 3] and Bernal-stacked bilayer graphene [4], the unprotected QBCPs have not been reported in any spinful system and their possible instabilities have not been discussed yet.

Besides, topological states, including quantum anomalous Hall (QAH) state, have attracted considerable research interest recently [6-13]. In spite of plenty of material proposals for QAH state [14-19], the observation of the QAH effect is still full of challenges and has been merely realized in a
few systems such as Cr-doped and V-doped (Bi,Sb)₂Te₃ thin films [20,21], magnetic topological insulator MnBi₂Te₄ [22], and twisted bilayer graphene (TBG) [23]. Previous theoretical studies also show that the QAH effect can be realized in graphene by introducing both exchange field and Rashba spin-orbit coupling (SOC) due to its unique linear Dirac band dispersions [15].

In recent years, MB₂ (M = transition metal) monolayers have been predicted to be 2D Dirac cone materials theoretically in the absence of SOC, such as TiB₂ [24], FeB₂ [25] and HfB₂ [26] monolayers. The FeB₂ bulk crystal has been grown [27]. The stability of the FeB₂ monolayer is predicted theoretically by structure searching, phonon spectra, and molecular dynamics [25,28,29]. Unlike graphene, the Dirac bands of FeB₂ originate from d states of the transition metal Fe, which has a substantial Rashba SOC effect and is very likely coupled to a magnetic field. A Chern insulator can be achieved once it is grown on an insulating magnetic substrate. In this article, we find that the FeB₂ monolayer is a nonmagnetic semimetal with QBCPs based on first-principle calculations. Without including SOC, there is a linearly dispersive Dirac node at K (resp. K') with a Berry phase π (resp. −π), protected by the combined symmetry of time reversal and twofold rotation (i.e., T⁶C₂h). Once including SOC, the Dirac node becomes a QBCP and its Berry phase becomes 2π (−2π) at K (K'). These characters can be captured by the k·p effective Hamiltonians. With an insulating magnetic substrate, the FeB₂ monolayer is turned to be a Chern insulator with two chiral edge states, which is stimulated by the fixed-moment calculations. More interestingly, once we introduce the Coulomb interactions, an instability towards a C = 2 QAH state with orbital moment ordering is found.

2 Calculation methods

We performed the first-principle calculations within the framework of the density functional theory (DFT) using the projector augmented wave (PAW) method [30,31], which is implemented in Vienna ab initio simulation package (VASP) [32,33]. The Perdew-Burke-Ernzerhof (PBE) generalized gradient approximation exchange-correlation functional [34] was implemented in calculations. The cut-off energy for plane wave expansion was 945 eV, and 12 × 12 × 1 k-point sampling grids were used in the self-consistent process. A vacuum layer of 20 Å was chosen to avoid interaction between neighboring layers. SOC was taken into account within the second variational method self-consistently. The irreducible representations (irreps) were obtained by the program IRVSP [35]. The maximally localized Wannier functions (MLWFs) were constructed by Fe-3d, B-2s and B-2p orbitals using Wannier90 package [36]. The edge states were calculated using surface Green's function of the semi-infinite system based on the iterative scheme [37-39].

3 Results and discussion

DFT results. The crystal structure of FeB₂ monolayer belongs to space group P6₃mm (No. 183), as shown in Figure 1(a). One unit cell (a = 3.171 Å) contains two B atoms and one Fe atom, which are located at 2b and 1a Wyckoff positions, respectively. B atoms are arranged in a honeycomb lattice, and Fe atoms are located in the middle of the hexagons. The distance of Fe atoms and B atoms plane is 0.628 Å. The PBE band structure of FeB₂ monolayer is shown in Figure 1(a), there is a linearly dispersive Dirac point at K near the Fermi level (E_F).

Therefore, FeB₂ monolayer was predicted to be a 2D Dirac semimetal [25,40]. The little point group at K is C₃ᵥ, and the twofold Dirac bands belong to G₃ irrep, which is consistent with ref. [40]. The total and projected density of states (DOS) are plotted in Figure 1(c). They show that the hybridization between Fe and B is strong, while the electronic states near E_F are mainly contributed by dₓ²−dᵧ² and dₓz−dᵧz electrons of Fe atoms (the orbital-resolved band structures are given in Supplementary Materials). Once including SOC, as shown in Figure 1(b) and (d), the two Dirac bands split into two non-degenerate bands (G₄ and G₃) and one doubly-degenerate band (G₅) at K, exhibiting quadratic band dispersion.

Low-energy effective models. Based on the theory of invariants, we derive the low-energy effective Hamiltonian H_k(k) (i.e., k is the offset momentum from K). Under the basis of G₃ irrep, e.g. (|dₓz + idᵧz⟩, |dₓz − idᵧz⟩), it reads,

\[ H_k(k) = \begin{pmatrix} M_1(k) & A_{k_+} \\ A_{k_-} & M_1(k) \end{pmatrix}. \]  

After considering the spin degree of freedom, the four-band Hamiltonian becomes (in the basis of (|↑⟩, |↓⟩) ⊗ (|dₓz + idᵧz⟩, |dₓz − idᵧz⟩)),

\[ H_k^{σ} (k) = σ_0 \otimes H_k(k) \]

\[ = \begin{pmatrix} M_2(k) & 0 \\ 0 & -M_2(k) \end{pmatrix} \begin{pmatrix} \begin{pmatrix} i M_3(k) \\ iB_+ \end{pmatrix} & \begin{pmatrix} iC(k) \\ iB_- \end{pmatrix} \end{pmatrix} \begin{pmatrix} \begin{pmatrix} \begin{pmatrix} 0 \\ M_2(k) \end{pmatrix} \end{pmatrix} & \begin{pmatrix} \begin{pmatrix} M_2(k) \\ iB_+ \end{pmatrix} \end{pmatrix} \end{pmatrix}, \]  

where \( k_+ = k_x \pm ik_y, C(k) = C_{1k_- + C_2k^2}, M_{σ=1,2,3}(k) = E_σ + F_σ k^2_σ \) with \( k^2_σ = k^2_x + k^2_y \), and \( σ_0 \) is the identity matrix in spin space. Since the second-order k terms are crucial for the
quadratic band dispersion in the following two-band model (which were omitted in ref. [40]), we have derived them in the four-band $k \cdot p$ model as well.

By fitting the DFT band structure in the vicinity of $K$, the parameters are obtained in Table 1 and the results are shown in Figure 2(a). The $k \cdot p$ model reproduces the QBCP at $K$, and the Berry phase for the QBCP is $2\pi$. The 2nd and 3rd bases form $G_2$ irrep of $C_3v$ double group, i.e., \( \{ |d_{xz} - id_{yz}, \rangle, |d_{xz} + id_{yz}, \rangle \} \). To evaluate the positions of Dirac points, a simple model under $G_6$ irrep can be obtained as below:

\[
H'_K(k) = \begin{pmatrix}
M_1(k) - M_2(k) - iC_1 k_x - iC_2 k_y^2 \\
C_1 k_x + iC_2 k_y^2 - M_1(k) - M_2(k)
\end{pmatrix}
\]

where $C_2$ is a modified parameter after downfolding. Its two eigenvalues are solved as $E_{\pm} = M_1(k) - M_2(k) \pm \sqrt{\Delta(k)}$ with

\[
\Delta(k) = C_2^2 k_+^4 + 2C_1 C_2 k_x(k_x^2 - 3k_y^2) + C_2^2 k_y^2.
\]

The gapless points satisfy the condition of $\Delta(k) = 0$. Assum-
ing \( k_x = 0 \), the equation is simplified to \( C_2^2 k_x^4 + 2 C_1 C_2^2 k_x^2 + C_1^2 k_x^2 = 0 \), giving rise to two Dirac points located at \( k_x = 0 \), \( -C_1/C_2 \). The detailed calculations show that the two Dirac points have opposite \( \pi \) Berry phase. The distance between them is \( d_0 = |C_1/C_2| \) in momentum space. Considering \( C_2 \) symmetry, there must be two additional Dirac points around \( K \), as shown in the inset of Figure 2(b). No other gapless point is found (see the proof in Supplementary Materials).

As the Dirac points and the quantized Berry phase of \( \pi \) are protected by the antunitary symmetry \( TC_{2z} \), the above discussion should be valid for the four-band model \( H^0_{K}(k) \) as well. In the band dispersions of Figure 2(a), we numerically get \( d_0 \sim 5.2 \times 10^{-3} \text{ Å}^{-1} \). The ratio \( d_0/d_{HK} \) is 0.004\% \( (d_{HK} = 1.321 \text{ Å}^{-1}) \), which is too small to identify in FeB\(_2\) monolayer. Therefore, it is rational to consider the K point is a double Dirac point with quadratic band dispersions in FeB\(_2\) monolayer, corresponding to a \( 2\pi \) Berry phase. As the quadratic band dispersion is not protected by rotational symmetry, it was previously considered as linear dispersion improperly [40]. Note that it is similar to the case in the magic-angle TBG, where the velocity of K becomes zero [41,42]. For comparison, we plot the band dispersions of the four-band model with different \( C_1 \) and \( C_2 \) parameters in Figure 2(b), from which \( d_0 \) is read to be 0.223 \( \text{ Å}^{-1} \) \( (~0.17d_{HK}) \). The iso-energy-gap contours are shown in the vicinity of K points in its inset. A Dirac point \( (-\pi, \pi) \) at K and three other Dirac points \( (\pi, \pi) \) are clearly shown.

With an external magnetic field, a Chern insulator can be achieved in FeB\(_2\) monolayer (e.g., grown on an insulating magnetic substrate). As shown in Figure 3(a) and (b), with an in-plane external magnetic field (keeping \( TC_{2z} \), the double Dirac point at K splits into two Dirac points with the same chirality. The positions of Dirac nodes with different strength and directions of the in-plane magnetic field are shown in Supplementary Materials. When the magnetism is out-of-plane, the FeB\(_2\) becomes a Chern insulator with two chiral edge states in Figure 3(c). The Zeeman’s coupling Hamiltonian is given in Supplementary Materials. To simulate the spin-polarized state of FeB\(_2\) induced by the out-of-plane magnetism of substrates, we have performed the DFT calculations with a fixed moment (e.g. 0.01 \( \mu_B \) on each Fe atom) in z-direction. Its spin-polarized band structure is obtained in Figure 3(d). The FeB\(_2\) monolayer becomes a Chern insulator, which is compatible with the result of graphene with both Rashba SOC and an exchange field [15]. Then, we construct the maximally localized Wannier functions (MLWFs) and calculate the edge spectra, as shown in Figure 3(e). Two chiral edge states connecting the conduction continuum and valence continuum indicate a Chern number of 2.

Orbital-moment-induced QAHE with interactions. Interestingly, once considering onsite Coulomb interaction, we find the instability towards a gapped phase with orbital moment ordering, and the system exhibiting a QAHE effect. Using \( d_{xz}, d_{yz} \) and \( d_{z^2} \) orbitals of Fe atoms, a spinful three-orbital tight-binding model is constructed to capture the DFT band structure (see more details in Supplementary Materials). The Coulomb interaction considered in \( d_{xz} \) and \( d_{yz} \) orbitals is written as:

\[
H_{\text{int}} = U \sum_{l} n_{l\alpha} n_{l\beta} + U' \sum_{l \alpha \neq \beta} n_{l\alpha} n_{l\beta},
\]

where \( n_{l\alpha} \) represents the electron density on orbital \( l \) with spin \( \alpha \) and \( \alpha, \beta = +, - \). We further employ the Hartree-Fock approximation to treat the Coulomb interaction (the results of the LDA+U method are discussed in Supplementary Materials). And the order parameters are defined as:

\[
M^l = \sum_{\alpha \neq \beta} \tau^l_{\alpha\beta} \sigma^l_{\alpha\beta} (d^\dagger_{l\alpha} d_{l\beta}).
\]

where the \( d^\dagger_{l\alpha} \) operator annihilates (creates) an electron in orbital \( l \) and spin \( \alpha \). \( \tau^l \) and \( \sigma^l \) \((\mu, \nu = x, y, z)\) are the identities with three Pauli matrices representing the orbital and spin degree of freedom respectively. We self-consistently investigate the zero-temperature phase diagram, and the results are shown in Figure 4.

In self-consistent calculations, we exclude the channels for SOC relevant order parameter \( M^C \) and the symmetric part of the electron density term \( M^{\rho} \), which are already considered in the DFT calculation. After considering all other order parameters, we find that the Coulomb interaction between \( d_{xz} \) and \( d_{yz} \) orbitals intrinsically stimulates orbital-magnetization phases respectively with order parameters \( M^{x}, M^{y} \) and \( M^{\rho} \). These three orderings break the \( TC_{2z} = i\tau_y \otimes \sigma_3 K \) symmetry and open the gap at the K point. The \( M^{x} \) phase and \( M^{y} \) phase are related by \( C_{6z} \) symmetry with relative higher energy, while the \( M^{\rho} \) phase with orbital moment ordering is the ground state. The gap width exponentially grows when increasing the Coulomb interaction strength \( U \) in Figure 4(a). The gapped system then becomes a \( C = 2 \) Chern insulator.

4 Conclusions

In conclusion, we have explored electronic structures and the topological property of the FeB\(_2\) monolayer. Without
SOC, the FeB$_2$ monolayer has linear band crossing points at K points. Upon including SOC, they become QBCPs with Berry phase $2\pi$. Based on effective Hamiltonians, we demonstrate that the QBCPs are not protected by rotational symmetry. The appearance of QBCPs (or zero velocity at K) is similar to the case in the magic-angle TBG. FeB$_2$ monolayer is a good platform for studying the instability of spinful QBCPs. Considering Coulomb interaction in the spinful model of FeB$_2$ with QBCPs, it turns out to be a $C = 2$ QAH insulator with orbital moment ordering.

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Supporting Information

The supporting information is available online at phys.sichina.com and link.springer.com. The supporting materials are published as submitted, without typing or editing. The responsibility for scientific accuracy and content remains entirely with the authors.

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