

Spin-orbital-momentum locking under odd-parity magnetic quadrupole orderingSatoru Hayami ¹ and Hiroaki Kusunose ²¹*Department of Applied Physics, The University of Tokyo, Tokyo 113-8656, Japan*²*Department of Physics, Meiji University, Kawasaki 214-8571, Japan*

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Odd-parity magnetic and magnetic toroidal multipoles in the absence of both spatial-inversion and time-reversal symmetries are sources of multiferroic and nonreciprocal optical phenomena. We investigate electronic states caused by an emergent odd-parity magnetic quadrupole (MQ) as a representative example of magnetic odd-parity multipoles. It is shown that spontaneous ordering of the MQ leads to an antisymmetric spin-orbital polarization in momentum space, which corresponds to a spin-orbital-momentum locking at each wave vector. By a symmetry argument, we show that the orbital or sublattice degree of freedom is indispensable to give rise to the spin-orbital-momentum locking. We demonstrate how the electronic band structures are modulated by the MQ ordering in the three-orbital system, in which the MQ is activated by the spin-dependent hybridization between the orbitals with different spatial parities. The spin-orbital-momentum locking is related to the microscopic origin of cross-correlated phenomena, e.g., the magnetic-field-induced symmetric and antisymmetric spin polarization in the band structure, the current-induced distortion, and the magnetoelectric effect. We also discuss similar spin-orbital-momentum locking in an antiferromagnet where the MQ degree of freedom is activated through the antiferromagnetic spin structure in a sublattice system.

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The interplay among internal degrees of freedom in electrons, such as charge, spin, and orbital, gives rise to unconventional physical phenomena in the strongly correlated electron system. The concept of the atomic-scale multipole can describe not only electronic order parameters but also resultant physical phenomena in a unified way [1–6]. There are four types of multipoles according to space- and time-inversion properties: electric, magnetic, electric toroidal, and magnetic toroidal multipoles [7–9]. Moreover, such atomic-scale multipoles have been generalized so as to describe anisotropic charge and spin distributions over multiple sites, which are denoted as a cluster multipole [10–15] and a bond multipole [16,17]. The generalization of the concept of the multipole is referred to as an augmented multipole, which opens a new direction of cross-correlated (multiferroic) physical phenomena in antiferromagnets, such as the anomalous Hall and Nernst effects in Mn_3Sn [11,18–22], current-induced magnetization in UNi_4B [23–26] and Ce_3TiBi_5 [27,28], and nonreciprocal magnon excitations in $\alpha\text{-Cu}_2\text{V}_2\text{O}_7$ [29–33].

The active multipole moments in real space are related to the electronic band structures in momentum space [4,17,34–36]. In other words, the band deformations and spin splittings at each wave vector are ascribed to the active multipole moments. For example, a lowering of the symmetry in the band structure caused by spontaneous electronic orderings, such as the Pomeranchuk instability [37–39] and the electronic nematic state [40–42], corresponds to the appearance of a particular type of active electric quadrupole. Another example is an antisymmetric band-bottom shift

without both spatial-inversion and time-reversal symmetries, which is accounted for by the emergent magnetic toroidal dipole moment [24,43–47].

The correspondence between the multipole and the band deformation is classified according to the space- and time-inversion symmetries [4]; the even-rank (odd-rank) electric (magnetic toroidal) multipole leads to symmetric (antisymmetric) band deformation, and the odd-rank magnetic (electric) multipole and even-rank magnetic toroidal (electric toroidal) multipole induce symmetric (antisymmetric) spin splittings with respect to the wave vector. A systematic classification of the band structure based on multipoles can lead to a further intriguing situation, such as symmetric and antisymmetric spin splittings even without spin-orbit coupling [17,35,36,48–54].

In this paper, we focus on the role of the magnetic quadrupole (MQ) in the electronic structures in momentum space. The MQ is characterized as a rank-2 axial tensor with time reversal odd among the magnetic multipoles. As this is a higher-rank multipole of the magnetic dipole, it is defined as the spatial distributions of the magnetic moments, such as the spin and orbital angular momenta. A typical example to exhibit the MQ is the antiferromagnetic ordering without the spatial-inversion symmetry, which has been discussed in the context of multiferroic materials in magnetic insulators [55–59], such as Cr_2O_3 [60–64], $\text{Ba}(\text{TiO})\text{Cu}_4(\text{PO}_4)_4$ [65–67], $\text{Co}_4\text{Nb}_2\text{O}_9$ [68–72], and KOsO_4 [73–75]. Meanwhile, such ordering has recently been discussed in magnetic metals [76–79], such as BaMn_2As_2 [80,81], as it could exhibit intriguing current-induced magnetization and distortion.

In generalization of the studies on the MQ from insulators to metals, there is a natural question as to how the MQ affects the electronic band structure microscopically and induces related physical phenomena. There is a missing link between the electronic band modulations and the odd-parity magnetic multipoles because the latter cannot be constructed by a simple product between the wave vectors and spin degrees of freedom [4]. To answer this naive question, we investigate the characteristic feature of the electronic band structure by the formation of the MQ ordering based on the simplest multi-orbital model. We show that there is a nontrivial spin-orbital entanglement once the MQ ordering occurs; the electric quadrupole polarization defined by the product of spin and orbital angular momenta appears with a dependence on the wave vector in an antisymmetric way. By analogy with the spin-momentum locking in noncentrosymmetric metals [82], we refer to the effective spin-orbital entanglement as “spin-orbital-momentum locking.” The spin-orbital-momentum locking becomes the origin of the antisymmetric spin polarization under the magnetic field. Moreover, we find that the spin-orbital-momentum locking provides a deep understanding of conductive phenomena in magnetic metals, such as the current-induced distortion. We also show that a similar spin-orbital-momentum locking is realized in the antiferromagnetic ordering by taking into account the sublattice degree of freedom instead of the orbital one.

The rest of this paper is organized as follows. In Sec. II, after introducing the expressions of the MQ in real space, we present them in momentum space, which indicates an origin of the spin-orbital-momentum locking. We discuss the realization of such spin-orbital-momentum locking by considering the multi-orbital and sublattice systems with the active MQ degree of freedom in Sec. III. We relate the spin-orbital-momentum locking to physical phenomena, such as the current-induced distortion and magnetoelectric effect, under the MQ ordering from the analysis of the linear response theory. Section IV is devoted to a summary.

II. MAGNETIC QUADRUPOLE

In this section, we show the expressions of the MQ in real and momentum spaces on the basis of multipole expansion and group theory. After briefly reviewing the expressions in real space in Sec. II A, we describe the band modulations under the MQ in Sec. II B. It is shown that the active MQ gives rise to the spin-orbital-momentum locking at each wave vector.

A. Expressions in real space

We start by reviewing the MQ in real space, whose expression is obtained in the second order of the multipole expansion for the vector potential [8,83,84]. The MQ is characterized by the rank-2 axial tensor with five components $\{M_u, M_v, M_{yz}, M_{zx}, M_{xy}\}$ with $u = 3z^2 - r^2$ and $v = x^2 - y^2$, which has the odd parities for both space- and time-inversion operations. The expressions are given by

$$M_u = 2zm_z - xm_x - ym_y, \quad (1)$$

TABLE I. The correspondence between the multipoles and the momentum in terms of the space-time-inversion symmetries. “Even” (“odd”) in parentheses represents the even-rank (odd-rank) multipoles. The first four rows of the table show the correspondence in the single-orbital system, while the last two rows show the correspondence in the multi-orbital system where $\mu, \nu = x, y, z$.

Momentum	\mathcal{P}	\mathcal{T}	Multipoles
\mathbf{k}^{2n}	+1	+1	electric (even)
\mathbf{k}^{2n+1}	-1	-1	magnetic toroidal (odd)
$\mathbf{k}^{2n}\mathbf{m}$	+1	-1	magnetic (odd) or magnetic toroidal (even)
$\mathbf{k}^{2n+1}\mathbf{m}$	-1	+1	electric (odd) or electric toroidal (even)
$\mathbf{k}^{2n}l_\mu\sigma_\nu$	+1	+1	electric (even) or electric toroidal (odd)
$\mathbf{k}^{2n+1}l_\mu\sigma_\nu$	-1	-1	magnetic (even) or magnetic toroidal (odd)

$$M_v = \sqrt{3}(xm_x - ym_y), \quad (2)$$

$$M_{yz} = \sqrt{3}(zm_y + ym_z), \quad (3)$$

$$M_{zx} = \sqrt{3}(xm_z + zm_x), \quad (4)$$

$$M_{xy} = \sqrt{3}(ym_x + xm_y), \quad (5)$$

where $\mathbf{r} = (x, y, z)$ is the position vector and $\mathbf{m} = (m_x, m_y, m_z)$ is the magnetic moment consisting of the dimensionless orbital- and spin-angular-momentum operators \mathbf{l} and $\boldsymbol{\sigma}/2$, as $\mathbf{m} = 2\mathbf{l}/3 + \boldsymbol{\sigma}$ [8]. One can confirm that the sign of the MQs in Eqs. (1)–(5) is reversed by the spatial-inversion or time-reversal operations, \mathcal{P} and \mathcal{T} , as \mathcal{P} (\mathcal{T}) reverses the sign of \mathbf{r} (\mathbf{m}). Meanwhile, the expressions in Eqs. (1)–(5) are invariant under the \mathcal{PT} operation. Although such space-time-inversion properties are common to the magnetic toroidal dipole proportional to $\mathbf{r} \times \mathbf{m}$, they are distinguished from the rotational property: The MQ is the rank-2 axial tensor, and the magnetic toroidal dipole is the rank-1 polar tensor. The real-space spin configurations of each MQ component projected onto a sphere are schematically shown in Fig. 1.

B. Spin-orbital-momentum locking

In contrast to the real-space expressions of the MQ in Sec. II A, it is nontrivial to deduce their momentum-space expressions owing to the opposite time-reversal parity between \mathbf{r} and the wave vector \mathbf{k} . Indeed, it is impossible to construct the counterparts of Eqs. (1)–(5) by replacing \mathbf{r} with \mathbf{k} . In fact, any contractions of the time-reversal-odd polar vector \mathbf{k} and the time-reversal-odd axial vector \mathbf{m} lead to the odd-rank electric multipoles or the even-rank electric toroidal multipoles with time-reversal-even rather than the time-reversal-odd rank-2 axial tensor, MQ. We summarize the correspondence between the multipoles and their \mathbf{k} dependence in terms of the space-time-inversion symmetries in the first four rows of Table I. Thus it is concluded that the appearance of the real-space MQ does not affect the electronic band structure within the product between \mathbf{k} and \mathbf{m} .

Such a situation is resolved by taking into account the product of two angular momenta, \mathbf{l} and $\boldsymbol{\sigma}$. Since both \mathbf{l} and

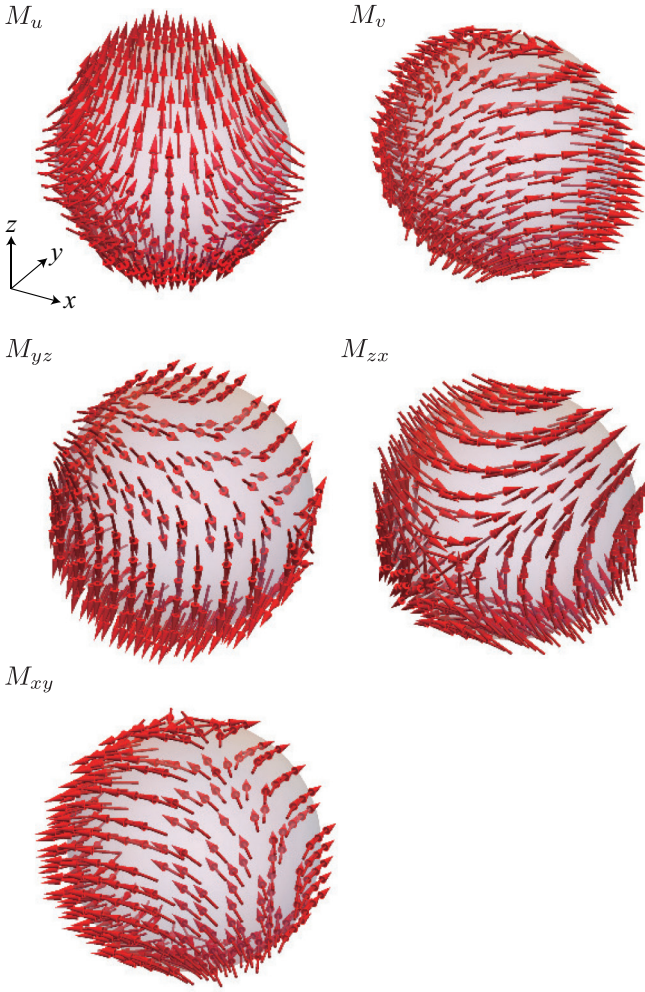


FIG. 1. Schematic pictures of the spin configuration of the MQs, $\{M_u, M_v, M_{yz}, M_{zx}, M_{xy}\}$, in Eqs. (1)–(5) projected onto a sphere. The arrows represent the direction of the magnetic moments.

σ are the same rank-1 axial tensors but they are independent of each other, their contraction expresses the rank-0 and rank-2 polar tensor $\mathcal{Q}_{\mu\nu} = (l_\mu\sigma_\nu + l_\nu\sigma_\mu)/\sqrt{2}$ for $\mu, \nu = x, y, z$ and rank-1 axial tensor $\mathcal{G} = \mathbf{l} \times \boldsymbol{\sigma}$ with time reversal even. By taking a further contraction between \mathbf{k} and \mathcal{G} or $\mathcal{Q}_{\mu\nu}$, one can construct the rank-2 axial tensor corresponding to the MQ in momentum space. In the case of the contraction between \mathbf{k} and \mathcal{G} , the MQ in momentum space is expressed as

$$M_u^{(1)}(\mathbf{k}) = 2\mathcal{G}_z k_z - \mathcal{G}_x k_x - \mathcal{G}_y k_y, \quad (6)$$

$$M_v^{(1)}(\mathbf{k}) = \sqrt{3}(\mathcal{G}_x k_x - \mathcal{G}_y k_y), \quad (7)$$

$$M_{yz}^{(1)}(\mathbf{k}) = \sqrt{3}(\mathcal{G}_y k_z + \mathcal{G}_z k_y), \quad (8)$$

$$M_{zx}^{(1)}(\mathbf{k}) = \sqrt{3}(\mathcal{G}_z k_x + \mathcal{G}_x k_z), \quad (9)$$

$$M_{xy}^{(1)}(\mathbf{k}) = \sqrt{3}(\mathcal{G}_x k_y + \mathcal{G}_y k_x). \quad (10)$$

In the case of the contraction between \mathbf{k} and $\mathcal{Q}_{\mu\nu}$, the MQ is expressed as

$$M_u^{(II)}(\mathbf{k}) = -3\mathcal{Q}_{yz}k_x + 3\mathcal{Q}_{zx}k_y, \quad (11)$$

$$M_v^{(II)}(\mathbf{k}) = \sqrt{3}(-\mathcal{Q}_{yz}k_x - \mathcal{Q}_{zx}k_y + 2\mathcal{Q}_{xy}k_z), \quad (12)$$

$$M_{yz}^{(II)}(\mathbf{k}) = \sqrt{3}[\sqrt{2}(\mathcal{Q}_{zz} - \mathcal{Q}_{yy})k_x + \mathcal{Q}_{xy}k_y - \mathcal{Q}_{zx}k_z], \quad (13)$$

$$M_{zx}^{(II)}(\mathbf{k}) = \sqrt{3}[\sqrt{2}(\mathcal{Q}_{xx} - \mathcal{Q}_{zz})k_y + \mathcal{Q}_{yz}k_z - \mathcal{Q}_{xy}k_x], \quad (14)$$

$$M_{xy}^{(II)}(\mathbf{k}) = \sqrt{3}[\sqrt{2}(\mathcal{Q}_{yy} - \mathcal{Q}_{xx})k_z + \mathcal{Q}_{zx}k_x - \mathcal{Q}_{yz}k_y]. \quad (15)$$

As $\{M_u^{(I)}(\mathbf{k}), M_v^{(I)}(\mathbf{k}), M_{yz}^{(I)}(\mathbf{k}), M_{zx}^{(I)}(\mathbf{k}), M_{xy}^{(I)}(\mathbf{k})\}$ and $\{M_u^{(II)}(\mathbf{k}), M_v^{(II)}(\mathbf{k}), M_{yz}^{(II)}(\mathbf{k}), M_{zx}^{(II)}(\mathbf{k}), M_{xy}^{(II)}(\mathbf{k})\}$ are the same spatial property, their linear combination, e.g., $c_1 M_u^{(I)}(\mathbf{k}) + c_2 M_u^{(II)}(\mathbf{k})$, where c_1 and c_2 are linear coefficients, is expected to appear once the MQ order occurs.

The expressions in Eqs. (6)–(15) indicate an emergent antisymmetric spin-orbital polarization with respect to \mathbf{k} in the band structure. The product of \mathbf{l} and $\boldsymbol{\sigma}$ in \mathcal{G} and $\mathcal{Q}_{\mu\nu}$ is a higher-rank coupling than the atomic spin-orbit coupling $\mathbf{l} \cdot \boldsymbol{\sigma}$. The \mathbf{k} dependences of these two couplings are qualitatively different from that of $\mathbf{l} \cdot \boldsymbol{\sigma}$: The present coupling shows an antisymmetric \mathbf{k} dependence, whereas the ordinary spin-orbit coupling does not. Besides, the coupling between the different components of \mathbf{l} and $\boldsymbol{\sigma}$ can emerge in the MQ ordered state, e.g., $\mathcal{G}_x = l_y\sigma_z - l_z\sigma_y$ and $\mathcal{Q}_{xy} = (l_x\sigma_y + l_y\sigma_x)/\sqrt{2}$. Since $\mathcal{Q}_{\mu\nu}$ has the same symmetry property as the quadrupole, this spin-orbital polarization is regarded as the antisymmetric quadrupole splitting. Thus the appearance of the MQ ordering connects between the momentum and the spin-orbital degrees of freedom, which is the microscopic origin of the current-induced distortion, as will be discussed in Sec. III A 4.

The above antisymmetric spin-orbital polarization is similar to the antisymmetric spin polarization in a nonmagnetic noncentrosymmetric lattice system with the Rashba or Dresselhaus spin-orbit interaction. In the case of the nonmagnetic systems, the antisymmetric spin splittings appear in the form of $\mathbf{k} \times \boldsymbol{\sigma}$ for the polar crystal and $k_\mu\sigma_\nu$ for the chiral or gyrotropic crystal. Owing to the momentum dependence in the spin splitting, the spin orientation is locked at the particular direction at each wave vector \mathbf{k} , which is called the spin-momentum locking [82]. In a similar way, the present antisymmetric spin-orbital polarization leads to the locking of the component of $l_\mu\sigma_\nu$ at the particular component at each \mathbf{k} . Thus we refer to the antisymmetric spin-orbital polarization in the MQ ordered state as the spin-orbital-momentum locking. It is noted that this spin-orbital momentum locking does not accompany the individual spin and orbital polarizations owing to the \mathcal{PT} symmetry. This situation can be regarded as the hidden spin polarization in the band structure, which is similar to that discussed in the staggered Rashba systems without local inversion symmetry at each lattice site [85–90], such as the zigzag [45,46,91,92], honeycomb [10,93–96], diamond [75,97,98], and layered systems [24,99–101]. In contrast to the staggered Rashba systems, the present spin-orbital polarization with hidden spin and orbital polarizations is activated by the spontaneous MQ ordering irrespective of the specific

lattice structure. It is noted that the hidden polarizations can be lifted easily by applying an external magnetic field.

Let us remark on the relevance to other multipole orderings. The antisymmetric spin-orbital-momentum locking can also appear in the odd-parity magnetic and magnetic toroidal multipoles, such as the magnetic toroidal dipole. For instance, the contraction of \mathbf{k} and \mathcal{G} includes the rank-1 polar tensor corresponding to the magnetic toroidal dipole, $\mathbf{k} \times \mathcal{G}$. There, however, is a clear difference in the band structure between the MQ and the magnetic toroidal dipole after tracing out the spin-orbital degree of freedom: The former shows the symmetric band structure, while the latter exhibits the antisymmetric one with respect to \mathbf{k} .

III. ACTIVE MAGNETIC QUADRUPOLE SYSTEM

In this section, we demonstrate that the MQ ordering gives rise to the spin-orbital-momentum locking by analyzing specific lattice models. We consider two intuitive systems including the MQ degree of freedom: One is the multiorbital system, where the MQ is activated by the spin-dependent hybridization between orbitals with different spatial parity in Sec. III A. The other is the sublattice system, where the MQ is activated by the antiferromagnetic ordering in Sec. III B.

A. Multiorbital system

In this section, we consider the MQ ordering in the multiorbital system. By constructing the multiorbital model consisting of the s , p_x , and p_y orbitals, where the MQ degree of freedom is described by the spin-dependent s - p hybridization in Sec. III A 1, we discuss the electronic band structure under the MQ ordering in Sec. III A 2. We show that the MQ ordering gives rise to a variety of the spin-orbital-momentum locking depending on the type of MQ as introduced in Sec. II B. The spontaneous MQ ordering induces the effective spin-orbit interaction similar to the atomic relativistic spin-orbit coupling. In Sec. III A 3, we show the effect of the magnetic field on the band structure in the MQ ordering. The symmetric and antisymmetric spin splittings in addition to the Zeeman splitting are induced by the magnetic field owing to the \mathcal{PT} symmetry breaking. We discuss the relation between the spin-orbital momentum locking and physical responses by exemplifying two cross-correlated phenomena: current-induced distortion in Sec. III A 4 and the magnetoelectric effect in Sec. III A 5.

1. Model

We construct a minimal multiorbital model to describe the MQ degree of freedom. We consider a three-orbital model consisting of the s , p_x , and p_y orbitals on a two-dimensional square lattice under the point group D_{4h} . We take the lattice constant as unity. The following results are straightforwardly generalized to a three-dimensional system. The wave functions of the s , p_x , and p_y orbitals are represented by ϕ_s , ϕ_x , and ϕ_y , respectively. Then, the tight-binding Hamiltonian for the basis $\{\phi_{s\sigma}, \phi_{x\sigma}, \phi_{y\sigma}\}$ is given by

$$\mathcal{H} = \sum_{\mathbf{k}, \alpha, \beta, \sigma} c_{\mathbf{k}\alpha\sigma}^\dagger H_\sigma^{\alpha\beta} c_{\mathbf{k}\beta\sigma}, \quad (16)$$

where $c_{\mathbf{k}\alpha\sigma}^\dagger$ ($c_{\mathbf{k}\alpha\sigma}$) is the creation (annihilation) operator of electrons at wave vector \mathbf{k} , orbital $\alpha = s, x, y$, and spin σ . The 3×3 Hamiltonian matrix spanned by the basis $\{\phi_{s\sigma}, \phi_{x\sigma}, \phi_{y\sigma}\}$ is given by

$$H_\sigma = \begin{pmatrix} 2t_s(c_x + c_y) & -2it_{sp}s_x & -2it_{sp}s_y \\ 2it_{sp}s_x & 2(t_\sigma c_x + t_\pi c_y) & 2t_{xy}s_x s_y - i\sigma\lambda \\ 2it_{sp}s_y & 2t_{xy}s_x s_y + i\sigma\lambda & 2(t_\sigma c_y + t_\pi c_x) \end{pmatrix}, \quad (17)$$

where $c_\eta = \cos k_\eta$ and $s_\eta = \sin k_\eta$ for $\eta = x, y$. There are five hopping parameters in the Hamiltonian in Eq. (17), $\{t_s, t_\sigma, t_\pi, t_{sp}, t_{xy}\}$ from the symmetry of the system: the nearest-neighbor hoppings between the s orbitals t_s , p orbitals t_σ and t_π , and s - p orbitals t_{sp} and the next-nearest-neighbor hopping between the p orbitals t_{xy} . λ is the constant for the atomic spin-orbit coupling where the factor 1/2 from the spin operator $\sigma/2$ is rescaled. We do not consider the atomic energy difference between s and p orbitals and the other hoppings for simplicity.

The spinful 6×6 Hamiltonian matrix spanned by $\{\phi_{s\uparrow}, \phi_{x\uparrow}, \phi_{y\uparrow}, \phi_{s\downarrow}, \phi_{x\downarrow}, \phi_{y\downarrow}\}$ has 36 independent electronic degrees of freedom. In spinless space, there are nine electronic degrees of freedom, whose irreducible representations are $2A_{1g}^+ \oplus A_{2g}^- \oplus B_{1g}^+ \oplus B_{2g}^- \oplus E_u^\pm$ where the superscript \pm denotes the time-reversal parity. Among them, the irreducible representations E_u^+ and E_u^- correspond to the odd-parity dipoles: the electric dipoles, $Q_x^{(h)}$ and $Q_y^{(h)}$, and magnetic toroidal dipoles, $T_x^{(h)}$ and $T_y^{(h)}$, respectively. Physically, they are expressed as the real and imaginary hybridizations between s and p orbitals, whose matrices are represented by

$$Q_x^{(h)} = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad Q_y^{(h)} = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \quad (18)$$

$$T_x^{(h)} = \begin{pmatrix} 0 & i & 0 \\ -i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad T_y^{(h)} = \begin{pmatrix} 0 & 0 & i \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{pmatrix}, \quad (19)$$

where the superscript (h) represents the hybrid multipoles that are active in the hybridized orbitals [8]. See also Fig. 2(a). It is noted that there is no MQ degree of freedom in spinless space.

The MQ degree of freedom with $(\mathcal{P}, \mathcal{T}) = (-1, -1)$ appears by considering the electronic degrees of freedom in spinful space, which is constructed from the product of the electric dipole with $(\mathcal{P}, \mathcal{T}) = (-1, 1)$ and spin operator with $(\mathcal{P}, \mathcal{T}) = (1, -1)$ [8,9]. Indeed, the product of the irreducible representation of the electric dipole E_u^+ and spin $A_{2g}^- \oplus E_g^-$ gives six odd-parity multipoles with time reversal odd; $E_u^+ \otimes (A_{2g}^- \oplus E_g^-) = A_{1u}^- \oplus A_{2u}^- \oplus B_{1u}^- \oplus B_{2u}^- \oplus E_u^-$. Among them, five out of six multipole degrees of freedom are expressed as MQs, whose expressions are given by

$$A_{1u}^-: M_u^{(h)} = -Q_x^{(h)}\sigma_x - Q_y^{(h)}\sigma_y, \quad (20)$$

$$B_{1u}^-: M_v^{(h)} = Q_x^{(h)}\sigma_x - Q_y^{(h)}\sigma_y, \quad (21)$$

$$E_u^-: M_{yz}^{(h)} = Q_y^{(h)}\sigma_z, \quad (22)$$

$$M_{zx}^{(h)} = Q_x^{(h)}\sigma_z, \quad (23)$$

$$B_{2u}^-: M_{xy}^{(h)} = Q_x^{(h)}\sigma_y + Q_y^{(h)}\sigma_x. \quad (24)$$

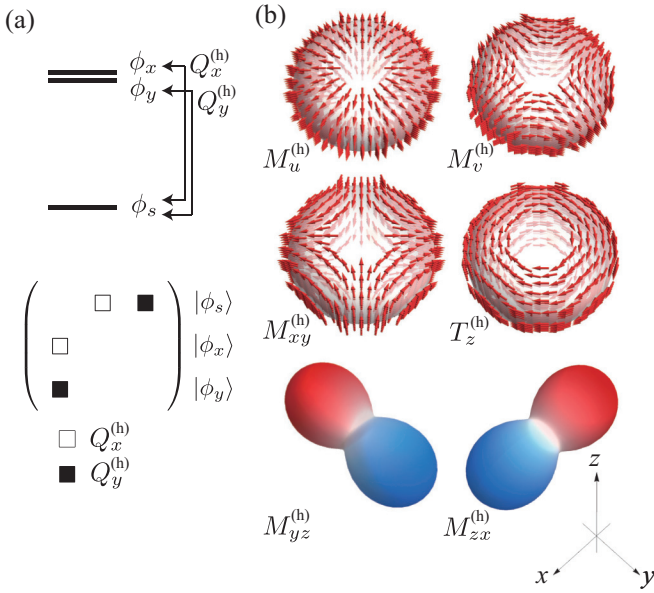


FIG. 2. (a) Multiorbital model consisting of s , p_x , and p_y orbitals, whose wave functions are denoted as ϕ_s , ϕ_x , and ϕ_y . The electric dipole degrees of freedom, $Q_x^{(h)}$ and $Q_y^{(h)}$, are defined by the off-diagonal elements between ϕ_s and ϕ_x (open squares) and ϕ_s and ϕ_y (solid squares). (b) The wave functions of the MQ $\{M_u^{(h)}, M_v^{(h)}, M_{yz}^{(h)}, M_{zx}^{(h)}, M_{xy}^{(h)}\}$ and magnetic toroidal dipole $T_z^{(h)}$ orderings in Eqs. (20)–(25). For visibility, we use arrows for the angle distribution of the xy spin moments for $M_u^{(h)}$, $M_v^{(h)}$, $M_{xy}^{(h)}$, and $T_z^{(h)}$, while a color map is used for the z spin moments for $M_{yz}^{(h)}$ and $M_{zx}^{(h)}$. The shapes represent the angle distributions of the electric charge density.

One can find that the expressions in Eqs. (20)–(24) correspond to those in Eqs. (1)–(5) in Sec. II A by replacing (x, y, z) and (m_x, m_y, m_z) with $(Q_x^{(h)}, Q_y^{(h)}, 0)$ and $(\sigma_x, \sigma_y, \sigma_z)$, respectively. It is noted that $M_{yz}^{(h)}$ and $M_{zx}^{(h)}$ belong to the same irreducible representation as the in-plane magnetic toroidal dipoles, T_x and T_y , respectively, which will be discussed in detail in Sec. III A 2.

The remaining multipole degree of freedom corresponds to the magnetic toroidal dipole degree of freedom $T_z^{(h)}$, which belongs to the irreducible representation A_{2u}^- . The expression of $T_z^{(h)}$ is given by the antisymmetric product between $\{Q_x^{(h)}, Q_y^{(h)}\}$ and $\{\sigma_x, \sigma_y\}$ as [8,102]

$$A_{2u}^-: T_z^{(h)} = Q_x^{(h)}\sigma_y - Q_y^{(h)}\sigma_x. \quad (25)$$

The above six multipoles satisfy the orthogonal relation $\text{Tr}[XY] = 0$, where $X, Y = M_u^{(h)}, M_v^{(h)}, M_{yz}^{(h)}, M_{zx}^{(h)}, M_{xy}^{(h)}, T_z^{(h)}$ and $X \neq Y$. In the following, we consider the situation where one of the six multipoles is ordered by the electron correlation. The amplitude of the mean field is given by h . We show schematic pictures of the wave functions with nonzero $M_u^{(h)}$, $M_v^{(h)}$, $M_{yz}^{(h)}$, $M_{zx}^{(h)}$, $M_{xy}^{(h)}$, and $T_z^{(h)}$ in Fig. 2(b). The shapes represent the electric charge density, while the arrows for $M_u^{(h)}$, $M_v^{(h)}$, $M_{xy}^{(h)}$, and $T_z^{(h)}$ [colors for $M_{yz}^{(h)}$ and $M_{zx}^{(h)}$] represent the angle distributions of the $xy(z)$ spin moments, which correspond well with the schematic spin polarization in Fig. 1.

2. Band structure

We investigate the change in the electronic band structure in the presence of the MQ orderings in the multiorbital model in Eq. (16). As the system is two dimensional ($k_z = 0$) and the Hamiltonian has only the z component of the angular momentum ($l_x = l_y = 0$), the spin-orbital-momentum locking in Eqs. (6)–(15) reduces to

$$M_u(\mathbf{k}) = -l_z\sigma_y k_x + l_z\sigma_x k_y, \quad (26)$$

$$M_v(\mathbf{k}) = -l_z\sigma_y k_x - l_z\sigma_x k_y, \quad (27)$$

$$M_{yz}(\mathbf{k}) = l_z\sigma_z k_x, \quad (28)$$

$$M_{zx}(\mathbf{k}) = -l_z\sigma_z k_y, \quad (29)$$

$$M_{xy}(\mathbf{k}) = l_z\sigma_x k_x - l_z\sigma_y k_y, \quad (30)$$

except for the numerical coefficient. Thus the spin-orbital-momentum locking with respect to the components of $l_z\sigma_x$, $l_z\sigma_y$, and $l_z\sigma_z$ is expected once the MQ order occurs.

Figures 3(a)–3(c) show the isoenergy surfaces in the band structure at the chemical potential $\mu = 1$ for the $M_u^{(h)}$, $M_v^{(h)}$, and $M_{xy}^{(h)}$ ordered states, respectively. The model parameters are taken as $t_\sigma = 0.8$, $t_\pi = 0.5$, $t_{xy} = 0.3$, $t_s = 1$, $t_{sp} = 0.6$, and $h = 0.3$. We neglect the effect of the atomic relativistic spin-orbit coupling $\lambda = 0$ unless otherwise stated. The spin-orbital polarizations $l_z\sigma_x$, $l_z\sigma_y$, and $l_z\sigma_z$ are calculated at each \mathbf{k} and are shown in the left, middle, and right columns in Fig. 3, respectively. Each band is doubly degenerate owing to the \mathcal{PT} symmetry.

The results clearly indicate the emergence of the spin-orbital-momentum locking expected from the symmetry argument in Eqs. (26)–(30) in each ordered state. The antisymmetric spin-orbital polarizations of $l_z\sigma_x$ and $l_z\sigma_y$ occur along the k_y and k_x directions, respectively, in the case of the $M_u^{(h)}$ ordered state in Fig. 3(a). Similarly, the antisymmetric spin-orbital polarizations in Eqs. (27) and (30) are found in the $M_v^{(h)}$ and $M_{xy}^{(h)}$ ordered states, as shown in Figs. 3(b) and 3(c), respectively.

The important hopping parameters for the spin-orbital-momentum locking are easily extracted by evaluating the following quantity at each wave vector \mathbf{k} : $\mathcal{O}_\mu(\mathbf{k}) = \text{Tr}[e^{-\beta\mathcal{H}_\mathbf{k}} l_z\sigma_\mu]$ for $\mu = x, y, z$ and $\mathcal{H} = \sum_{\mathbf{k}} \mathcal{H}_\mathbf{k}$, where β is the inverse temperature. In the high-temperature expansion of $\mathcal{O}_\mu(\mathbf{k})$, the necessary hopping parameters for the spin-orbital-momentum locking are systematically obtained [17,36]. For the $M_u^{(h)}$ ordered state, the lowest-order contributions of $\mathcal{O}_x(\mathbf{k})$ and $\mathcal{O}_y(\mathbf{k})$ are given by $-ht_{sp} \sin k_y$ and $ht_{sp} \sin k_x$, respectively, which indicates that the antisymmetric spin-orbital polarization is induced by the effective coupling between the order parameter h and the s - p hopping t_{sp} .

Notably, there is a symmetric spin-orbital polarization in terms of the $l_z\sigma_z$ component even without the atomic spin-orbit coupling, as shown in Figs. 3(a)–3(c). This is because the order parameters in Eqs. (20), (21), and (24) are described by two spin components, σ_x and σ_y . In this case, the term proportional to $l_z\sigma_z$ appears as the even-order product of the mean-field term in the expansion of $\mathcal{O}_z(\mathbf{k})$. Indeed, the lowest-order contribution of $\mathcal{O}_z(\mathbf{k})$ is proportional to h^2 . The

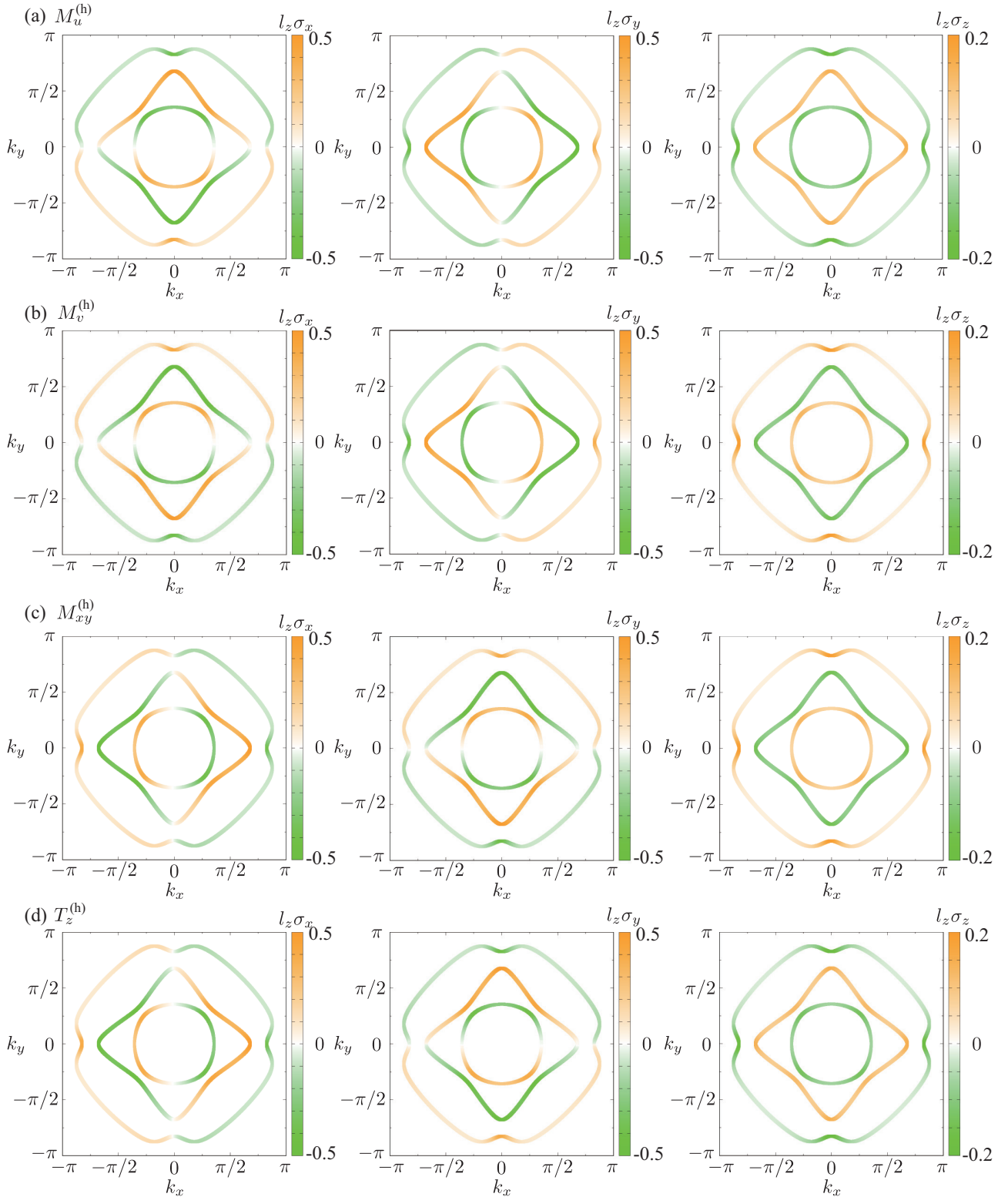


FIG. 3. The isoenergy surfaces at $\mu = 1$, $t_\sigma = 0.8$, $t_\pi = 0.5$, $t_{xy} = 0.3$, $t_s = 1$, $t_{sp} = 0.6$, and $\lambda = 0$ in the (a) $M_u^{(h)}$, (b) $M_v^{(h)}$, (c) $M_{xy}^{(h)}$, and (d) $T_z^{(h)}$ states with the molecular field $h = 0.3$. The color map shows the spin-orbital polarization of the $l_z \sigma_x$ (left), $l_z \sigma_y$ (middle), and $l_z \sigma_z$ (right) components at each wave vector.

opposite sign of $l_z \sigma_z$ between the $M_u^{(h)}$ and the other two ordered states is due to the opposite vorticity of the vector $\mathcal{Q}(\mathbf{k}) = (\langle l_z \sigma_x(\mathbf{k}) \rangle, \langle l_z \sigma_y(\mathbf{k}) \rangle, \langle l_z \sigma_z(\mathbf{k}) \rangle)$ in \mathbf{k} space: The direction of $(\mathcal{Q}_x, \mathcal{Q}_y)$ shows a (counter)clockwise rotation for the

$M_v^{(h)}$ and $M_{xy}^{(h)}$ ($M_u^{(h)}$) ordered states for the counterclockwise path on the circular Fermi surfaces, as schematically shown in Fig. 4. As the almost uniform distribution of $l_z \sigma_z$ in \mathbf{k} space resembles the atomic spin-orbit coupling, this is regarded as

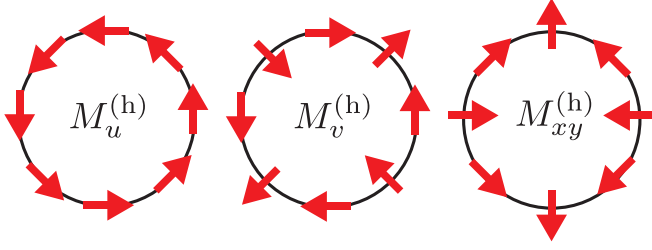


FIG. 4. The schematic spin-orbital-momentum locking on the circular Fermi surfaces for the $M_u^{(h)}$, $M_v^{(h)}$, and $M_{xy}^{(h)}$ ordered states. The arrows represent the direction of (Q_x, Q_y) .

the emergent spin-orbit coupling arising from the MQ ordering. Thus the magnitude of the atomic spin-orbit coupling can be controlled by the magnitude of the MQ order parameter.

Similar to the MQ ordering, the magnetic toroidal dipole ordering $T_z^{(h)}$ in Eq. (25) also shows the antisymmetric spin-orbital polarization, as shown in Fig. 3(d). The functional form of the antisymmetric spin-orbital polarization is represented by $l_z\sigma_x k_x + l_z\sigma_y k_y$, which is obtained by replacing σ_x with $-\sigma_x$ in the expression of $M_{xy}(\mathbf{k})$ in Eq. (30). Although the asymmetric bottom shift along the k_z direction is expected with the onset of $T_z^{(h)}$, it does not appear in the present two-dimensional system.

The remaining MQs, $M_{yz}^{(h)}$ and $M_{zx}^{(h)}$, also show the spin-orbital-momentum locking. The antisymmetric spin-orbital polarization of $l_z\sigma_z$ appears with respect to the k_x (k_y) direction in the $M_{yz}^{(h)}$ ($M_{zx}^{(h)}$) ordered state, as shown in Fig. 5(a) [Fig. 5(b)]. In contrast to the result in Fig. 3, there is no symmetric polarization of $l_z\sigma_z$ owing to the one spin component in Eqs. (22) and (23).

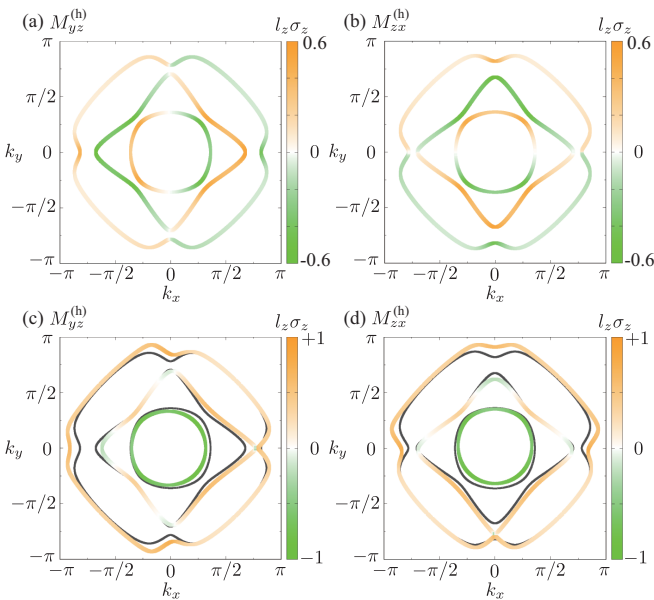


FIG. 5. Same as Fig. 3, but in the (a) and (c) $M_{yz}^{(h)}$ and (b) and (d) $M_{zx}^{(h)}$ states. The same model parameters as in Fig. 3 are used in (a) and (b), and the effect of the spin-orbit coupling λ is added as $\lambda = 0.5$ in (c) and (d). The solid black curves in (c) and (d) represent the isoenergy surfaces in (a) and (b), respectively.

It is noteworthy that $M_{yz}^{(h)}$ and $M_{zx}^{(h)}$ belong to the same irreducible representations of $T_x^{(h)}$ and $T_y^{(h)}$ under the point group D_{4h} . Nevertheless, there is no antisymmetric band bottom shift along the k_x and k_y directions in Figs. 5(a) and 5(b). The antisymmetric band deformation appears only when introducing the atomic spin-orbit coupling λ in Eq. (17), as shown in Figs. 5(c) and 5(d). Indeed, the effective coupling between λ and ht_{sp} appears in the expansion of $\text{Tr}[e^{-\beta\mathcal{H}_k}]$: $-ht_{sp}\lambda \sin k_x$ for the $M_{yz}^{(h)}$ state and $ht_{sp}\lambda \sin k_y$ for the $M_{zx}^{(h)}$ state. This result indicates that the magnetic toroidal dipoles, $T_x^{(h)}$ and $T_y^{(h)}$, are secondarily induced in the presence of the spin-orbit coupling in the MQ state.

3. Spin splittings under a magnetic field

Although the MQ ordered state exhibits the antisymmetric spin-orbital polarization, it does not show any spin splittings owing to the presence of the \mathcal{PT} symmetry. The degeneracy is lifted by the \mathcal{PT} -breaking field, which results in additional momentum-dependent spin splittings in the band structure. Hereafter, we demonstrate that various symmetric and antisymmetric spin splittings are induced by an external magnetic field by focusing on the $M_{xy}^{(h)}$ ordered state. We introduce the Zeeman coupling to spin, $-\mathbf{H} \cdot \sum_{i\alpha\sigma\sigma'} c_{i\alpha\sigma}^\dagger \sigma_{\sigma\sigma'} c_{i\alpha\sigma'}$, where we neglect the Zeeman coupling to orbital angular momentum without loss of generality.

Figures 6(a), 6(b), and 6(c) show the isoenergy surfaces in the presence of the magnetic field along the x , y , and z directions, respectively, with the magnitude of $|\mathbf{H}| \equiv H = 0.1$. The three panels in each figure correspond to the spin polarization of σ_x , σ_y , and σ_z . The other parameters are the same as those in the previous section.

When the magnetic field is turned on along the x direction, the spin polarization emerges owing to the \mathcal{PT} symmetry breaking, as shown in Fig. 6(a), although the \mathbf{k} dependence of the spin polarization is different for the different spin components. The x spin component parallel to the magnetic field shows the ordinary Zeeman splitting, whereas the y and z spin components perpendicular to the magnetic field give rise to the symmetric and antisymmetric spin splittings, whose functional forms are given by $k_x k_y \sigma_y$ and $k_x \sigma_z$ in the limit of $\mathbf{k} \rightarrow \mathbf{0}$, respectively.

Reflecting the different forms of spin splittings, the necessary model parameters are different. We extract the essential model parameters for the spin splittings by calculating $\mathcal{S}_\mu(\mathbf{k}) = \text{Tr}[e^{-\beta\mathcal{H}_k} \sigma_\mu]$ [17,36]. In the y spin component, the lowest-order contribution in $\mathcal{S}_y(\mathbf{k})$ for $\beta\mathcal{H}_k \ll 1$ is given by $h^2 H t_{xy} \sin k_x \sin k_y$ or $h^2 H t_{sp}^2 \sin k_x \sin k_y$, whereas that in the z spin component $\mathcal{S}_z(\mathbf{k})$ is given by $h^3 H t_{sp} \sin k_x$. From these expressions, one can find that the s - p hopping t_{sp} is necessary for the antisymmetric spin splitting, while it is not necessary for the symmetric spin splitting. Moreover, the domain formation is irrelevant (relevant) to the (anti)symmetric spin splitting as $\mathcal{S}_y(\mathbf{k})$ [$\mathcal{S}_z(\mathbf{k})$] is proportional to h^2 (h^3). These additional \mathbf{k} -dependent spin splittings are related to the active multipoles: Symmetric spin splitting such as $k_x k_y \sigma_y$ corresponds to the magnetic toroidal quadrupole with the zx component, and antisymmetric spin splitting such as $k_x \sigma_z$ corresponds to the electric dipole along the y direction [4]. In particular, the latter electric dipole induced by the magnetic

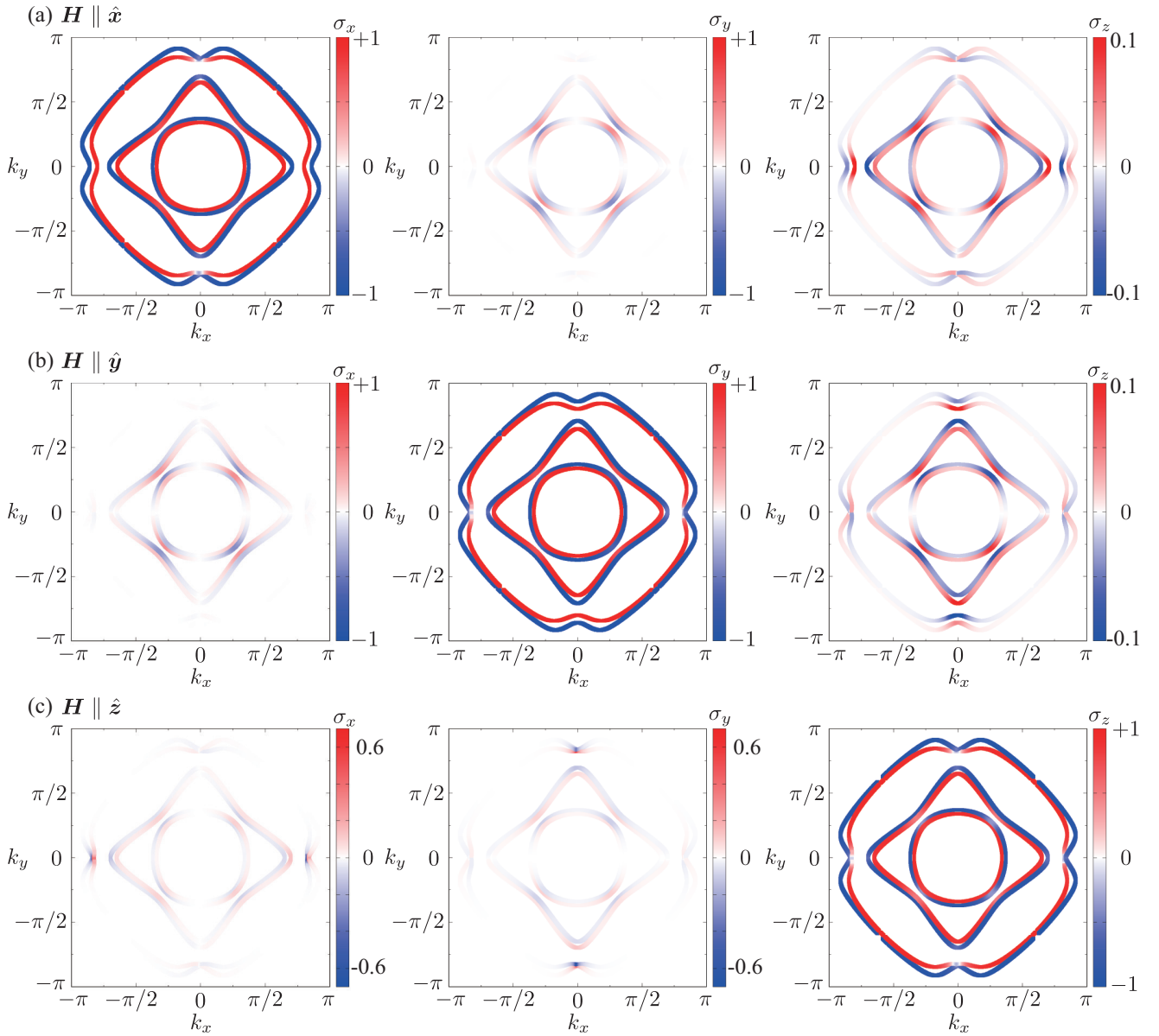


FIG. 6. The isoenergy surfaces in the $M_{xy}^{(h)}$ state in the external magnetic field along the (a) x , (b) y , and (c) z directions with $|\mathbf{H}| = 0.1$. The color map shows the spin polarization of the x (left), y (middle), and z (right) components at each wave vector. The other parameters are the same as in Fig. 3.

field implies the magnetoelectric effect in metals, which is relevant to the discussion in Sec. III A 5.

Similar band modulations also occur under the magnetic field along the y and z directions, as shown in Figs. 6(b) and 6(c), respectively. For $\mathbf{H} \parallel \hat{y}$, the symmetric (antisymmetric) spin splitting in the form of $k_x k_y$ (k_y) is found in the x (z) spin component in addition to the Zeeman splitting in the y spin component. This indicates that the yz component of the magnetic toroidal quadrupole and the x component of the electric dipole are activated by the magnetic field along the y direction.

For $\mathbf{H} \parallel \hat{z}$, the antisymmetric spin splitting occurs in both σ_x and σ_y components in Fig. 6(c), whose functional form is represented by $k_x \sigma_x - k_y \sigma_y$. Indeed, by calculating \mathcal{S}_x and \mathcal{S}_y , we obtain the coupling form as $\hbar^3 H t_{sp} (\sin k_x \sigma_x - \sin k_y \sigma_y)$. It is noteworthy that this type of antisymmetric spin splitting

indicates the active axial electric toroidal quadrupole rather than the polar electric dipole. The appearance of the electric toroidal quadrupole is related to the optical rotation.

4. Current-induced distortion

Next, we discuss physical phenomena related by the spin-orbital-momentum locking under the MQ ordering. We here consider the piezoelectric effect where the symmetric distortion ϵ_ζ is induced by the electric field E_ν , i.e., $\epsilon_\zeta = \sum_\nu \Lambda_{\zeta\nu} E_\nu$ for $\zeta = u, v, yz, zx, xy$. The current-induced distortion tensor $\Lambda_{\zeta\nu}$ is calculated by the linear response theory as [10,80,103]

$$\Lambda_{\zeta\nu} = \sum_{\mathbf{k}} \sum_{pq} \Pi_{pq}(\mathbf{k}) Q_{\zeta\mathbf{k}}^{pq} v_{\nu\mathbf{k}}^{qp}, \quad (31)$$

where

$$\Pi_{pq}(\mathbf{k}) = \frac{e\hbar}{iV} \frac{f[\varepsilon_p(\mathbf{k})] - f[\varepsilon_q(\mathbf{k})]}{[\varepsilon_p(\mathbf{k}) - \varepsilon_q(\mathbf{k})][\varepsilon_p(\mathbf{k}) - \varepsilon_q(\mathbf{k}) + i\hbar\delta]}, \quad (32)$$

with the eigenenergy $\varepsilon_p(\mathbf{k})$ and the Fermi distribution function $f[\varepsilon_p(\mathbf{k})]$. e is the electron charge, $\hbar = h/2\pi$ is the Plank constant divided by 2π , V is the system volume, and δ is the broadening factor. $Q_{\zeta\mathbf{k}}^{pq} = \langle p\mathbf{k} | \hat{Q}_\zeta | q\mathbf{k} \rangle$ and $v_{\nu\mathbf{k}}^{pq} = \langle p\mathbf{k} | v_{\nu\mathbf{k}} | q\mathbf{k} \rangle$ are the matrix elements of the electric quadrupole and velocity $\hat{v}_{\mu\mathbf{k}} = \partial \hat{\mathcal{H}} / (\hbar \partial k_\mu)$, respectively. We regard $l_\mu \sigma_\nu$ as the electric quadrupole degree of freedom \hat{Q}_ζ from the symmetry viewpoint. We take $e = \hbar = 1$, $\delta = 0.01$, and the temperature $T = 1/\beta = 0.01$ in the following calculations.

The current-induced distortion tensor $\Lambda_{\zeta\nu}$ becomes nonzero in the absence of the spatial-inversion symmetry in the system. $\Lambda_{\zeta\nu}$ consists of two parts: One is the intraband Fermi surface contribution $p = q$, and the other is the interband Fermi sea contribution $p \neq q$, where their time-reversal

parities are opposite to each other. Reflecting the different time-reversal properties, the relevant multipoles are different in each contribution. The odd-parity magnetic and magnetic toroidal multipoles contribute to the intraband process, while the odd-parity electric and electric toroidal multipoles contribute to the interband process. In the present model in Eq. (17), the intraorbital contribution plays an important role in $\Lambda_{\zeta\nu}$, as the odd-parity electric and electric toroidal multipoles are not activated in the MQ ordered state owing to the \mathcal{PT} symmetry.

The 15 independent matrix elements of $\Lambda_{\zeta\nu}$ are characterized by the active rank-1–3 odd-parity multipoles with time reversal odd: the magnetic toroidal dipole $\{T_x, T_y, T_z\}$, MQ $\{M_u, M_v, M_{yz}, M_{zx}, M_{xy}\}$, and magnetic toroidal octupole $\{T_{xyz}, T_x^\alpha, T_y^\alpha, T_z^\alpha, T_x^\beta, T_y^\beta, T_z^\beta\}$. By using the multipole notation, the matrix form of $\Lambda_{\zeta\nu}$ is represented by [4]

$$\Lambda = \begin{pmatrix} T_x + M_{yz} - T_x^\alpha - T_x^\beta & T_y - M_{zx} - T_y^\alpha + T_y^\beta & -2T_z + 2T_z^\alpha \\ -3T_x + M_{yz} + 3T_x^\alpha - T_x^\beta & 3T_y + M_{zx} - 3T_y^\alpha - T_y^\beta & -2M_{xy} + 2T_z^\beta \\ -3M_u - M_v + T_{xyz} & -3T_z - M_{xy} - 2T_z^\alpha - 2T_z^\beta & -3T_y + M_{zx} - 2T_y^\alpha + 2T_y^\beta \\ -3T_z + M_{xy} - 2T_z^\alpha + 2T_z^\beta & 3M_u - M_v + T_{xyz} & -3T_x - M_{yz} - 2T_x^\alpha - 2T_x^\beta \\ -3T_y - M_{zx} - 2T_y^\alpha - 2T_y^\beta & -3T_x + M_{yz} - 2T_x^\alpha + 2T_x^\beta & 2M_v + T_{xyz} \end{pmatrix}, \quad (33)$$

where the rows (columns) of the matrix represent the components of $\{E_x, E_y, E_z\}$ ($\{\epsilon_u, \epsilon_v, \epsilon_{yz}, \epsilon_{zx}, \epsilon_{xy}\}$).

Once the MQ ordering occurs, nonzero $\Lambda_{\zeta\mu}$ is obtained according to the types of the orderings. It is noted that the magnetic toroidal dipole and/or octupole belonging to the same irreducible representation of the MQ can be additionally activated, which also contributes to nonzero $\Lambda_{\zeta\mu}$. For example, in the case of M_{xy} ordering, the magnetic toroidal octupole T_z^β is simultaneously activated, which indicates two independent matrix elements in $\Lambda_{\zeta\mu}$, $\Lambda_{zxx} = -\Lambda_{zyy}$ and Λ_{vz} . The relation between the MQ ordering and nonzero Λ in each irreducible representation is listed in Table II. In the following, we discuss the behavior of Λ by focusing on the $M_{xy}^{(h)}$ ordered state in the model in Eq. (16).

Figure 7 shows the μ dependence of Λ_{zxx} ($= -\Lambda_{zyy}$) (solid red lines) in the $M_{xy}^{(h)}$ ordered state. The results for different h are plotted in Fig. 7(a) at $h = 0.5$, Fig. 7(b) at $h = 2$, and Fig. 7(c) at $h = 5$. The hopping parameters are $t_\sigma = 0.8$, $t_\pi =$

0.5 , $t_{xy} = 0.3$, $t_s = 1$, $t_{sp} = 0.6$, and $\lambda = 0$, which are the same as those in Sec. III A 2. It is noted that $\Lambda_{vz} = 0$ because of the two-dimensional system.

Λ_{zxx} takes a finite value for nonzero h , as shown in Figs. 7(a)–7(c). However, it vanishes in the insulating region without the Fermi surfaces, e.g., $2.7 < |\mu| < 3.7$ for $h = 5$ in Fig. 7(c), since the intraband process at the Fermi surface is important in the presence of the MQ, as mentioned above. The overall behavior of Λ_{zxx} against μ is similar: Λ_{zxx} shows a positive value for the small Fermi surface (small electron-hole filling), while it becomes negative for the large Fermi surface (close to half filling). For larger $h = 2$ and 5 , Λ_{zxx} is characterized by two broad maxima and one broad minimum, whose positions become closer to the eigenvalues of the mean-field Hamiltonian, i.e., $\pm\sqrt{2}h, 0$, for larger h . Meanwhile, there are four maxima and three minima for $h = 0.5$ in Fig. 7(a). These behaviors are understood by decomposing Λ_{zxx} into the contribution for the p th band, $\Lambda_{zxx}^{(p)}$ ($p = 0-5$), i.e., $\Lambda_{zxx} = \sum_p \Lambda_{zxx}^{(p)}$. When the bands are well separated by $\pm\sqrt{2}h$ for large $h = 5$ in Fig. 7(c), two maxima arise from the lower ($p = 0, 1$) and higher ($p = 4, 5$) bands, and one minimum arises from the middle band ($p = 2, 3$). With a decrease in h , the separated bands become closer to each other, and then they are overlapped at the band edge, as shown in Fig. 7(b). With a further decrease in h , the sum of the different band contributions results in complicated behavior, as shown in Fig. 7(a).

To examine the behavior of Λ_{zxx} in the MQ ordered state in detail, we compare it with the order parameter $\langle M_{xy}^{(h)} \rangle$, plotted as a function of μ at $h = 5$ in Fig. 7(d). $|\langle M_{xy}^{(h)} \rangle|$ increases while $|\mu|$ decreases and appears almost constant for $|\mu| < 3.7$. This result indicates that the behaviors of $\langle M_{xy}^{(h)} \rangle$ do

TABLE II. The irreducible representation (irrep.) of the magnetic and magnetic toroidal multipoles from rank 0 to rank 3 under the point group D_{4h} . The nonzero matrix elements of the current-induced distortion tensor Λ and the magnetoelectric tensor α are also shown.

Irrep.	Multipoles	$\Lambda_{\eta\mu}$	$\alpha_{\mu\nu}$
A_{1u}^-	M_0, M_u	$\Lambda_{yzx} = -\Lambda_{zxy}$	$\alpha_{xx} = \alpha_{yy}, \alpha_{zz}$
A_{2u}^-	T_z, T_z^α	$\Lambda_{zxx} = \Lambda_{zyy}, \Lambda_{uz}$	$\alpha_{xy} = -\alpha_{yx}$
B_{1u}^-	M_v, T_{xyz}	$\Lambda_{yzx} = \Lambda_{zxy}, \Lambda_{xyz}$	$\alpha_{xx} = -\alpha_{yy}$
B_{2u}^-	M_{xy}, T_z^β	$\Lambda_{zxx} = -\Lambda_{zyy}, \Lambda_{vz}$	$\alpha_{xy} = \alpha_{yx}$
E_u^-	$M_{yz}, T_x, T_x^\alpha, T_x^\beta$	$\Lambda_{ux}, \Lambda_{vx}, \Lambda_{xyy}, \Lambda_{zxx}$	α_{yz}, α_{zy}
	$M_{zx}, T_y, T_y^\alpha, T_y^\beta$	$\Lambda_{uy}, \Lambda_{vy}, \Lambda_{xyx}, \Lambda_{yzz}$	α_{zx}, α_{xz}

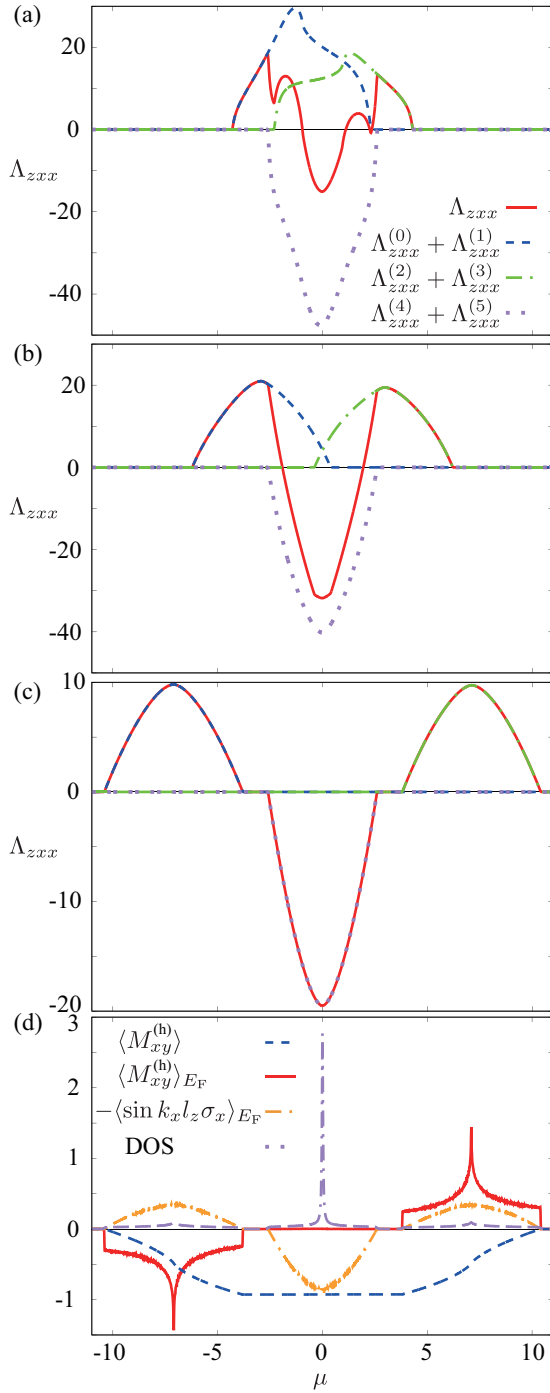


FIG. 7. (a)–(c) μ dependence of the coefficient of the current-distortion correlation, Λ_{zxx} , in the $M_{xy}^{(h)}$ state at temperature $T = 0.01$ and with damping factor $\delta = 0.01$ for (a) $h = 0.5$, (b) 2, and (c) 5. $\Lambda_{zxx}^{(p)}$ represents the intraband contribution from the p th band. The other parameters are the same as in Fig. 3. (d) μ dependences of the order parameter $\langle M_{xy}^{(h)} \rangle$, its contribution near the Fermi level $\langle M_{xy}^{(h)} \rangle_{E_F}$, the spin-orbital polarization near the Fermi level $\langle \sin k_x l_z \sigma_x \rangle_{E_F}$, and the density of states (DOS). Arbitrary units are used for $\langle M_{xy}^{(h)} \rangle_{E_F}$ and $\langle \sin k_x l_z \sigma_x \rangle_{E_F}$.

not have a simple correlation such as $\Lambda_{zxx} \propto \langle M_{xy}^{(h)} \rangle$ except in the region of low or high electron density. Besides, we also compare Λ_{zxx} with the μ derivative of $\langle M_{xy}^{(h)} \rangle$, $\langle M_{xy}^{(h)} \rangle_{E_F}$, since Λ_{zxx} is characterized by the intraband process at the Fermi

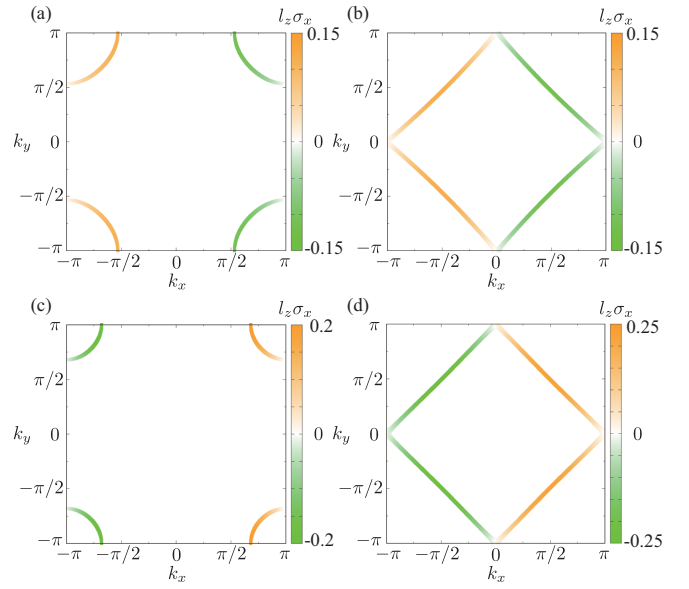


FIG. 8. The $l_z \sigma_x$ polarization of the isoenergy surfaces in the M_{xy} state for (a) $\mu = -9$, (b) $\mu = -7.1$, (c) $\mu = -2$, and (d) $\mu = 0$. The other parameters are $t_\sigma = 0.8$, $t_\pi = 0.5$, $t_{xy} = 0.3$, $t_s = 1$, $t_{sp} = 0.6$, and $h = 5$.

surface. As shown in Fig. 7(d), $\langle M_{xy}^{(h)} \rangle_{E_F}$ is enhanced at the inflection points with $|\mu| \simeq 7.1$, but it vanishes in the region for $|\mu| < 3.7$. Thus Λ_{zxx} do not have a simple correlation with $\langle M_{xy}^{(h)} \rangle_{E_F}$ either.

On the other hand, we find that Λ_{zxx} has a strong correlation with the antisymmetric spin-orbital polarization at the Fermi surface $-\langle \sin k_x l_z \sigma_x \rangle_{E_F}$ when the Fermi surface has the simple form, as shown in Fig. 7(d); there are two broad maxima at $|\mu| \simeq 7.1$ and a broad minimum at $\mu = 0$. This result indicates that the quantity of $-\langle \sin k_x l_z \sigma_x \rangle_{E_F}$, which is related to the spin-orbital-momentum locking, becomes the appropriate measure of the current-induced distortion. In other words, a large response is expected when the degree of the spin-orbital-momentum locking becomes large. There are two possibilities to reach a large value of Λ_{zxx} : One is the large value of $\mathcal{O}_\mu(\mathbf{k})$ at the Fermi surface, and the other is the large density of states (DOS) denoted as the dotted lines in Fig. 7(d). For the former $\mathcal{O}_\mu(\mathbf{k})$, a larger s - p hopping is preferable as discussed in Sec. III A 2. Meanwhile, for the latter, a large enhancement of the density of states, such as the van Hove singularity or flat band, is required. Indeed, Λ_{zxx} shows an increase by approaching $\mu \simeq 0, \pm\sqrt{2}h$, where the small circular Fermi surface close to the band edge in Figs. 8(a) and 8(c) gradually changes to the large square-shaped one at the van Hove singularity arising from the square-lattice geometry in Figs. 8(b) and 8(d).

5. Magnetoelectric effect

Next, we consider another cross-correlated response in the MQ ordered state. We investigate the magnetoelectric effect where the magnetization M_μ is induced by the electric field E_ν , i.e., $M_\mu = \sum_\nu \alpha_{\mu\nu} E_\nu$ for $\mu, \nu = x, y, z$. The tensor $\alpha_{\mu\nu}$ is

calculated by the linear response theory as

$$\alpha_{\mu\nu} = \sum_{\mathbf{k}} \sum_{pq} \Pi_{pq}(\mathbf{k}) M_{\mu\mathbf{k}}^{pq} v_{\nu\mathbf{k}}^{qp}, \quad (34)$$

where $M_{\mu\mathbf{k}}^{pq} = \langle p\mathbf{k} | \sigma_{\mu} | q\mathbf{k} \rangle$ is the matrix element of the spin. We here take into account only the spin component in $M_{\mu\mathbf{k}}^{pq}$ for simplicity.

Similar to the current-induced distortion tensor $\Lambda_{\zeta\nu}$ in the previous section, the magnetoelectric tensor $\alpha_{\mu\nu}$ becomes nonzero in the absence of the spatial-inversion symmetry. Since the time-reversal property between $\Lambda_{\zeta\nu}$ and $\alpha_{\mu\nu}$ is opposite, the odd-parity magnetic and magnetic toroidal multipoles with time reversal odd contribute to the interband process $p \neq q$. By using the active rank-0–2 odd-parity multipoles, the magnetic monopole M_0 , the magnetic toroidal dipole $\{T_x, T_y, T_z\}$, and the MQ $\{M_u, M_v, M_{yz}, M_{zx}, M_{xy}\}$, the matrix form of $\alpha_{\mu\nu}$ is represented by

$$\alpha = \begin{pmatrix} M_0 - M_u + M_v & M_{xy} + T_z & M_{zx} - T_y \\ M_{xy} - T_z & M_0 - M_u - M_v & M_{yz} + T_x \\ M_{zx} + T_y & M_{yz} - T_x & M_0 + 2M_u \end{pmatrix}, \quad (35)$$

where the rows (columns) of the matrix represent the components of $\{E_x, E_y, E_z\}$ ($\{M_x, M_y, M_z\}$). The nonzero matrix elements under the MQ ordering are shown in Table II. In the following, we focus on the behavior of $\alpha_{\mu\nu}$ in the $M_{xy}^{(h)}$ ordered state with $\alpha_{xy} = \alpha_{yx}$.

Figure 9 shows the μ dependence of α_{yx} ($= \alpha_{xy}$) denoted by the red solid lines in the $M_{xy}^{(h)}$ ordered state for $h = 0.5$ [Fig. 9(a)], $h = 2$ [Fig. 9(b)], and $h = 5$ [Fig. 9(c)]. The other parameters are common in Sec. III A 2. The result shows that α_{yx} is induced by nonzero h as Λ_{zxx} . In contrast to Λ_{zxx} , α_{yx} takes a finite value in the insulating region for $2.7 < |\mu| < 3.7$ and $h = 5$ in addition to the metallic region, since the interband process dominates in α_{yx} . As compared with the results in Figs. 9(a)–9(c), α_{yx} tends to be smaller for larger h , which is reasonable in terms of the interband process: The larger energy difference in the denominator in Eq. (34) for larger h suppresses α_{yx} . Although nonzero α_{yx} exists in the presence of the antisymmetric spin-orbital polarization under the MQ ordering, its behavior is mainly determined by the details of the electronic band structure, as discussed below.

As each band is doubly degenerate owing to the \mathcal{PT} symmetry, the total of six bands are separated into three two-degenerate bands under the MQ ordering. Then, α_{yx} is decomposed into three parts according to the different interband processes, $\alpha_{yx} = \alpha_{yx}^{(LM)} + \alpha_{yx}^{(MU)} + \alpha_{yx}^{(LU)}$, where the superscripts L, M, and U represent the lower two bands $p = 0, 1$, middle two bands $p = 2, 3$, and upper two bands $p = 4, 5$, respectively. In other words, $\alpha_{yx}^{(LM)}$ includes the contribution of the interband process between the lower two bands and middle two bands, for instance. For small $h = 0.5$, the contribution of $\alpha_{yx}^{(MU)}$ ($\alpha_{yx}^{(LM)}$) is dominant for the negative (positive) peak at $\mu \simeq -2.33$ (2.32), while $\alpha_{yx}^{(LU)}$ is less important. The large enhancement at $\mu \simeq -2.33$ and 2.32 is attributed to the small band gap in the electronic band structure for small h , as shown in Fig. 10(a). The band structure in Fig. 10(a) indicates that the dominant contribution comes from near the

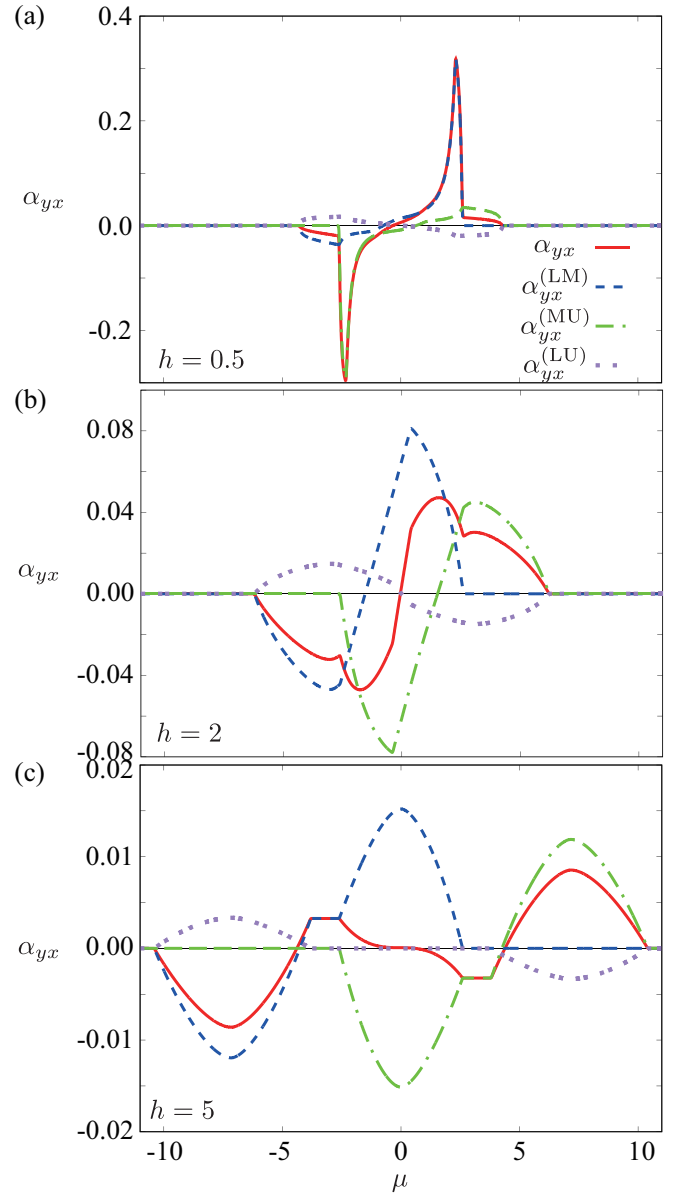


FIG. 9. μ dependence of the coefficient of the current-magnetization correlation, α_{yx} , in the $M_{xy}^{(h)}$ state at temperature $T = 0.01$ and with damping factor $\delta = 0.01$ for (a) $h = 0.5$, (b) 2, and (c) 5. $\alpha_{yx}^{(LM)}$, $\alpha_{yx}^{(MU)}$, and $\alpha_{yx}^{(LU)}$ represent the interband contribution for the specific bands. L, M, and U represent the lower two bands ($p = 0, 1$), middle two bands ($p = 2, 3$), and upper two bands ($p = 4, 5$), respectively. For example, $\alpha_{yx}^{(LM)}$ stands for the interband process between the lower two bands and middle two bands. The other parameters are the same as in Fig. 3.

$\mathbf{k} = (\pi, \pi)$ [$\mathbf{k} = (0, 0)$] point at $\mu \simeq -2.33$ (2.32), which is originally fourfold degenerate at $h = 0$. When the three bands are separated by increasing h , the contribution of $\alpha_{yx}^{(LM)}$ ($\alpha_{yx}^{(MU)}$) becomes important for low (high) electron density, as shown in Figs. 9(b) and 9(c). For large h , all the \mathbf{k} points below the Fermi level contribute to $\alpha_{yx}^{(LM)}$ irrespective of $\mathcal{Q}(\mathbf{k})$, since the energy difference between the lower and middle bands at each \mathbf{k} takes similar values, as shown in Fig. 10(b). The broad peaks at $\mu \simeq -7.16$ and 7.17 for $h = 5$ are attributed to

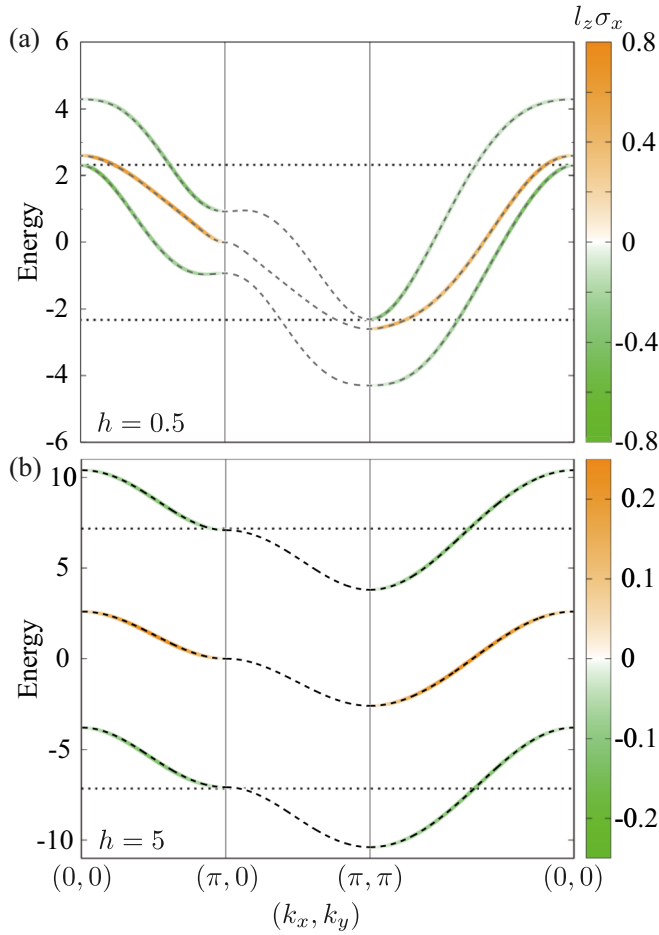


FIG. 10. The band structure at (a) $h = 0.5$ and (b) 5. The dashed curves show the band dispersions, and the color map shows the spin-orbital polarization of the $l_z \sigma_x$ component at each wave vector. The horizontal dotted lines show the energy where $|\alpha_{yx}|$ is maximized.

the van Hove singularity, as shown in Fig. 8(b). Meanwhile, α_{yx} is negligibly small close to the half filling owing to the cancellation of the contributions of $\alpha_{yx}^{(LM)}$ and $\alpha_{yx}^{(MU)}$, as shown in Fig. 9(c).

B. Sublattice system

Next, we investigate another situation with the active MQ degree of freedom in the sublattice system. We consider a four-sublattice model in the tetragonal system in Sec. III B 1. In Sec. III B 2, we show that a similar spin-orbital-momentum locking occurs in the MQ ordering even without the atomic orbital degree of freedom.

1. Model

In this section, we consider another electronic degree of freedom to activate the MQ. In particular, we focus on the sublattice degree of freedom instead of the orbital one, where the MQ is activated with the antiferromagnetic ordering. We examine the four-sublattice system in the tetragonal lattice structure, as shown in Fig. 11(a), where the point group is D_{4h} as in Sec. III A. Also in this sublattice case, the extension to a three-dimensional system is straightforward. The lattice

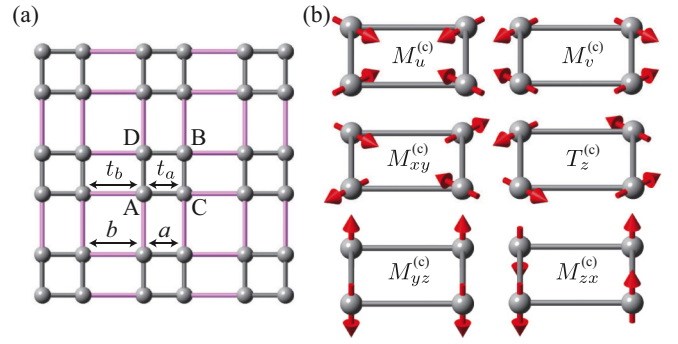


FIG. 11. (a) Sublattice model consisting of four sublattices A–D in the tetragonal lattice structure with the lattice constant $a + b$. (b) The spin patterns of the odd-parity cluster MQs $\{M_u^{(c)}, M_v^{(c)}, M_{xy}^{(c)}, M_{yz}^{(c)}, M_z^{(c)}\}$ and magnetic toroidal dipole $T_z^{(c)}$ in Eqs. (40)–(45). The arrows represent the direction of magnetic moments.

constant is taken as $a = b = 1/2$ for notational simplicity, and the difference between a and b is expressed as the different hopping amplitudes, t_a and t_b . When there is no orbital degree of freedom at each sublattice, the tight-binding Hamiltonian is given by

$$\mathcal{H} = \sum_{\mathbf{k}, \gamma, \gamma', \sigma} c_{\mathbf{k}\gamma\sigma}^\dagger H_{\sigma}^{\gamma\gamma'} c_{\mathbf{k}\gamma'\sigma}, \quad (36)$$

where $c_{\mathbf{k}\gamma\sigma}^\dagger$ ($c_{\mathbf{k}\gamma\sigma}$) is the creation (annihilation) operator of electrons at wave vector \mathbf{k} , sublattice $\gamma = A-D$, and spin σ . The 4×4 Hamiltonian matrix spanned by the four-sublattice basis $\{\phi_{A\sigma}, \phi_{B\sigma}, \phi_{C\sigma}, \phi_{D\sigma}\}$ is given by

$$H_{\sigma} = \begin{pmatrix} 0 & 0 & f_x^* & f_y^* \\ 0 & 0 & f_y & f_x \\ f_x & f_y^* & 0 & 0 \\ f_y & f_x^* & 0 & 0 \end{pmatrix}, \quad (37)$$

where $f_{\eta} = t_a e^{ik_{\eta}/2} + t_b e^{-ik_{\eta}/2}$ for $\eta = x, y$.

The Hamiltonian in Eq. (36) has 64 independent electronic degrees of freedom. Similar to the discussion in Sec. III A, one can construct the MQ degree of freedom by the product of the odd-parity electronic degree of freedom in spinless space and spin σ . The spinless odd-parity electronic degree of freedom is expressed as the spatial distribution of the on-site potential with the same magnitude but different sign, which corresponds to the odd-parity electric dipoles, $Q_x^{(c)}$ and $Q_y^{(c)}$. The matrix forms of $Q_x^{(c)}$ and $Q_y^{(c)}$ are given by

$$Q_x^{(c)} = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}, \quad (38)$$

$$Q_y^{(c)} = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \quad (39)$$

where the superscript (c) means the cluster multipole that is defined in the sublattice cluster [10–12]. We here do not explicitly consider the other electric dipole degree of freedom,

e.g., the bond degree of freedom, and we here focus on the antiferromagnetic ordering, which is represented by the contraction of $\{Q_x^{(c)}, Q_y^{(c)}\}$ and σ . By taking a linear combination of them, we obtain the expressions for five MQs as

$$A_{1u}^-: M_u^{(c)} = -Q_x^{(c)}\sigma_x - Q_y^{(c)}\sigma_y, \quad (40)$$

$$B_{1u}^-: M_v^{(c)} = Q_x^{(c)}\sigma_x - Q_y^{(c)}\sigma_y, \quad (41)$$

$$E_u^-: M_{yz}^{(c)} = Q_y^{(c)}\sigma_z, \quad (42)$$

$$M_{zx}^{(c)} = Q_x^{(c)}\sigma_z, \quad (43)$$

$$B_{2u}^-: M_{xy}^{(c)} = Q_x^{(c)}\sigma_y + Q_y^{(c)}\sigma_x \quad (44)$$

and the magnetic toroidal dipole as

$$A_{2u}^-: T_z^{(c)} = Q_x^{(c)}\sigma_y - Q_y^{(c)}\sigma_x. \quad (45)$$

The corresponding spin patterns are shown in Fig. 11(b), where $M_u^{(c)}$, $M_v^{(c)}$, $M_{xy}^{(c)}$, and $T_z^{(c)}$ exhibit the noncollinear magnetic textures, while $M_{yz}^{(c)}$ and $M_{zx}^{(c)}$ are the collinear magnetic textures. It is noted that $M_{yz}^{(c)}$ and $M_{zx}^{(c)}$ are also regarded as the magnetic toroidal dipole ordering $T_x^{(c)}$ and $T_y^{(c)}$, respectively, which belong to the same irreducible representation under the point group D_{4h} .

2. Band structure

Since there is no orbital degree of freedom in the system, orbital angular momentum l is inactive as the electronic degree of freedom in the Hamiltonian. Nevertheless, a similar pseudo-orbital angular momentum is defined as the degree of freedom over the sublattices. Since the electron hoppings on the closed loop in the square plaquette as $A \rightarrow C \rightarrow B \rightarrow D$ give rise to the magnetic flux to the electrons in the out-of-plane direction, the matrix of the pseudo-orbital angular momentum is defined as

$$l_z^{(c)} = \begin{pmatrix} 0 & 0 & -i & i \\ 0 & 0 & i & -i \\ i & -i & 0 & 0 \\ -i & i & 0 & 0 \end{pmatrix}. \quad (46)$$

By using $l_z^{(c)}$ instead of l_z in Eqs. (26)–(30), one can obtain similar physics to that in Sec. III A.

We show a similar spin-orbital-momentum locking in the model in Eq. (36) under the MQ ordering. We here focus on the M_{xy} ordered state in Fig. 11(b) with the molecular field h as an example. Figure 12 shows the isoenergy surfaces at $\mu = -0.5$, $t_a = 1$, $t_b = 0.5$, and $h = 0.3$ in the M_{xy} ordered state. Similar to the result in Fig. 3(c), the band structure exhibits the antisymmetric spin-orbital polarization of $l_z^{(c)}\sigma_x$ and $l_z^{(c)}\sigma_y$, which corresponds to the spin-orbital-momentum locking. The component of $l_z^{(c)}\sigma_x$ is asymmetric with respect to the k_x direction, while that of $l_z^{(c)}\sigma_y$ is asymmetric with respect to the k_y direction. The necessary hopping parameters are also obtained by evaluating $\mathcal{O}_\mu(\mathbf{k}) = \text{Tr}[e^{-\beta H_\mu} l_z^{(c)} \sigma_\mu]$. The lowest-order contributions are given by

$$-h(t_a - t_b) \left(\sin \frac{k_x}{2} l_z^{(c)} \sigma_x + \sin \frac{k_y}{2} l_z^{(c)} \sigma_y \right), \quad (47)$$

which indicates that the relation $t_a \neq t_b$ is necessary for the spin-orbital-momentum locking besides $h \neq 0$. Also in this

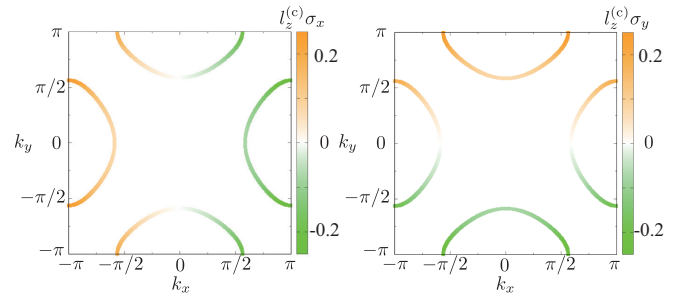


FIG. 12. The isoenergy surfaces at $\mu = -0.5$, $t_a = 1$, $t_b = 0.5$, and $h = 0.3$ in the M_{xy} state. The color map shows the spin-orbital polarization of $l_z^{(c)}\sigma_x$ (left) and $l_z^{(c)}\sigma_y$ (right) at each wave vector.

case, the effective spin-orbit coupling in the form of $l_z^{(c)}\sigma_z$ emerges even without the effect of the atomic relativistic spin-orbit coupling in the tight-binding model (not shown). The contribution is represented by $h^2(t_a + t_b)(\cos k_x/2 + \cos k_y/2)$.

Once the spin-orbital-momentum locking occurs by the MQ ordering, similar physics to that discussed in Sec. III A is expected, such as the antisymmetric spin polarization by the magnetic field and linear responses. We briefly discuss the electronic band structure in the presence of the magnetic field. Although similar symmetric and antisymmetric spin splittings to those shown in Fig. 6 are expected because of the same symmetry, the necessary model parameters are different from those of the multiorbital case. When the magnetic field is applied along the x direction, the $k_x k_y \sigma_y$ -type symmetric and $k_x \sigma_z$ -type antisymmetric spin splittings are expected, but they do not show up within the model Hamiltonian in Eq. (36). Such spin splittings under the magnetic field appear when the additional diagonal hopping between A and B (and C and D) and/or the effective spin-dependent hopping from the atomic relativistic spin-orbit coupling exist. Considering such terms within the plaquette, we obtain the former Hamiltonian matrix as

$$H_\sigma^{\text{diag}} = \begin{pmatrix} 0 & f_{xy}^* & 0 & 0 \\ f_{xy} & 0 & 0 & 0 \\ 0 & 0 & 0 & f_{xy}^* \\ 0 & 0 & f_{xy}' & 0 \end{pmatrix}, \quad (48)$$

where $f_{xy} = t_a' e^{i(k_x + k_y)/2}$ and $f_{xy}' = t_a' e^{i(-k_x + k_y)/2}$, and the latter Hamiltonian matrix as

$$H_\sigma^{\text{SOC}} = \lambda \begin{pmatrix} 0 & 0 & -ie^{-ik_x/2} & ie^{-ik_y/2} \\ 0 & 0 & ie^{ik_y/2} & -ie^{ik_x/2} \\ ie^{ik_x/2} & -ie^{-ik_y/2} & 0 & 0 \\ -ie^{ik_y/2} & ie^{-ik_x/2} & 0 & 0 \end{pmatrix}. \quad (49)$$

By evaluating $\mathcal{O}_\mu(\mathbf{k})$, we obtain the necessary effective coupling for the symmetric spin splitting $k_x k_y \sigma_y$ as $h^2 H_x t_b^2 t_a' \sin k_x \sin k_y$ and the antisymmetric spin splitting $k_x \sigma_z$ as the superposition of $h H_x \lambda t_b \sin k_x$ and $h^3 H_x t_a t_b' \sin k_x$. Thus t_a' is necessary for both the symmetric and antisymmetric spin splittings, while λ is the antisymmetric spin splitting. In a similar way, the antisymmetric spin splitting $k_x \sigma_x - k_y \sigma_y$ in a magnetic field along the z axis is caused by introducing t_a' and λ , e.g., the coupling $-h H_z \lambda t_b \sin k_x \sigma_x$ and $h^3 H_z t_a t_b' \sin k_x \sigma_x$.

IV. SUMMARY

To summarize, we have investigated the electronic states and related physical phenomena induced by the MQ orderings. We found that the MQ ordered state exhibits a peculiar spin-orbital entanglement in momentum space; the spin-orbital polarization is antisymmetrically locked at the particular component at each wave vector, which is dubbed the spin-orbital-momentum locking. The present spin-orbital-momentum locking is driven by the onset of the MQ orderings in contrast to the spin-momentum locking that exists in the nonmagnetic noncentrosymmetric lattice systems. We show two typical examples for the MQ orderings by considering the multiorbital and sublattice systems. We demonstrate that the spin-orbital-momentum locking occurs under the MQ orderings, which causes various cross-correlated physical phenomena, such as the magnetic-field-induced symmetric and antisymmetric spin polarization in the band structure, the current-induced distortion, and the magnetoelectric effect. We discuss the relevant model parameters in each phenomenon. As the spin-orbital-momentum locking is expected to be found in odd-parity magnetic materials not only

in the MQ phase but also in other magnetic and magnetic toroidal multipole phases, our study will stimulate a further exploration of functional spintronics materials, which have recently been extensively studied. BaMn_2As_2 [104–107] (UNi_4B [23,26,108,109] and Ce_3TiBi_5 [27,28]) is then a candidate material to exhibit the spin-orbital-momentum locking under the MQ (magnetic toroidal dipole) ordering.

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