

## Multipole order in two-dimensional altermagnets

Tenta Tani<sup>1,\*</sup> and Ulrich Zülicke<sup>2,†</sup>

<sup>1</sup>*Department of Physics, The University of Osaka, Toyonaka, Osaka 560-0043, Japan*

<sup>2</sup>*MacDiarmid Institute, School of Chemical and Physical Sciences, Victoria University of Wellington, P.O. Box 600, Wellington 6140, New Zealand*



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We theoretically investigate the magnetic-multipole orders in two-dimensional (2D) altermagnets, focusing on two representative models: a generic minimal three-site model and a four-site model representative of monolayer FeSe. We construct low-energy effective Hamiltonians for both systems and calculate their respective multipole indicators to characterize the underlying magnetic order. Our analysis reveals an intriguing contrast between the two systems. We find that the generic minimal model exhibits the expected nonzero magnetic-octupole order. In the monolayer-FeSe model, however, the magnetic-octupole order vanishes globally, and a magnetic-hexadecapole order is present instead. The emergence of altermagnetic splitting in the band structure then arises via the interplay with a sublattice-isospin degree of freedom. Our work demonstrates how the classification and comprehensive understanding of 2D altermagnetic materials transcends bulk descriptions.

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### I. INTRODUCTION

Altermagnetism [1–5] has recently been introduced as a term to designate magnetically ordered materials that have no bulk magnetization but still exhibit spin splitting in the electronic band structure. Altermagnets are thus different from ferromagnets (which have a finite spontaneous magnetization and associated uniform exchange spin splitting of electron states) and the more ordinary antiferromagnets (which also lack a bulk magnetization but retain spin degeneracy in their band structure because time inversion combined with a translation or with space inversion remains a good symmetry).

Physical ramifications of altermagnetism are currently attracting considerable attention. The altermagnetic properties of several materials have been intensively investigated, including RuO<sub>2</sub> [6–10], MnTe [11–13], and CrSb [14–16]. For example, spin-to-charge conversion [8], thermal transport [9], and magnons [6] have been examined for RuO<sub>2</sub>. Two-dimensional (2D) altermagnets are also increasingly coming into focus [17–21], with proposed materials including MnPSe<sub>3</sub> [22], Cr<sub>2</sub>SO [23] and V<sub>2</sub>SeTeO [24].

Conceptually, altermagnetism in bulk materials can be understood as a manifestation of hidden multipole order [4,25–27] that is space-inversion symmetric but breaks time inversion. In contrast to ferromagnets that are characterized by a macroscopic magnetic-dipole density (the magnetization),

altermagnets have been shown to exhibit spontaneous ordering of higher-odd-rank magnetic multipoles (octupoles, triakontadipoles, etc.) [4,26,27] or even-rank magnetotoroidal multipoles [4,28].

In the present work, we investigate the connection to multipole order for low-dimensional altermagnet realizations. For this purpose, we consider two specific microscopic models. The first one is the minimal model for a 2D altermagnet introduced in Ref. [17] and illustrated in Fig. 1(a), with two magnetic atoms and an additional nonmagnetic atom per unit cell. The second model is representative of monolayer FeSe, which was shown to become an altermagnet in the presence of a perpendicular electric field [22]. See Fig. 2 for the corresponding crystal structure, which can be regarded just as the minimal model [17] displayed in Fig. 1(a) with one additional nonmagnetic atom in the unit cell.

Our theoretical descriptions build upon previous foundational work: the minimal model for 2D altermagnetism proposed in Ref. [17] and the density-functional-theory (DFT) study of monolayer FeSe [22]. However, these prior studies did not investigate the nature of the magnetic-multipole orders that are intrinsically linked to the altermagnetic phases in these systems. The primary goal of this work is to fill this gap. To this end, we make two key contributions: (1) For the model from Ref. [17], we derive the effective low-energy Hamiltonian and identify the characteristic magnetic-octupole order. (2) For monolayer FeSe, we construct a tight-binding model that captures the essential low-energy features of the DFT results [22], and we demonstrate that this system hosts a hidden magnetic-hexadecapole order that is linked to the altermagnetic spin splitting. Through these analyses, we clarify the essential role of multipole physics in these prototypical 2D altermagnets.

We treat each model by first diagonalizing their respective tight-binding Hamiltonians that include nearest-neighbor

\*Contact author: [tenta.tani@qp.phys.sci.osaka-u.ac.jp](mailto:tenta.tani@qp.phys.sci.osaka-u.ac.jp)

†Contact author: [uli.zuelicke@vuw.ac.nz](mailto:uli.zuelicke@vuw.ac.nz)

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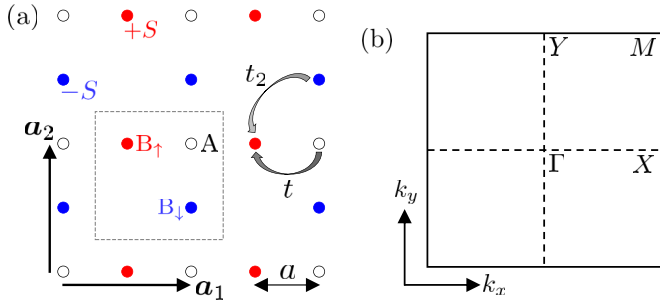


FIG. 1. Minimal model for a 2D altermagnet [17]. (a) Square lattice with sites having a localized spin-up (red), spin-down (blue), or no magnetization (white). Primitive lattice vectors  $\mathbf{a}_1, \mathbf{a}_2$  are shown as black arrows, and a (next-)nearest-neighbor hopping process with parameter  $t$  ( $t_2$ ) is depicted by gray arrows. (b) First Brillouin zone of the 2D square lattice.

and next-nearest-neighbor hopping terms, as well as local exchange-energy splittings at the magnetic sites. (For the case of monolayer FeSe, the electrostatic potential arising from the perpendicular electric field is also included.) This yields the known altermagnetic band structures for the two model systems [17,22]. We then derive a faithful effective envelope-function-Hamiltonian description for the low-energy subbands by adapting the standard subband- $\mathbf{k} \cdot \mathbf{p}$  theory that was originally devised for treating 2D-electron states in semiconductor heterostructures [29,30]. We identify terms in the effective low-energy model Hamiltonian that are representative of the hidden multipole order and derive the associated band-structure indicators using the method proposed in Sec. II E of Ref. [26]. This enables quantification of higher-order magnetic-multipole densities in the 2D altermagnetic structures considered here. Our analytical results reveal intriguing parametric dependencies of the multipole order.

The remainder of this article is organized as follows. Section II is devoted to analyzing the minimal model for 2D altermagnets proposed in Ref. [17] and shown in Fig. 1(a). We derive the effective low-energy effective model for the band structure and obtain the indicator of the magnetic-octupole density that is associated with altermagnetism in this structure. The magnitude of the latter is then calculated both analytically and numerically. In Sec. III, we consider the simple model for 2D FeSe depicted in Fig. 2 and derive its effective model. Surprisingly, we find that the magnetic-octupole density vanishes globally, while a magnetic-hexadecapole density represents hidden order in the FeSe system. Altermagnetic band splitting is shown to arise from the intricate interplay between the hexadecapolar order and the perpendicular electric field. Finally, Sec. IV presents our conclusions.

## II. MAGNETIC-OCTUPOLE ORDER IN A MINIMAL MODEL FOR 2D ALTERMAGNETS

To obtain generic insights into 2D altermagnets, we consider the minimal model proposed in Ref. [17]. As shown in Fig. 1(a), the model consists of a nonmagnetic site  $A$  and two magnetic sites  $B_\uparrow$  and  $B_\downarrow$ . The unit cell is indicated by the dashed square, and the primitive lattice vectors are

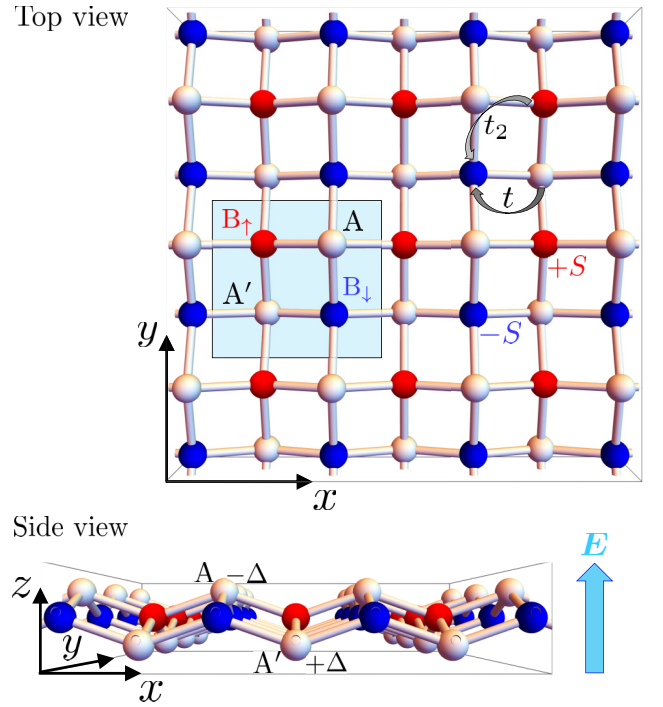


FIG. 2. Structure representing monolayer FeSe. The unit cell (indicated by the cyan square) contains two Fe atoms (red and blue) and two Se atoms (white). In the tight-binding model, nearest-neighbor ( $t$ ) and second-nearest-neighbor ( $t_2$ ) hopping parameters are included. The Fe sites are assumed to have localized spins  $\pm S$ . By applying a perpendicular electric field  $E$ , the two Se sites acquire different potentials  $\pm\Delta$ .

$\mathbf{a}_1 = (2a, 0)$  and  $\mathbf{a}_2 = (0, 2a)$ . In momentum space, reciprocal-lattice vectors are given by  $\mathbf{b}_1 = (\pi/a, 0)$  and  $\mathbf{b}_2 = (0, \pi/a)$ . In Fig. 1(b), the first Brillouin zone with labeled high-symmetry points is shown.

The electron Hamiltonian of the model is given by

$$\mathcal{H} = \sum_{\sigma=\pm} \left( t \sum_{\langle i,j \rangle} c_{i,\sigma}^\dagger c_{j,\sigma} + t_2 \sum_{\langle\langle i,j \rangle\rangle} c_{i,\sigma}^\dagger c_{j,\sigma} - J_{sd} \sigma \sum_i S_i c_{i,\sigma}^\dagger c_{i,\sigma} \right) \quad (1)$$

where  $c_{i,\sigma}^\dagger$  and  $c_{i,\sigma}$  are the creation and annihilation operators of an electron with spin  $\sigma = \pm 1$  at lattice site  $i$ . The parameter  $t$  quantifies hopping between nearest-neighbor pairs  $\langle i, j \rangle$ , and  $t_2$  is the corresponding hopping parameter between second-nearest-neighbor sites  $\langle\langle i, j \rangle\rangle$ . Examples for these hopping processes are illustrated in Fig. 1(a). The prefactor  $J_{sd}$  of the third term is the exchange coupling between localized and itinerant electrons. The respective localized-electron spins of atoms on the  $A$ ,  $B_\uparrow$ , and  $B_\downarrow$  sites are given by  $S_i = 0, S$ , and  $-S$ , respectively. Taking Bloch states  $\{|A\rangle, |B_\uparrow\rangle, |B_\downarrow\rangle\}$  as the basis, the Bloch Hamiltonian is written as

$$H(\mathbf{k}, \sigma) = \begin{pmatrix} 0 & 2 \cos k_x & 2 \cos k_y \\ 2 \cos k_x & -J\sigma & 4t_2 \cos k_x \cos k_y \\ 2 \cos k_y & 4t_2 \cos k_x \cos k_y & J\sigma \end{pmatrix}, \quad (2)$$

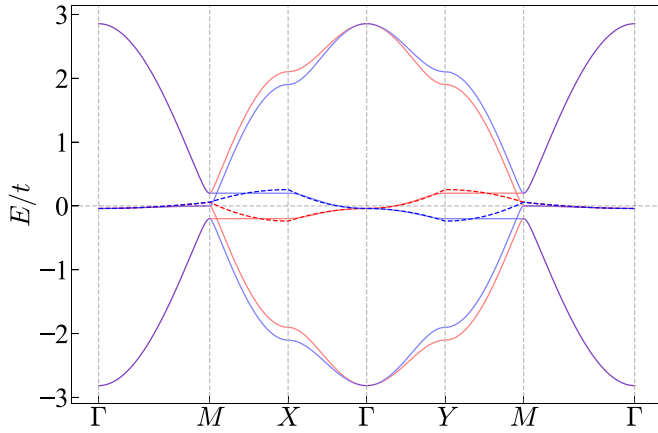


FIG. 3. Band structure for the minimal 2D-altermagnet model. The six bands plotted as the solid lines are calculated from the original Hamiltonian (2). The dispersions shown as dashed lines are obtained from the effective Hamiltonian (7). The red (blue) color indicates spin-up (spin-down) bands. The hopping parameters are set to be  $J/t = 0.2$  and  $t_2/t = 0.01$ .

where  $J = J_{sd}S$ , and we set  $a = 1$ ,  $t = 1$  for simplicity. From this Hamiltonian, the electronic band structure is obtained

$$H'(\mathbf{k}, \sigma) = \begin{pmatrix} -4t_2C_xC_y + J\sigma(C_x - C_y) & C_x - C_y + \frac{J\sigma}{\sqrt{2}}(1 - C_y) & -C_x + C_y + \frac{J\sigma}{\sqrt{2}}(1 - C_y) \\ C_x - C_y + \frac{J\sigma}{\sqrt{2}}(1 - C_y) & -\sqrt{2}(C_x + C_y) + 2t_2C_xC_y - \frac{J}{2}(3C_x + C_y) & 2t_2C_xC_y + \frac{J}{2}(C_x - C_y) \\ -C_x + C_y + \frac{J\sigma}{\sqrt{2}}(1 - C_y) & 2t_2C_xC_y + \frac{J}{2}(C_x - C_y) & \sqrt{2}(C_x + C_y) + 2t_2C_xC_y - \frac{J}{2}(3C_x + C_y) \end{pmatrix}, \quad (5)$$

where we used the abbreviations  $C_x \equiv \cos k_x$  and  $C_y \equiv \cos k_y$ . When we further neglect  $\mathcal{O}(J)$  and  $\mathcal{O}(t_2)$  corrections to terms of  $\mathcal{O}(1)$ , we find

$$H'(\mathbf{k}, \sigma) = \begin{pmatrix} -4t_2C_xC_y & C_x - C_y & -C_x + C_y \\ C_x - C_y & -\sqrt{2}(C_x + C_y) & 2t_2C_xC_y \\ -C_x + C_y & 2t_2C_xC_y & \sqrt{2}(C_x + C_y) \end{pmatrix} + J\sigma(C_x - C_y) \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1/2 \\ 0 & 1/2 & 0 \end{pmatrix}. \quad (6)$$

In Eq. (6), the coupling between the  $E = \mathcal{O}(t_2) \approx 0$  band and the bands with energies  $|E| \approx 2\sqrt{2}$  is negligible in the vicinity of the  $\Gamma$  point, and the effective low-energy Hamiltonian is found as

$$H_{\text{eff}}(\mathbf{k}) = J\sigma_z(\cos k_x - \cos k_y) - 4t_2 \cos k_x \cos k_y \approx -\frac{J}{2}\sigma_z(k_x^2 - k_y^2) + 4t_2(\mathbf{k}^2/2 - 1). \quad (7)$$

Here,  $\sigma_z$  denotes the Pauli matrix in spin space. The band structure obtained from this effective Hamiltonian is shown by the dashed curves in Fig. 3, where the red (blue) color corresponds to the spin-up (spin-down) electron states. We find that the effective bands fit the original dispersions fairly

as shown in Fig. 3 by the solid curves, using parameters  $J/t = 0.2$  and  $t_2/t = 0.01$ . Red (blue) curves are for the spin-up (spin-down) sector; these exhibit the altermagnetic spin splitting.

We now focus on the low-energy spectrum around the  $\Gamma$  point. An effective two-band Hamiltonian  $H_{\text{eff}}$  describing states near the Fermi level is constructed as follows. Exactly at the  $\Gamma$  point, the Hamiltonian (2) becomes

$$H_{\Gamma}(\sigma) = \begin{pmatrix} 0 & 2 & 2 \\ 2 & -J\sigma & 4t_2 \\ 2 & 4t_2 & J\sigma \end{pmatrix}. \quad (3)$$

If we set  $t_2 = 0$ ,  $H_{\Gamma}$  can be analytically diagonalized. Assuming further  $J \ll 1$  and neglecting  $\mathcal{O}(J^2)$  terms, the eigenenergies are  $E_1 = 0$ ,  $E_2 = -2\sqrt{2}$ , and  $E_3 = 2\sqrt{2}$ . We transform the original Hamiltonian (2) to this band basis. The unitary matrix  $U$  for this transformation reads

$$U = \frac{1}{4} \begin{pmatrix} -\sqrt{2}J\sigma & -2\sqrt{2} - J\sigma & 2\sqrt{2} - J\sigma \\ -2\sqrt{2} & 2 + \sqrt{2}J\sigma & 2 - \sqrt{2}J\sigma \\ 2\sqrt{2} & 2 & 2 \end{pmatrix}. \quad (4)$$

Hence, the Hamiltonian in the new basis is obtained by  $H'(\mathbf{k}, \sigma) = U^\dagger H(\mathbf{k}, \sigma)U$ , which can be written as

well and reproduce the altermagnetic spin splitting. The spin-dependent Fermi surface of the model is depicted in Fig. 4(a), for  $J < 4t_2$ , which has been called the weak-altermagnet phase [31,32]. The shapes of the Fermi surfaces are ellipses with a semimajor axis  $k_{F>} = [2/(1 + J/4t_2)]^{1/2}$  and a semiminor axis  $k_{F<} = [2/(1 - J/4t_2)]^{1/2}$ .

The connection between altermagnetism and multipole order is embodied in the spin-splitting term  $\propto \sigma_z(k_x^2 - k_y^2)$  in the Hamiltonian (7). Specifically, the quantity

$$\mathcal{I}^{(m,3)}(\mathbf{k}, \sigma) = \sigma(k_x^2 - k_y^2) \quad (8)$$

constitutes the band-structure indicator for a magnetic-octupole density [26,28] that is compatible with the system's magnetic-point-group symmetry  $D_{4h}(D_{2h})$  [17]. The indicator's expectation value is straightforwardly calculated as

$$\begin{aligned} \langle \mathcal{I}^{(m,3)} \rangle &= \sum_{\sigma} \int_{\text{BZ}} \frac{d\mathbf{k}}{(2\pi)^2} \mathcal{I}^{(m,3)}(\mathbf{k}, \sigma) f(E_{\mathbf{k}\sigma}) \\ &= \int_{\text{BZ}} \frac{d\mathbf{k}}{(2\pi)^2} (k_x^2 - k_y^2) [f(E_{\mathbf{k}+}) - f(E_{\mathbf{k}-})], \end{aligned} \quad (9)$$

where  $f(E)$  is the Fermi distribution function and  $E_{\mathbf{k}\sigma}$  the band dispersions close to the Fermi energy.

The expectation value  $\langle \mathcal{I}^{(m,3)} \rangle$  directly quantifies the magnetic-octupole density present in the system. (This

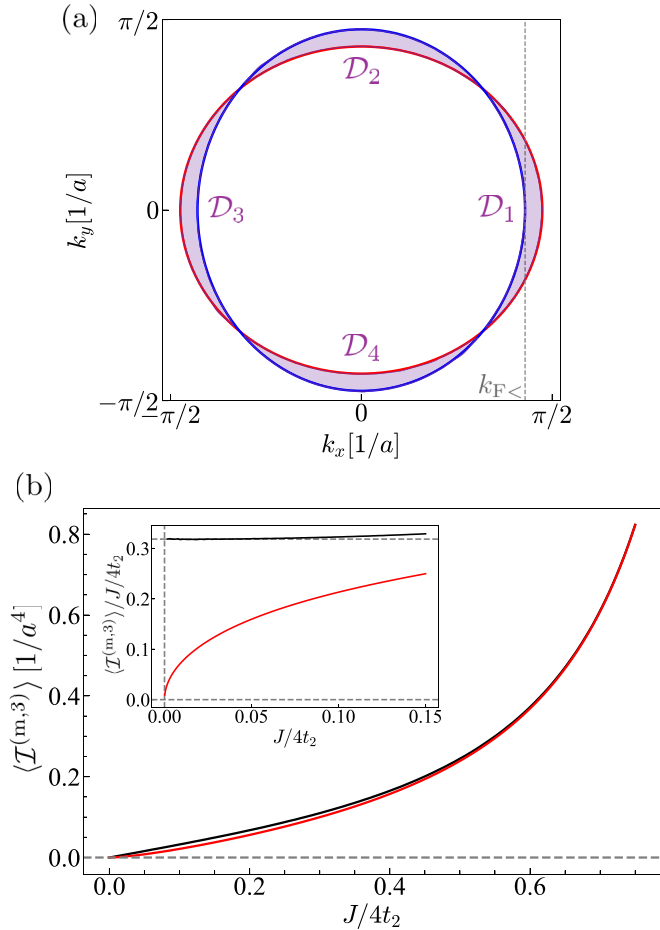


FIG. 4. (a) Fermi surfaces for spin-up (red) and spin-down (blue) states for the effective low-energy Hamiltonian (7) derived for the generic 2D-altermagnet model [17] with parameters  $J/4t_2 = 0.1$ . Purple shading indicates the four regions with spin-polarized occupation. (b) Expectation value of the magnetic-octupole indicator  $\langle \mathcal{I}^{(m,3)} \rangle$ . The black (red) curve plots the numerical (analytical) result.

is entirely analogous to how a finite expectation value of  $\mathcal{I}^{(m,1)} = \sigma$  quantifies the magnetization. Obviously,  $\langle \mathcal{I}^{(m,1)} \rangle \equiv 0$  in the present case.) We now calculate  $\langle \mathcal{I}^{(m,3)} \rangle$  in the zero-temperature limit, where the difference of Fermi functions in the expression (9) is finite only for states occupied by either spin-up or spin-down electrons. Considering the shape of the Fermi surface [Fig. 4(a)], the four purple regions  $\mathcal{D}_1$  to  $\mathcal{D}_4$  contribute equally. Thus, Eq. (9) can be rewritten as

$$\langle \mathcal{I}^{(m,3)} \rangle = \frac{4}{(2\pi)^2} \int_{\mathcal{D}_1} d\mathbf{k} (k_x^2 - k_y^2). \quad (10)$$

To obtain an approximate analytical expression, we only integrate over the region with  $k_x > k_{F<}$  [see the gray vertical line in Fig. 4(a)], which is a good approximation for larger  $J$ . After some computations, we find

$$\begin{aligned} \langle \mathcal{I}^{(m,3)} \rangle &= \frac{1}{(2\pi)^2} \left[ \left( \frac{\pi}{2} - \arcsin \frac{k_{F<}}{k_{F>}} \right) k_{F<} k_{F>} (k_{F>} + k_{F<}) (k_{F>} - k_{F<}) \right. \\ &\quad \left. - \frac{k_{F<}^2}{3} \sqrt{1 - \frac{k_{F<}^2}{k_{F>}^2}} \left( k_{F<}^2 - 3k_{F>}^2 + \frac{2k_{F<}^4}{k_{F>}^2} \right) \right]. \quad (11) \end{aligned}$$

In Fig. 4(b), we compare the numerical result (9) (black curve) and the analytical result (11) (red curve). The agreement between both is good for larger  $J/4t_2$ , as expected from the approximation used in the analytical calculation. Deviations become apparent in the small- $J$  regime ( $J/4t_2 \ll 1$ ), where we have

$$k_{F>} \approx \frac{\sqrt{2}}{a} \left( 1 + \frac{J/4t_2}{2} \right), \quad k_{F<} \approx \frac{\sqrt{2}}{a} \left( 1 - \frac{J/4t_2}{2} \right), \quad (12)$$

so that Eq. (11) reduces to

$$\langle \mathcal{I}^{(m,3)} \rangle \approx \frac{16\sqrt{2}}{3\pi^2 a^4} \left( \frac{J}{4t_2} \right)^{3/2}. \quad (13)$$

As seen in the inset of Fig. 4(b), the asymptotic behavior of the numerical result is  $\langle \mathcal{I}^{(m,3)} \rangle \propto J/(4t_2)$ , and this is not reproduced by the analytical form (13). This discrepancy arises because the area left out of the integration range in the analytical calculation becomes significant in the small- $J$  limit.

### III. ALTERMAGNETIC MONOLAYER FeSe

In this section, we investigate monolayer FeSe. Its crystal structure is shown in Fig. 2. It has coplanar magnetic (Fe) sites and a buckling that renders the two Se sites in the unit cell inequivalent. As was done in Ref. [22], we assume checkerboard-antiferromagnetic order to be present. The system is then characterized by the magnetic point group  $C_{4h}(S_4)$ , which has the combination of space inversion and time inversion as a good symmetry. As a result, the band dispersions are spin degenerate and asymmetric around the  $\Gamma$  point. Application of a perpendicular electric field was shown to render the material an altermagnet [22].

We construct a tight-binding model for checkerboard-antiferromagnetic FeSe simply by adding an additional nonmagnetic site  $A'$  to the minimal 2D-altermagnet model discussed in Sec. II. An external perpendicular electric field is introduced via onsite potentials  $\pm\Delta$  on the Se sites. We thus obtain a  $4 \times 4$  Bloch Hamiltonian,

$$\begin{aligned} H(\mathbf{k}, \sigma) &= \begin{pmatrix} -\Delta & 0 & 2 \cos k_x & 2 \cos k_y \\ 0 & \Delta & 2 \cos k_y & 2 \cos k_x \\ 2 \cos k_x & 2 \cos k_y & -J\sigma & 4t_2 \cos k_x \cos k_y \\ 2 \cos k_y & 2 \cos k_x & 4t_2 \cos k_x \cos k_y & J\sigma \end{pmatrix}, \quad (14) \end{aligned}$$

with basis states  $\{|A\rangle, |A'\rangle, |B_\uparrow\rangle, |B_\downarrow\rangle\}$ . The band structure calculated from this Hamiltonian for some sample parameters is plotted by the solid curves in Fig. 5. Around the  $M$  point, this model reproduces the DFT band structure calculated in Ref. [22].

At the  $M$  point, the Hamiltonian (14) is diagonal with eigenenergies  $[E_{1\sigma}^{(0)}, E_{2\sigma}^{(0)}, E_{3\sigma}^{(0)}, E_{4\sigma}^{(0)}] = [-\Delta, \Delta, -J\sigma, J\sigma]$ . In order to derive a low-energy effective Hamiltonian, we apply second-order perturbation theory to these eigenstates. This yields the energy dispersions

$$E_{k i \sigma} = E_{i \sigma}^{(0)} + \sum_{j \neq i} \frac{\langle u_i^{(0)} | H' | u_j^{(0)} \rangle}{E_{i \sigma}^{(0)} - E_{j \sigma}^{(0)}}, \quad (15)$$

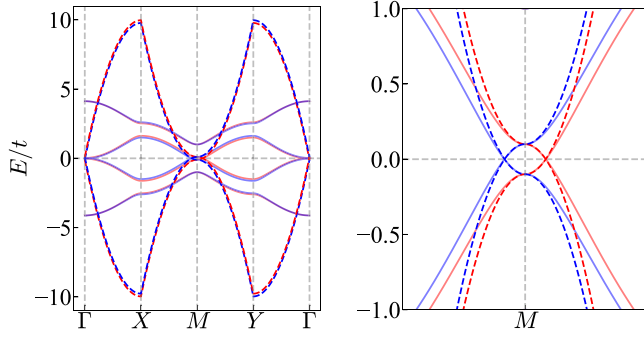


FIG. 5. Band structure of the four-site model for monolayer FeSe. The eight bands depicted by the solid lines are calculated from the original Hamiltonian (14), while the four bands shown by the dashed lines are obtained from the effective Hamiltonian (18). Red (blue) color represents the spin-up (spin-down) dispersion. The right panel is a magnification around the  $M$  point. Parameters used in the calculation are  $J/t = 1$ ,  $t_2/t = 0$ , and  $\Delta/t = 0.1$ .

for  $i = 1, 2, 3, 4$ .  $H'$  is defined via  $H = H_0 + H'$  and  $H_0 = H(\mathbf{k} = M)$ .  $|u_i^{(0)}\rangle$  is the  $i$ th eigenvector of  $H_0$ .

Here, we are interested in the two bands with  $i = 1, 2$ , which represent the band structure closest to the Fermi energy  $E = 0$ . When we relabel  $i = 1, 2$  in terms of a pseudospin quantum number  $\tau = \pm 1$ , we have

$$E_{k\tau\sigma} = \tau \left[ \Delta + 4 \frac{(\Delta + J\sigma) \cos^2 k_x + (\Delta - J\sigma) \cos^2 k_y}{\Delta^2 - J^2} \right]. \quad (16)$$

We can derive an effective Hamiltonian considering the limit of a small perpendicular electric field. For  $J \gg \Delta$ ,

$$H_{\text{eff}}(\mathbf{k}) = \tau_z [\Delta - (4/J) \sigma_z (\cos^2 k_x - \cos^2 k_y)], \quad (17)$$

where  $\tau_z$  is the Pauli matrix in the low-energy two-band space. When we take the  $M$  point to be the origin of  $\mathbf{k}$  space, we have

$$H_{\text{eff}}(\mathbf{k}) = \tau_z [\Delta - (4/J) \sigma_z (k_x^2 - k_y^2)], \quad (18)$$

for small  $\mathbf{k}$ . Plotting the band dispersions for the effective Hamiltonian (18) by dashed lines in Fig. 5, we see that they coincide with the original low-energy bands close to the  $M$  point.

The Fermi surface calculated from the effective Hamiltonian (18) for the  $\tau = +$  band is shown in Fig. 6(a). It consists of hyperbolas  $k_x^2/k_{F0}^2 - k_y^2/k_{F0}^2 = \pm 1$ , where the  $+/-$  signs are for the spin-up/spin-down electrons, respectively. Here, we introduced the scale  $k_{F0} = \sqrt{J\Delta/2}$ . Spin-up (spin-down) states are occupied in the regions  $\mathcal{D}_1$  and  $\mathcal{D}_3$  ( $\mathcal{D}_2$  and  $\mathcal{D}_4$ ). Such a Fermi-surface shape is indicative of a strong altermagnet [31,32].

In the effective Hamiltonian (18),  $\sigma_z$  corresponds to the electron spin, whereas  $\tau_z$  is a sublattice-pseudospin degree of freedom distinguishing the Se sites  $\{A, A'\}$ . Therefore,  $\tau_z$  has the characteristics of the spatial coordinate  $z$ , including its transformational properties under space inversion (odd) and time inversion (even). Consequently, the quantity

$$\mathcal{I}^{(m,4)}(\mathbf{k}, \tau, \sigma) = \tau \sigma (k_x^2 - k_y^2) \quad (19)$$

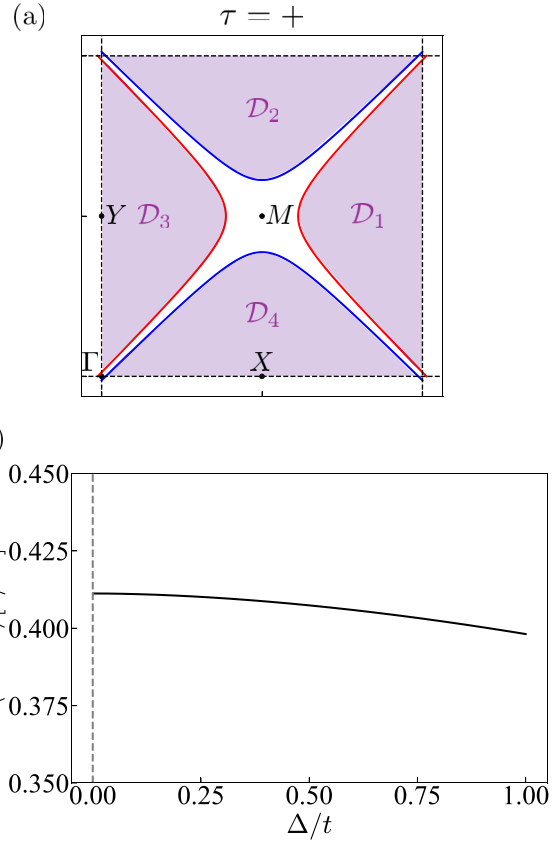


FIG. 6. (a) Fermi surfaces of the minimal model for FeSe at the  $M$  point. Here, we plot the  $\tau = +$  sector only. Regions  $\mathcal{D}_1$  and  $\mathcal{D}_3$  ( $\mathcal{D}_2$  and  $\mathcal{D}_4$ ) are occupied by spin-up (spin-down) states. Parameters used are  $J/t = 1$ ,  $t_2/t = 0$ , and  $\Delta/t = 0.5$ . (b) Expectation value  $\langle \mathcal{I}^{(m,4)} \rangle$  of the magnetic-hexadecapole indicator (19), plotted as a function of the electric-potential magnitude  $\Delta$ .

constitutes a band-structure indicator for a rank-4 multipole that is odd under both space inversion and time inversion, i.e., a magnetic hexadecapole.

The possibility of real-space quantities, such as sublattice-related pseudospins, appearing in effective Hamiltonians and energy dispersions for 2D systems enlarges the palette of band-structure indicators for multipole order beyond those that have previously been constructed for 3D crystals [26,28]. Magnetic-hexadecapole order is a case in point. In a bulk crystalline solid, its indicator must be an odd-order polynomial in wave-vector components [28] and cannot involve spin. The fact that, for a 2D system, the combination  $\tau_z \sigma_z$  transforms like a wave-vector component enables a substitution  $k_j \rightarrow \tau \sigma$ , leading to the form as given in Eq. (19). For more explicit illustration of this point, we now characterize both the magnetic-octupole and the magnetic-hexadecapole order in the FeSe model system.

### A. Magnetic octupole

The indicator for a macroscopic magnetic-octupole density is given in Eq. (8). Its expectation value for the FeSe system

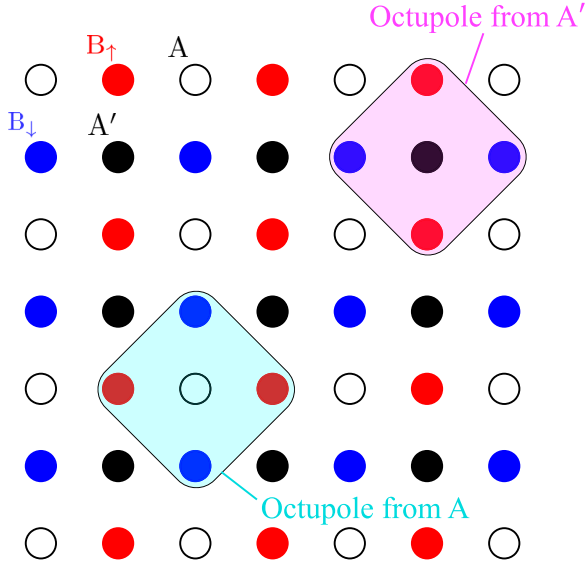


FIG. 7. Schematic illustration of the atomic structure of monolayer FeSe with opposite microscopic magnetic-octupole contributions from the A and A' sublattices indicated by the cyan and magenta regions. The cancellation of the two sublattice's spatially shifted magnetic-octupole densities produces magnetic-hexadecapole order.

is obtained by evaluating

$$\langle \mathcal{I}^{(m,3)} \rangle = \sum_{\tau\sigma} \int_{\text{BZ}} \frac{d\mathbf{k}}{(2\pi)^2} \mathcal{I}^{(m,3)}(\mathbf{k}, \sigma) f(E_{k\tau\sigma}). \quad (20)$$

At zero temperature, Eq. (18) implies  $\sum_{\tau\sigma} \sigma f(E_{k\tau\sigma}) \equiv \sum_{\sigma} \sigma = 0$ . Hence, the integrand from Eq. (20) vanishes identically, and so does  $\langle \mathcal{I}^{(m,3)} \rangle$ . This result means that the contributions to a magnetic-octupole density from the two sublattices  $\tau = \pm$  cancel out. Figure 7 is a conceptual illustration of the globally vanishing magnetic octupole, with the two contributions from the A sublattice (cyan) and the A' sublattice (magenta) cancelling each other. However, as we now demonstrate, a magnetic-hexadecapole density emerges as the remnant of this cancellation.

### B. Magnetic hexadecapole

The expectation value of the magnetic-hexadecapole indicator (19) for the FeSe system is obtained from

$$\langle \mathcal{I}^{(m,4)} \rangle = \sum_{\tau\sigma} \int_{\text{BZ}} \frac{d\mathbf{k}}{(2\pi)^2} \mathcal{I}^{(m,4)}(\mathbf{k}, \tau, \sigma) f(E_{k\tau\sigma}). \quad (21)$$

In this integral, contributions for  $\tau = \pm$  do not cancel, as we find

$$\sum_{\tau\sigma} \tau \sigma f(E_{k\tau\sigma}) = 2 \sum_{\sigma} \sigma f(E_{k+\sigma}). \quad (22)$$

Considering the shape of Fermi surfaces for the  $\tau = +$  bands [Fig. 6(a)], the expectation value (21) is obtained via

$$\langle \mathcal{I}^{(m,4)} \rangle = \frac{8}{(2\pi)^2} \int_{\mathcal{D}_1} d\mathbf{k} (k_x^2 - k_y^2), \quad (23)$$

since the four regions  $\mathcal{D}_1$  to  $\mathcal{D}_4$  contribute equally to the result. We can exactly integrate this to get an expression

$$\langle \mathcal{I}^{(m,4)} \rangle = \frac{k_{\text{F0}}^4}{2\pi^2} \left[ \frac{\pi}{6k_{\text{F0}}a} \sqrt{\frac{\pi^2}{4k_{\text{F0}}^2a^2} - 1} \left( \frac{\pi^2}{k_{\text{F0}}^2a^2} + 2 \right) - 2 \ln \left( \frac{\pi}{2k_{\text{F0}}a} + \sqrt{\frac{\pi^2}{4k_{\text{F0}}^2a^2} - 1} \right) \right]. \quad (24)$$

The  $\Delta$  dependence of  $\langle \mathcal{I}^{(m,4)} \rangle$  is plotted in Fig. 6(b). Note that it stays finite in the limit  $\Delta = 0$ ; i.e., it is a property of the FeSe crystal itself. However, the associated altermagnetic spin splitting emerges only for  $\Delta \neq 0$  when the combined spin and sublattice-pseudospin degeneracy is lifted. The finite magnetic-hexadecapole order could be experimentally observed via the magneto-piezoelectric effect, as proposed in Ref. [33].

Our finding that the altermagnetic phase in the monolayer-FeSe model is characterized by a magnetic hexadecapole looks surprising from the standpoint of conventional wisdom. Even-rank magnetic multipoles preserve the combination of space inversion and time inversion and, thus, have previously been associated with spin-degenerate,  $+\mathbf{k}/-\mathbf{k}$  asymmetric band structures [2,26] that are not of altermagnetic form. However, our work reveals a mechanism arising in the 2D FeSe system where the sublattice degree of freedom provides a crucial coupling  $\tau_z \sigma_z$ . This coupling enables the magnetic-hexadecapole order to generate a spin-dependent term in the effective Hamiltonian, which in turn drives the spin splitting. This result thus identifies a pathway to altermagnetism, expanding the classes of magnetic multipole orders known to host this phase.

In principle, the same scenario as discussed here for a specific 2D system could occur more generally in any situation with a time-inversion-invariant pseudospin degree of freedom transforming like an odd-rank polar tensor. This usually requires band-edge degeneracies and/or band edges located away from the  $\Gamma$  point.

## IV. CONCLUSION

We have investigated multipole order in a minimal model for generic 2D altermagnets and for a model system representing monolayer FeSe. Consistent with crystal symmetry, the former is shown to exhibit magnetic-octupole order, whereas the latter hosts a macroscopic magnetic-hexadecapole density. Both orders are quantified based on their respective band-structure indicators, given in Eqs. (8) and (19), respectively.

In contrast to previously considered situations for 3D crystals where magnetic-hexadecapole order is indicated by band dispersions that are asymmetric in wave-vector components but always remain spin degenerate, such order in a 2D system can give rise to altermagnetic spin splitting. We link such fundamental differences in physical ramifications for the same type of multipole order to the possibility to have 2D band-structure invariants that involve pseudospins that are equivalent to real-space (e.g., sublattice) positions. Future work could focus on incorporating more

systematically any possible pseudospin degrees of freedom into the construction of band-structure indicators in 2D crystals.

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### DATA AVAILABILITY

The data that support the findings of this article are not publicly available upon publication because it is not technically feasible and/or the cost of preparing, depositing, and hosting the data would be prohibitive within the terms of this research project. The data are available from the authors upon reasonable request.

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