Theory of orbital magnetic quadrupole moment and magnetoelectric susceptibility

Atsuo Shitade
RIKEN Center for Emergent Matter Science, 2-1 Hirosawa, Wako, Saitama 351-0198, Japan

Hikaru Watanabe and Youichi Yanase
Department of Physics, Graduate School of Science, Kyoto University, Kyoto 606-8502, Japan
(Dated: July 17, 2018)

We derive a quantum-mechanical formula of the orbital magnetic quadrupole moment (MQM) in periodic systems by using the gauge-covariant gradient expansion. This formula is valid for insulators and metals at zero and nonzero temperature. We also prove a direct relation between the MQM and magnetoelectric (ME) susceptibility for insulators at zero temperature. It indicates that the MQM is a microscopic origin of the ME effect. Using the formula, we quantitatively estimate these quantities for room-temperature antiferromagnetic semiconductors BaMn$_2$As$_2$ and CeMn$_2$Ge$_2-x$Si$_x$. We find that the orbital contribution to the ME susceptibility is comparable with or even dominant over the spin contribution.

In classical electromagnetism, electric and magnetic multipole moments characterize the anisotropy of the charge and charge current densities. Spin is also an important origin of the magnetic dipole moment. When electric or magnetic dipole moments align in a certain direction, it is called a ferroelectric or a ferromagnet. In several decades, we have witnessed the importance of higher-order multipole moments in strongly correlated electron systems [1, 2]. More recently, higher-order topological insulators with electric multipole moments were theoretically proposed [3–6] and soon later realized in a metamaterial [7] and a microwave circuit [8]. Multipole moments are now more ubiquitous than in the 19th century when classical electromagnetism was established.

Among multipole moments, the magnetic quadrupole moment (MQM) has been believed to be an important ingredient for the magnetoelectric (ME) effect [9–11]. In this phenomenon, the charge polarization is induced by a magnetic field, and the magnetization is induced by an electric field. Both the inversion and time-reversal symmetries should be broken. Although the multipole order observed in some f-electron systems [1, 2] does not break the inversion symmetry, the symmetry conditions are satisfied in the presence of the MQM. Cr$_2$O$_3$ was the first material in which the ME effect was theoretically predicted [12] and experimentally observed [13–16]. So far, the toroidal moment, which is the antisymmetric part of the MQM, was investigated in Ga$_{2−x}$Fe$_x$O$_3$ [17, 18], LiCoPO$_4$ [19, 20], and Ni$_{0.4}$Mn$_{0.6}$TiO$_3$ [21], and the symmetric MQM in Ba(TiO)$_2$Cu$_4$(PO$_4$)$_4$ [22]. We also note that the ME effect has been intensively studied in the field of multiferroics since the celebrated discoveries of BiFeO$_3$ thin films [23] and TbMnO$_3$ [24]. Theoretically, an expression of the spin MQM was derived using an adiabatic deformation [25, 26]. However, it is not gauge invariant, nor does it take spin-orbit interactions into account, and another expression was thermodynamically derived using the semiclassical theory [27].

Although the above materials are magnetic insulators, the MQM also appears in electron systems. In a zigzag chain [28, 29] and a honeycomb lattice [30–32], the inversion symmetry may be broken by a magnetic order, leading to the spin MQM and ME effect. It was pointed out that a spin magnetic hexadecapole moment appears in antiferromagnetic (AFM) semiconductor BaMn$_2$As$_2$ [33]. In these theoretical studies, the orbital contribution has been neglected although it may not be negligible.

When we calculate the electric or magnetic multipole moments quantum mechanically in periodic systems, we suffer from the fact that the position operator is unbounded. This difficulty can be solved in several ways. The charge polarization $P^i$ was formulated by calculating the charge current density $J^i$ induced by an adiabatic deformation of the Hamiltonian [34–36]. This idea relies on the electromagnetic relation $J^i = P^i + \epsilon^{ijk}\partial_{X_j}M_k$, in which $\epsilon^{ijk}$ is the totally antisymmetric tensor. The result is expressed by the Berry connection and valid only for insulators at zero temperature. Later, it was reformulated using the Green’s function [37–39]. On the other hand, the orbital magnetization $M_k$ was defined by the thermodynamic relation $M_k = -\partial\Omega/\partial B^k$ [40], in which $\Omega$ is the grand potential, and $B^k$ is a magnetic field. The result is expressed by the Berry curvature and magnetic moment and is valid for insulators, without or with the Chern number, and metals at zero and nonzero temperature. Effects of disorder and interactions were studied with the help of the Green’s function [37, 41, 42].

In this Rapid Communication, we derive a quantum-mechanical formula of the orbital MQM in periodic systems. First, we define the MQM and prove a direct relation to the ME susceptibility based on thermodynamic relations. This relation indicates that the MQM is a microscopic origin of the ME effect. Next, we calculate the orbital MQM in the Bloch basis using the gauge-covariant gradient expansion of the Keldysh Green’s function [43–45]. Finally, we apply these results to the AFM semiconductors BaMn$_2$As$_2$ and CeMn$_2$Ge$_2-x$Si$_x$. We find that the orbital contribution to the ME susceptibility is com-
parable with or even dominant over the spin contribution.

We begin with the thermodynamic relation of the grand potential \( \Omega \equiv E - TS - \mu N \),

\[
d\Omega = -SdT - M_\mu dB^k - N d\mu,
\]

in which \( S, N \) are the entropy and particle number, and \( T, \mu \) are temperature and the chemical potential. Supposing a magnetic field \( B(X) \) is nonuniform and varies slowly compared with a length scale of the lattice constants, then we can extend Eq. (1) to a local relation,

\[
d\Omega = -SdT - (M_k - \partial_X M^l_k) dB^k - N d\mu.
\]

\( M^l_k \) is the MQM and in general not symmetric over \( l \) and \( k \). The magnetic toroidal and monopole moments are also included in the \( 3 \times 3 = 9 \) components of \( M^l_k \). By integrating by parts, we obtain a general definition of the MQM,

\[
M^l_k \equiv -\frac{\partial \Omega}{\partial (\partial_X B^k)},
\]

together with the well-known relations \( S = -\partial \Omega/\partial T \) and \( N = -\partial \Omega/\partial \mu \). We also obtain the Maxwell relations,

\[
\begin{align*}
-\frac{\partial^2 \Omega}{\partial T \partial (\partial_X B^k)} &= \frac{\partial S}{\partial (\partial_X B^k)} = \frac{\partial M^l_k}{\partial T}, \\
-\frac{\partial \Omega}{\partial (\partial_X B^k) \partial \mu} &= \frac{\partial M^l_k}{\partial \mu} = \frac{\partial N}{\partial (\partial_X B^k)}.
\end{align*}
\]

The first relation (4a) is practically important. To see this, we define a related quantity,

\[
\tilde{M}^l_k \equiv -\frac{\partial K}{\partial (\partial_X B^k)},
\]

which involves the energy \( K \equiv E - \mu N = \Omega + TS \). Using Eq. (4a), these two are related by

\[
\tilde{M}^l_k = -\frac{\partial \Omega}{\partial (\partial_X B^k)} - T \frac{\partial S}{\partial (\partial_X B^k)} = M^l_k - T \frac{\partial M^l_k}{\partial T} = \frac{\partial (\beta M^l_k)}{\partial \beta}.
\]

We calculate Eq. (5) and solve Eq. (6) to obtain the MQM. A similar relation is known for the orbital magnetization [40].

A direct relation between the MQM and ME susceptibility follows from the second relation (4b). When the system is an insulator at zero temperature, the charge density can be expressed by \( q N = -\partial_X P^\mu \), with \( q \) being the electron charge, and Eq. (4b) is reduced to

\[
-q \frac{\partial M^l_k}{\partial \mu} = \frac{\partial (\partial_X P^\mu)}{\partial (\partial_X B^k)} = \alpha^l_k.
\]

\( \alpha^l_k = \partial P^l / \partial B^k \) is the linear ME susceptibility. If the system is a metal or at nonzero temperature, the polarization charge is screened by the itinerant or thermally excited charge, and hence this relation does not make sense. This relation is valid for the orbital and spin contributions and indicates that the MQM is a microscopic origin of the ME effect. Gao et al. obtained the same relation but restricted their discussion to the spin toroidal moment [27].

Let us comment on the Středa formula for the MQM. The Středa formula relates the Hall conductivity to the orbital magnetization as \( \partial J^i / \partial E_j = q e^{ijk} \partial M_k / \partial \mu = q e^{ijk} \partial N / \partial B^k \) [46]. The first equality is explained by the magnetization current \( J^i = e^{ijk} \partial X_j \partial X_k \partial M_k / \partial \mu \) and identifying \( \partial X_j / q \) as an electric field \( E_j \). The second equality follows from the Maxwell relation. Similarly, the magnetization is expressed by \( M_k = -\partial X_j \partial M_k^l = -(\partial X_j / \mu) (\partial M_k^l / \partial \mu) \), leading to \( \partial M_k / \partial E_l = -q \partial M_k^l / \partial \mu \). This electric-field-induced magnetization is defined in insulators and metals at zero and nonzero temperature. However, in the above identification, we do not take into account the dissipation effect caused by the electric field on the Fermi surface.

The Středa formula is known as such Fermi-surface terms. Therefore, the Středa formulas are valid only for insulators at zero temperature. Combining Eq. (7), we obtain

\[
\partial M_k / \partial E_l = -q \partial M_k^l / \partial \mu = \partial P^l / \partial B^k.
\]

This is not trivial because the charge polarization is not a thermodynamic quantity but a geometric one, while the magnetization is a thermodynamic one. Note that the above discussion holds for disordered and interacting systems because it relies on thermodynamics. Below, we microscopically prove Eq. (8) for the orbital contribution in the absence of disorder or interactions.

Here, we derive the quantum-mechanical formula of the orbital MQM. To calculate the energy in the nonuniform magnetic field, we use the gauge-covariant gradient expansion [43–45]. In this method, we attach the Wilson line to the Keldysh Green’s function, which guarantees the gauge covariance, and express the gauge-covariant Keldysh Green’s function in terms of the center-of-mass coordinate \( X \) and the relative momentum \( p \). As a result, the convolution in the Dyson equation turns into the noncommutative Moyal product. In the absence of disorder or interactions, the variation of the energy due to the nonuniform magnetic field is given by [51].
\[
K_{DF} = -\frac{i\hbar^2}{6} \frac{1}{\partial X} \frac{d^4 p}{(2\pi\hbar)^4} \int \frac{dx}{2\pi} f(\xi) \times \text{tr} \left[ \partial_0^R \partial_{p_i}(g_0^R)^{-1} \partial_{p_j}(g_0^R)^{-1} \partial_{p_k}(g_0^R)^{-1} \right] + y_0^R \partial_{p_i}(g_0^R)^{-1} - y_0^R \partial_{p_j}(g_0^R)^{-1} - y_0^R \partial_{p_k}(g_0^R)^{-1} \right] + c.c., \quad (9)
\]

in which \( F_{ij} = q\epsilon_{ijk}B^k \) is the magnetic field, \( d \) is the space dimension, and \( g_0^R(\xi, \vec{p}) = [\xi - \mathcal{H}(\vec{p}) + \mu + i\eta]^{-1} \) is the retarded Green's function of the Hamiltonian \( \mathcal{H}(\vec{p}) \). By expanding the trace in Eq. (9) with respect to the Bloch basis that satisfies \( \mathcal{H}(\vec{p})|\epsilon_n(\vec{p})\rangle = \epsilon_n(\vec{p})|\epsilon_n(\vec{p})\rangle \), we obtain
\[
M_i^j = \frac{q}{\hbar^2} \epsilon_{ijk} \sum_n \int \frac{d^4 p}{(2\pi\hbar)^4} \left\{ A_{ij}^n f_n(\epsilon_n - \mu) + m_{ij}^n [f_n + f_n^\prime(\epsilon_n - \mu)] + \gamma_{ij}^n [2f_n^\prime + f_n^{\prime\prime}(\epsilon_n - \mu)] \right\}, \quad (10a)
\]
\[
A_{ij}^n = \frac{q^3}{2} \sum_{m, r, (\neq n)} \frac{\langle u_n|v^{|r_{m}}\rangle \langle u_{m}|v^{|r_{r}}\rangle \langle u_{r}|v^{|r_{n}}\rangle}{(\epsilon_n - \epsilon_m)^2(\epsilon_n - \epsilon_r)} + \frac{\hbar^3}{2} \sum_{m(\neq n)} \frac{\langle u_n|v^{|m}\rangle \langle u_{m}|v^{|m}\rangle \langle u_{n}|v^{|m}\rangle}{(\epsilon_n - \epsilon_m)^3} + c.c. - (i \leftrightarrow j), \quad (10b)
\]
\[
m_{ij}^n = -\frac{q^3}{6} \sum_{m, r, (\neq n)} \frac{\langle \partial_{p_{m}} u_n |\omega_{r}| u_{m} |\partial_{p_{r}} (\epsilon_n + \mathcal{H}) Q_{n} |\partial_{p_{n}} u_{m} \rangle}{(\epsilon_n - \epsilon_m)(\epsilon_n - \epsilon_r)} + \frac{\hbar^3}{3} \sum_{m(\neq n)} \frac{\langle u_n|v^{|m}\rangle \langle u_{m}|v^{|m}\rangle \langle u_{n}|v^{|m}\rangle}{(\epsilon_n - \epsilon_m)^2} + c.c. - (i \leftrightarrow j), \quad (10c)
\]
\[
\gamma_{ij}^n = \frac{q^3}{12} \sum_{m(\neq n)} \frac{\langle u_n|v^{|m}\rangle \langle u_{m}|v^{|m}\rangle \langle u_{n}|v^{|m}\rangle}{\epsilon_n - \epsilon_m} + c.c. - (i \leftrightarrow j), \quad (10d)
\]

Here, \( v^{|i} \equiv \partial_{p_i} \mathcal{H} \) is the velocity operator, \( f_n \equiv f(\epsilon_n - \mu) \) is the Fermi distribution function, and \( Q_n \equiv 1 - |u_n\rangle \langle u_n| \) is the projection operator, which guarantees the gauge invariance. For degenerate bands, we have to modify the projection operator as \( Q_n \equiv 1 - \sum_s |u_{n_s}\rangle \langle u_{n_s}| \), in which \( s \) indicates the index of degenerate bands with energy \( \epsilon_n \). The arguments \( \xi, \vec{p} \) are dropped for simplicity. By solving Eq. (6), we obtain our central result on the orbital MQM,
\[
M_i^j = \frac{q}{\hbar^2} \epsilon_{ijk} \sum_n \int \frac{d^4 p}{(2\pi\hbar)^4} \left[ -A_{ij}^n \int_{\epsilon_n - \mu}^\infty dz f(z) + m_{ij}^n f_n + \gamma_{ij}^n f_n \right]. \quad (11)
\]

The third term seems to be a Fermi-surface term unlike thermodynamic quantities. However, it can be integrated by parts because \( \gamma_{ij}^n \) is proportional to \( \partial_{p_i} \epsilon_n \). Therefore, the second and third terms are Fermi-sea terms.

For insulators at zero temperature, where we can drop the derivatives of the Fermi distribution function, we obtain
\[
-\frac{q}{\hbar^2} \frac{1}{\epsilon_{ijk}} \sum_n \int \frac{d^4 p}{(2\pi\hbar)^4} A_{ij}^n = \alpha_i^j. \quad (12)
\]

This formula is identical to the orbital ME susceptibility derived by using an adiabatic deformation in the context of topological insulators [52, 53], except for the isotropic Chern-Simons 3-form. Our formula is gauge invariant and hence does not include such a gauge-dependent term. Thus, we have microscopically proved Eq. (8) for the orbital contribution. The full ME susceptibility of \( \text{Cr}_2\text{O}_3 \) including spin and lattice [54] was calculated by first principles. Our formula of the orbital MQM Eq. (11) is based on the Bloch basis, and thus it enables a first-principles calculation of the orbital MQM.

It is suggestive to compare Eq. (11) with the quantum-mechanical formula of the orbital magnetization [40] that consists of the Berry-curvature and magnetic-moment terms. These are interpreted as magnetizations arising from the itinerant and local circulations, respectively, in the semiclassical [55, 56] and Wannier-basis theories [57, 58]. Similarly, the first term in Eq. (11) is the itinerant contribution to the orbital MQM, while the second and third terms are the local ones. In fact, according to Eq. (5) in Ref. [53], \( A_{ij}^n \) is rewritten by a virtual process from an occupied band \( n \) to an unoccupied band \( m \) via the electric dipole moment \( \vec{r}^d \) and magnetic dipole moment \( \vec{r}^d \times \vec{v} \) and is consistent with the group-theoretical analysis. Such an interband process is allowed not only in metals but also in insulators. Therefore, the itinerant
contribution is important even in insulators, as demonstrated below.

Let us apply our formula to real materials. First, we focus on an AFM semiconductor BaMn$_2$As$_2$ [59–61]. In this material, since two Mn sites are crystallographically inequivalent even in the paramagnetic phase, the AFM order breaks the time-reversal and inversion symmetries instead of the translation symmetry. By hole doping, Ba$_{1-x}$K$_x$Mn$_2$As$_2$ becomes a metal, but the AFM order is robust up to $x < 0.16$ [62, 63]. The group-theoretical analysis and microscopic calculation revealed that this seemingly conventional AFM order is in fact the ferroic order of the magnetic hexadecapole moment and MQM [33]. The ferroic MQM suggests a room-temperature ME effect below the Néel temperature $T_N = 625$ K.

We use an effective model of Mn 3$d_{x^2−y^2}$ orbitals [33],
\[
\mathcal{H}(\vec{q}) = \epsilon(\vec{q}) + V(\vec{q})\rho^z + [\vec{g}(\vec{q}) - \vec{h}] \cdot \rho^\sigma,
\]
\[
\epsilon(\vec{q}) = -2t_1(\cos q_x + \cos q_y) - 8t_2 \cos q_x/2 \cos q_y/2 \cos q_z/2,
\]
\[
V(\vec{q}) = -4\nu_1 \cos q_x/2 \cos q_y/2 - 2\nu_2 \cos q_z/2,
\]
\[
\vec{g}(\vec{q}) = \begin{bmatrix}
2\alpha_1 \sin q_x + 8\alpha_2 \sin q_y/2 \sin q_y/2 \sin q_z/2 \\
2\alpha_1 \sin q_x + 8\alpha_2 \sin q_y/2 \sin q_y/2 \sin q_z/2 \\
8\alpha_3 \sin q_x/2 \sin q_y/2 \sin q_z/2
\end{bmatrix},
\]
in which $\rho^z, \rho^\sigma$ are the Pauli matrices for the sublattice and spin degrees of freedom. $q_x = k_x a, q_y = k_y a, q_z = k_z c$ are the dimensionless wave numbers with $a,c$ being the lattice constants. $t_1, t_2$ and $\nu_1, \nu_2$ are the intra- and inter-sublattice transfer integrals, respectively. $\vec{g}(\vec{q})$ represents the spin-orbit interaction, and $\vec{h}$ is the AFM mean field. This model correctly captures the low-energy physics of magnetic hexadecapole moment and MQM [33]. The ferroic MQM suggests a room-temperature ME effect below the Néel temperature $T_N = 625$ K.

Note added. Recently, we became aware of a related paper by Gao and Xiao [67]. Their results on the orbital MQM, derived by the semiclassical theory, agree with ours. They discuss a role of the orbital MQM in nonlinear anomalous thermoelectric transport.

A.S. thanks N. Nagaosa for discussions on the Sředa formula and A. Daido for pointing out that Eq. (12) does not include the Chern-Simons 3-form. This work was supported by Grants-in-Aid for Scientific Research on Innovative Areas “J-Physics” (Grant No. JP15H05884) and “Topological Materials Science” (Grant No. JP16H00991) from the Japan Society for the Promotion of Science (JSPS), and by JSPS KAKENHI.
FIG. 1. Chemical potential dependence of the nonzero orbital MQM (a) for $\vec{h} = h\vec{z}$ and (b), (c) for $\vec{h} = h\vec{x}$ in the unit of $qh/\hbar$. The black star shows the total orbital MQM, the red square shows the itinerant contribution given by the first term in Eq. (11), and the blue circle and magenta triangle show the local contributions given by the second and third terms. The gray region shows that the system is an insulator.

(Grants No. JP15K05164 and No. JP15H05745). A.S. was supported by the RIKEN Special Postdoctoral Researcher Program.

[1] P. Santini, S. Carretta, G. Amoretti, R. Caciuffo, N. Magnani, and G. H. Lander, Rev. Mod. Phys. 81, 807 (2009).
[2] Y. Kuramoto, H. Kusunose, and A. Kiss, J. Phys. Soc. Jpn. 78, 072001 (2009).
[3] W. A. Benalcazar, B. A. Bernevig, and T. L. Hughes, Science 357, 61 (2017).
[4] W. A. Benalcazar, B. A. Bernevig, and T. L. Hughes, Phys. Rev. B 96, 245115 (2017).
[5] J. Langbehn, Y. Peng, L. Trifunovic, F. von Oppen, and P. W. Brouwer, Phys. Rev. Lett. 119, 246401 (2017).
[6] Z. Song, Z. Fang, and C. Fang, Phys. Rev. Lett. 119, 246402 (2017).
[7] M. Serra-Garcia, V. Peri, R. Ssstrunk, O. R. Bilal, T. Larsen, L. G. Villanueva, and S. D. Huber, Nature (London) 555, 342 (2018).
[8] C. W. Peterson, W. A. Benalcazar, T. L. Hughes, and G. Bahl, Nature (London) 555, 346 (2018).
[9] C. Ederer and N. A. Spaldin, Phys. Rev. B 76, 214404 (2007).
[10] N. A. Spaldin, M. Fiebig, and M. Mostovoy, J. Phys.: Condens. Matter 20, 434203 (2008).
[11] N. A. Spaldin, M. Fechner, E. Bousquet, A. Balatsky, and L. Nordström, Phys. Rev. B 88, 094429 (2013).
[12] I. E. Dzyaloshinskii, Zh. Eksp. Teor. Fiz. 37, 881 (1960) [Sov. Phys. JETP 10, 628 (1960)].
[13] D. N. Astrov, Zh. Eksp. Teor. Fiz. 38, 984 (1960) [Sov. Phys. JETP 11, 708 (1960)].
[14] D. N. Astrov, Zh. Eksp. Teor. Fiz. 40, 1035 (1961) [Sov. Phys. JETP 13, 729 (1961)].
[15] V. J. Folen, G. T. Rado, and E. W. Stalder, Phys. Rev. Lett. 6, 607 (1961).
[16] G. T. Rado and V. J. Folen, Phys. Rev. Lett. 7, 310 (1961).
[17] Y. F. Popov, A. M. Kadomtseva, G. P. Vorob’ev, V. A. Timofeeva, D. M. Ustinin, A. K. Zvezdin, and M. M. Tegeranchi, Zh. Eksp. Teor. Fiz. 114, 263 (1998) [Sov. Phys. JETP 87, 146 (1998)].
[18] T. Arima, J.-H. Jung, M. Matsubara, M. Kubota, J.-P. He, Y. Kaneko, and Y. Tokura, J. Phys. Soc. Jpn. 74, 1419 (2005).
[19] B. B. V. Aken, J.-P. Rivera, H. Schmid, and M. Fiebig, Nature (London) 449, 702 (2007).
[20] A. S. Zimmermann, D. Meier, and M. Fiebig, Nat. Commun. 5, 4796 (2014).
[21] Y. Yamaguchi and T. Kimura, Nat. Commun. 4, 2063 (2013).
[22] K. Kimura, P. Babkevich, M. Sera, M. Toyoda, K. Yamachi, G. S. Tucker, J. Martius, T. Fennell, P. Manuel, D. D. Khalyavin, R. D. Johnson, T. Nakano, Y. Nozue, H. M. Ronnow, and T. Kimura, Nat. Commun. 7, 13039 (2016).
[23] J. Wang, J. B. Neaton, H. Zheng, V. Nagarajan, S. B. Ogale, B. Liu, D. Viehland, V. Vaithyanathan, D. G. Schlom, U. V. Waghmare, N. A. Spaldin, K. M. Rabe, M. Wattig, and R. Ramesh, Science 299, 1719 (2003).
[24] T. Kimura, T. Goto, H. Shintani, T. Arima, Y. Yamaguchi, and Y. Tokura, Nature (London) 426, 55 (2003).
[25] C. D. Batista, G. Ortiz, and A. A. Aligia, Phys. Rev. Lett. 101, 077203 (2008).
[26] F. Thöle, M. Fechner, and N. A. Spaldin, Phys. Rev. B 93, 195167 (2016).
[27] Y. Gao, D. Vanderbilt, and D. Xiao, Phys. Rev. B 97, 134423 (2018).
[28] Y. Yanase, J. Phys. Soc. Jpn. 83, 014703 (2014).
[29] S. Hayami, H. Kusunose, and Y. Motome, Phys. Rev. B 84, 064477 (2015).
[30] S. Hayami, H. Kusunose, and Y. Motome, Phys. Rev. B 90, 024432 (2014).
[31] S. Hayami, H. Kusunose, and Y. Motome, Phys. Rev. B 90, 081115 (2014).
[32] S. Hayami, H. Kusunose, and Y. Motome, J. Phys.: Condens. Matter 28, 395601 (2016).
[33] H. Watanabe and Y. Yanase, Phys. Rev. B 96, 064432 (2017).
[34] R. D. King-Smith and D. Vanderbilt, Phys. Rev. B 47, 1651 (1993).
[35] D. Vanderbilt and R. D. King-Smith, Phys. Rev. B 48, 4442 (1993).
[36] R. Resta, Rev. Mod. Phys. 66, 899 (1994).
[37] K.-T. Chen and P. A. Lee, Phys. Rev. B 84, 205137 (2011).
[38] R. Nourafkan and G. Kotliar, Phys. Rev. B 88, 155121 (2013).
[39] A. Shitade, J. Phys. Soc. Jpn. 83, 033708 (2014).
[40] J. Shi, G. Vignale, D. Xiao, and Q. Niu, Phys. Rev. Lett. 99, 197202 (2007).
[41] G. Zhu, S. A. Yang, C. Fang, W. M. Liu, and Y. Yao, Phys. Rev. B 86, 214415 (2012).
[42] R. Nourafkan, G. Kotliar, and A.-M. S. Tremblay, Phys. Rev. B 90, 125132 (2014).
[43] M. Levanda and V. Fleurov, J. Phys.: Condens. Matter 6, 7889 (1994).
[44] M. Levanda and V. Fleurov, Ann. Phys. 292, 199 (2001).
[45] A. Shitade, arXiv:1708.03424.
[46] P. Streda, J. Phys. C 15, L717 (1982).
[47] V. M. Edelstein, Solid State Commun. 73, 233 (1990).
[48] A. G. Aronov and Y. B. Lyanda-Geller, Pis’ma Zh. Eksp. Teor. Fiz. 50, 398 (1989) [JETP Lett. 50, 431 (1989)].
[49] T. Yoda, T. Yokoyama, and S. Murakami, Sci. Rep. 5, 12024 (2015).
[50] S. Zhong, J. E. Moore, and I. Souza, Phys. Rev. Lett. 116, 077201 (2016).
[51] See Supplemental Material at [URL] for the derivation of the gauge-covariant gradient expansion and the orbital MQM.
[52] A. M. Essin, J. E. Moore, and D. Vanderbilt, Phys. Rev. Lett. 102, 146805 (2009).
[53] A. M. Essin, A. M. Turner, J. E. Moore, and D. Vanderbilt, Phys. Rev. B 81, 205104 (2010).
[54] A. Malashevich, S. Coh, I. Souza, and D. Vanderbilt, Phys. Rev. B 86, 094430 (2012).
[55] D. Xiao, J. Shi, and Q. Niu, Phys. Rev. Lett. 95, 137204 (2005).
[56] D. Xiao, Y. Yao, Z. Fang, and Q. Niu, Phys. Rev. Lett. 97, 026603 (2006).
[57] T. Thonhauser, D. Ceresoli, D. Vanderbilt, and R. Resta, Phys. Rev. Lett. 95, 137205 (2005).
[58] D. Ceresoli, T. Thonhauser, D. Vanderbilt, and R. Resta, Phys. Rev. B 74, 024408 (2006).
[59] J. An, A. S. Sefat, D. J. Singh, and M.-H. Du, Phys. Rev. B 79, 075120 (2009).
[60] Y. Singh, A. Ellern, and D. C. Johnston, Phys. Rev. B 79, 094519 (2009).
[61] Y. Singh, M. A. Green, Q. Huang, A. Kreyssig, R. J. McQueeney, D. C. Johnston, and A. I. Goldman, Phys. Rev. B 80, 100403 (2009).
[62] A. Pandey, R. S. Dhaka, J. Lamsal, Y. Lee, V. K. Anand, A. Kreyssig, T. W. Heitmann, R. J. McQueeney, A. I. Goldman, B. N. Harmon, A. Kaminski, and D. C. Johnston, Phys. Rev. Lett. 108, 087005 (2012).
[63] J. Lamsal, G. S. Tucker, T. W. Heitmann, A. Kreyssig, A. Jesche, A. Pandey, W. Tian, R. J. McQueeney, D. C. Johnston, and A. I. Goldman, Phys. Rev. B 87, 144418 (2013).
[64] H. Kusunose, J. Phys. Soc. Jpn. 77, 064710 (2008).
[65] M.-T. Suzuki, T. Koretsune, M. Ochi, and R. Arita, Phys. Rev. B 95, 094406 (2017).
[66] M. F. Md Din, J. L. Wang, Z. X. Cheng, S. X. Dou, S. J. Kennedy, M. Avdeev, and S. J. Campbell, Sci. Rep. 5, 11288 (2015).
[67] Y. Gao and D. Xiao, arXiv:1803.06726.