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Unlocking of time reversal, space-time inversion and rotation invariants in magnetic materials

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Time reversal (T) and space inversion are symmetries of our universe in the low-energy limit. Fundamental theorems relate their corresponding quantum numbers to the spin for elementary particles: $\hat{T}^2 = (\hat{P}\hat{T})^2 = -1$ for half-odd-integer spins and $\hat{T}^2 = (\hat{P}\hat{T})^2 = +1$ for integer spins. Here we show that for elementary excitations in magnetic materials, this "locking" between quantum numbers is lifted: $\hat{T}^2$ and $(\hat{P}\hat{T})^2$ take all four combinations of $+1$ and -1 regardless of the value of the spin, where T now represents the composite symmetry of time reversal and lattice translation. Unlocked quantum numbers lead to new forms of minimal coupling between these excitations and external fields, enabling novel physical phenomena such as the"cross-Lamor precession", indirectly observable in a proposed light-absorption experiment. We list the magnetic space groups with certain high-symmetry momenta where such excitations may be found.

Introduction Spatial inversion (P) and time reversal (T) are considered as fundamental symmetries of our universe at low energy (but are broken in weak forces)[1]. As operators, inversion acts on the spatial degrees of freedom of particles, and time reversal the internal ones: they naturally commute $[\hat{P}, \hat{T}] = 0$. (We use hatted letters for operators in Hilbert space, and unhatted ones for symmetries themselves.) Restricting the discussion to the single-particle sector of the Hilbert space, we understand that inversion squares to unity, $\hat{P}^2 = 1$, because (i) two consecutive inversions equal identity and (ii) inversion does not act on spin. Time reversal, on the other hand, an anti-unitary symmetry reversing time and inverting spin, is represented by $\hat{T} = e^{i\hat{S}_y\pi}K$, where $\hat{S}_y$ is the y-component of the spin operator. Therefore we have $\hat{T}^2 = (-1)^{2s}$, where $s(s+1)\hbar^2 = \hat{\mathbf{S}}^2$.

Symbolically, we have

$$[\hat{P}, \hat{T}] = 0, \hat{P}^2 = 1, \hat{T}^2 = (-1)^{2s}. \tag{1}$$

Eq.(1) relates the space-inversion, the time-reversal and the rotation invariants for particles in vacuum. These relations can be more concisely represented by three *invariants* $\chi_T := \hat{T}^2$, $\chi_{PT} := (\hat{P}\hat{T})^2$ and $\chi_S := (-1)^{2s}$:

$$\chi_T = \chi_{PT} = \chi_S. \tag{2}$$

For a given type of particle with spin-s, χ_T and χ_{PT} are completely fixed to be $+1$ if s is an integer (particle being boson) and -1 if s is a half-odd-integer (particle being fermion). Eq.(2) applies for any Lorentz-invariant theory given that $\hat{P}$ and $\hat{T}$ do not act on the species degrees of freedom [2, 3].

In this paper, we show that for elementary excitations in certain lattices with magnetic ordering, the three invariants, χ_S (the definition of which is modified due to the absence of continuous rotation), χ_T and χ_{PT}, are independent from each other, and can take all eight combinations, in contrast to being locked with each other as in Eq.(2) in real vacuum. Here, what T represents is not time reversal, broken by the magnetic order, but a composite symmetry of time reversal and some lattice translation, which is present in many antiferromagnets. The properties of elementary excitations having unlocked invariants are demonstrated through the example of quasiparticle excitations in magnetic space group 222.103. The unlocked invariants enable unconventional linear responses to electromagnetic field. We show that polarization operators and magnetization operators together furnish an $SO(4)$ algebra unseen, to our best knowledge, in previous studies. The $SO(4)$ algebra leads to a new type of Larmor precession, where a precession of polarization is driven by a magnetic field, and a precession of magnetization by an electric field. We propose a light-absorption experiment to observe this "cross-Larmor precession".

Invariants on a non-magnetic lattice When we put any theory on a lattice, the three-dimensional-rotation symmetry reduces to a point group symmetry, so the rotation invariant χ_S is no longer well-defined. For a modified version, we require the point group in question to contain at least three orthogonal twofold rotation axes. For example, the group D_{2h}, having three such twofold axes $C_{2x,2y,2z}$, satisfies our constraint, while the group C_{2h}, having only one, does not. The redefined rotation invariant χ_S is

$$\hat{C}_{2m}\hat{C}_{2n} = \chi_S \hat{C}_{2n}\hat{C}_{2m}, \tag{3}$$

where $m \neq n$ take values x, y, z.

In real vacuum, for any stable theory, the lowest particle excitations are near zero momentum, because this is the only special point having higher symmetry than its neighborhood. However, on a lattice, the elementary excitation may also appear at the corners of the Brillouin

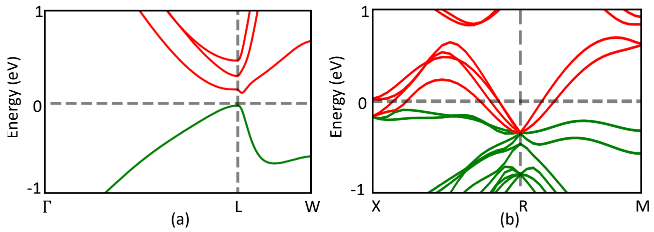

FIG. 1: Electron excitations centering at BZ corners. (a) In SnTe, the conduction bottom (and valence top) is located at L instead of Γ. (b) In BaPPt, the conduction and the valence bands touch each other at R. In both cases, there are bands of elementary excitations centering at some nonzero and high-symmetry momentum. These band structures are downloaded from http://materiae.iphy.ac.cn

zone (BZ), which are nonzero crystal momenta with highest symmetry in the neighborhood[4]. This is the case when, for example, the band bottom of the conduction band appears at a BZ corner [Fig.1(a)], or when the conduction and the valence bands touch each other at some BZ corner [Fig.1(b)].

Yet another complication in lattices is that some spatial symmetries are neither point-group operations nor lattice translations, but are composite operations of a point-group operation and a fractional lattice translation. Lattice symmetry groups containing these spatial symmetries are called nonsymmorphic space groups[5]. Consider for example space group $Pbca$, generated by three orthogonal lattice translations $t_{\mathbf{x},\mathbf{y},\mathbf{z}}$ along x,y,z-directions with lattice constants a,b,c, respectively, space inversion about the origin, P, and three twofold screw axes parallel to x,y,z-axes, $C_{2x}\rightarrow 2_{100}t_{\mathbf{x}/2+\mathbf{y}/2}, C_{2y}\rightarrow 2_{010}t_{\mathbf{y}/2+\mathbf{z}/2}, C_{2z}\rightarrow 2_{001}t_{\mathbf{x}/2+\mathbf{z}/2}$; 2_{mnl} represents a π-rotation on both spatial coordinates and spin components about the $[mnl]$-direction, where $[mnl]$ are Miller indices. $t_{d_1\mathbf{x}+d_2\mathbf{y}+d_3\mathbf{z}}$ represents translation by $d_1\mathbf{x}a+d_2\mathbf{y}b+d_3\mathbf{z}c$ where $\mathbf{x},\mathbf{y},\mathbf{z}$ are unit vectors and a,b,c lattice constants. It is straightforward to check that $\hat{C}_{2x}\hat{C}_{2y}=(-1)^{2s_0}\hat{C}_{2y}\hat{C}_{2x}\hat{t}_{-\mathbf{x}+\mathbf{y}+\mathbf{z}}$. Here s_0 is the physical spin of the particle, $2s_0\in even$ for bosons and $2s_0\in odd$ for fermions. Consider excitations at $\mathbf{R}=(\pi/a,\pi/b,\pi/c)$, where $\hat{t}_{-\mathbf{x}+\mathbf{y}+\mathbf{z}}=-1$, then we have $\chi_S=-(-1)^{2s_0}$. The additional minus sign means that the half-lattice translations give a "twist" to the rotation invariant, making integer spins look like half-odd-integer spins, and vice versa[6].

However, on a nonmagnetic, centrosymmetric lattice, similar twist does not occur in the invariants (χ_T,χ_{PT}). For excitations on any nonmagnetic lattice, we always have $\chi_T=\chi_{PT}=(-1)^{2s_0}$. Therefore, for excitations at $\mathbf{R}=(\pi/a,\pi/b,\pi/c)$ in space group $Pbca$, we have

$$\chi_T=\chi_{PT}=-\chi_S. \tag{4}$$

Further unlocking of invariants on a magnetic lattice Is it possible to further unlock the values of χ_T and χ_{PT} from the constraint $\chi_T=\chi_{PT}$? We seek this possibility in elementary excitations in magnetically ordered lattices, the band topology of which has recently become a research focus[7–14]. While the physical time reversal is broken by magnetism, many antiferromagnetic materials preserve a symmetry in the form $T\rightarrow T_{phy}t_{\mathbf{L}/2}$, where T_{phy} is pure time reversal operator acting only on internal degrees of freedom, and $\mathbf{L}/2$ is a lattice vector (which becomes a half-lattice vector in the magnetic unit cell)[7, 8]. Symmetries of magnetic systems are classified by magnetic space groups, and when the above T is a symmetry, the magnetic space groups are called type-IV[15]. When this is the case, excitations at any time-reversal invariant momentum in the magnetic Brillouin zone (mBZ) have this T symmetry. We then naturally redefine χ_T as $\chi_T\equiv\hat{T}^2=(\hat{T}_{phy}\hat{t}_{\mathbf{L}/2})^2$. As expected, the translation part in T in general changes the value of χ_T, and could also make P and T not commute[7, 12]. One can use the theory of projective representations to show that (χ_T,χ_{PT}) can take all possible values of $(+1,+1)$, $(+1,-1)$, $(-1,+1)$ and $(-1,-1)$, irrespective of the rotation invariant χ_S. Let us use an example to illustrate one of these possibilities here, and defer the general proof in Table S3 of supplementary materials (SM).

In Fig.2, a conjectured magnetic structure of NdZn[13, 16] (magnetic space group 222.103) is shown. Looking from O or O', the magnetic structure is invariant under all proper rotations of a cube (point group O); the structure is also centro-symmetric about I, and has a composite symmetry $T\rightarrow T_{phy}t_{(\mathbf{x}+\mathbf{y}+\mathbf{z})/2}$, where $(\mathbf{x}+\mathbf{y}+\mathbf{z})/2$ is a lattice vector of the nonmagnetic lattice. It is straightforward to check $\hat{T}^2=(-1)^{2s_0}\hat{t}_{\mathbf{x}+\mathbf{y}+\mathbf{z}}$, $\hat{P}\hat{T}=\hat{t}_{\mathbf{x}+\mathbf{y}+\mathbf{z}}\hat{T}\hat{P}$, and $\chi_S=(-1)^{2s_0}$. Therefore, at mBZ corner $\mathbf{R}=(\pi/a,\pi/a,\pi/a)$, we have

$$\chi_T=-\chi_{PT}=-\chi_S. \tag{5}$$

For magnons on this lattice, we have $(\chi_S,\chi_T,\chi_{PT})=(+1,-1,+1)$, and for electrons $(-1,+1,-1)$, neither of which is possible on nonmagnetic lattices.

Effective theory with minimal coupling In quantum field theory, particles couple to an external source (field) if there exists a bilinear of particle field operators that carries the same symmetry representation as the one carried by the source. The form of coupling hence depends on the projective representation carried by particle field, as well as the linear representation carried by the external field (generally some tensor representation). The symmetry invariants $\chi_{S,T,PT}$ do not denote specific representations, but classes of representations. For example, for group $SO(3)$, all integer spins belong to one class ($\chi_S=1$) while all half-odd-integer spins to another class ($\chi_S=-1$).

We postpone the former definition of "classes of repre-

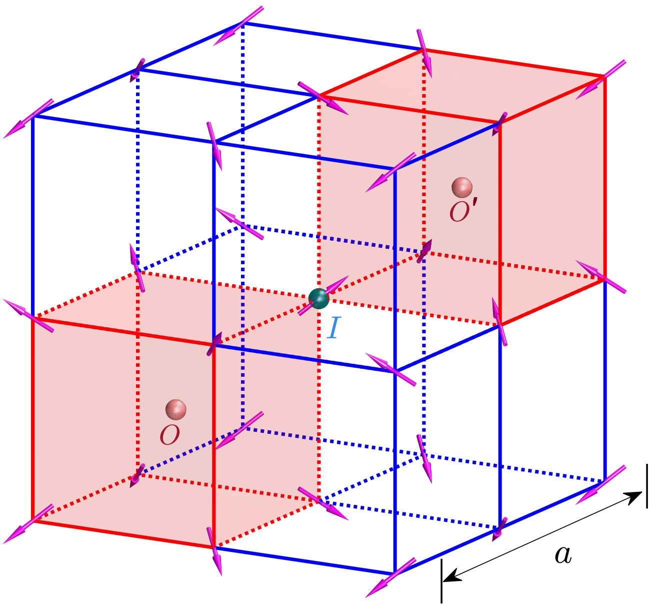

FIG. 2: The magnetic unit cell with lattice constant a of a magnetic structure having magnetic space group 222.103, conjectured as the symmetry for the magnetic ground state of NdZn. Yellow circles O, O' are body centers of point group symmetry O, and orange circle I is an inversion center. T is time reversal combined with a lattice translation that relates the two cubes outlined in red. The local moments are polarized so that they are all-out with respect to O and all-in with respect to O'.

sentations" and invariants to a later part. For now, we only need that fact that new invariants unlocked in magnetic systems allow new classes of representations for field operators, which in turn bring about new forms of linear coupling to external sources such as applied electromagnetic field and strain tensor field. We restrict the discussion to electron excitations, $s_0 = 1/2$, linearly coupled to an electromagnetic field. Physically, since electrons have charge, the electromagnetic field has two effects: the orbital effect that changes the crystal momentum of the electron in a fixed band structure, and the Zeeman effect which modifies the periodic part of Bloch wavefunctions at each momentum, thereby modifying the band structure itself[17]. The invariants, $\chi_{S,T,PT}$, have little to do with the first effect, so we focus on the second, altogether ignoring the change of crystal momentum by the external fields.

Again let us use the magnetic lattice in Fig.2 as the example, and focus on mBZ corner $\mathbf{R} = (\pi/a, \pi/a, \pi/a)$ having little co-group $G_{\mathbf{R}} = O_h \times Z_2^T$. There are three different irreducible representations, $R_{1/2}$ and $R^{\pm}_{3/2}$, of $G_{\mathbf{R}}$, all satisfying $(\chi_S, \chi_T, \chi_{PT}) = (-1, +1, -1)$. Here we pick one representation $R_{1/2}$ for our analysis, where the generators are given by

$$\begin{aligned}
\hat{T} &= \tau_y\sigma_y K, \\
\hat{P} &= i\tau_y, \\
\hat{C}_{2x} &= i\sigma_x, \\
\hat{C}_{31} &\equiv \hat{C}_{3,111} = -\exp(-i\sigma_{111}\pi/3), \\
\hat{C}_{4z} &= i\tau_z \exp(-i\sigma_z\pi/4),
\end{aligned} \tag{6}$$

where $C_{3,111}$ is the threefold rotation about the [111]-direction, and $\sigma_{111} \equiv (\sigma_x + \sigma_y + \sigma_z)/\sqrt{3}$. Group theory allows us to classify all hermitian bilinears of field operators in the form $\psi^\dagger\tau_\mu\sigma_\nu\psi$ into the representations of the symmetry group, listed in Table I. On the other hand, all monomials of crystal momentum relative to $\mathbf{R}$, $\mathbf{q} = \mathbf{k} - \mathbf{R}$, and the components of electric, magnetic and strain fields can also be put into these representations, also summarized in Table I.

Matching the representations between fermion bilinear operators and monomials of momenta and of fields, we find the effective theory with minimal couplings. The free part of the theory is obtained by matching the monomials of momenta to the bilinears:

$$h_0[\psi] = -\frac{1}{2m}\int dr^3 \psi^\dagger \tau_y(\sigma_x\partial^2_{yz} + \sigma_y\partial^2_{zx} + \sigma_z\partial^2_{xy})\psi. \tag{7}$$

The minimal coupling terms to the electric field are

$$h_E[\psi, \mathbf{E}] = -\lambda_E \mathbf{E} \cdot \int dr^3 \psi^\dagger \tau_z \boldsymbol{\sigma}\psi; \tag{8}$$

the minimal coupling terms to the magnetic field

$$h_B[\psi, \mathbf{B}] = -\lambda_B \mathbf{B} \cdot \int dr^3 \psi^\dagger \boldsymbol{\sigma}\psi, \tag{9}$$

where $\lambda_{E,B}$ are coupling constants. From Eq.(8,9), we have the effective polarization and magnetization operators:

$$\begin{aligned}
\hat{P}_i &= -\frac{\delta\,(h_0 + h_E + h_B)}{\delta E_i} = \lambda_E \tau_z \sigma_i, \\
\hat{M}_i &= -\frac{\delta\,(h_0 + h_E + h_B)}{\delta B_i} = \lambda_B \sigma_i.
\end{aligned} \tag{10}$$

We note that Eq. (10) implies the quantum nature of polarization $\hat{P}_i$ in this minimal effective theory, as different components do not commute

$$[\hat{p}_i, \hat{p}_j] = i\epsilon_{ijk}\hat{m}_k, [\hat{p}_i, \hat{m}_j] = i\epsilon_{ijk}\hat{p}_k, \tag{11}$$

where we have defined the dimensionless reduced dipole operator $\hat{p}_i \equiv \hat{P}_i/(2\lambda_E)$ and magnetization operator $\hat{m}_i \equiv \hat{M}_i/(2\lambda_B)$.

Hidden $SO(4)$ algebra, cross-Larmor precession and absorption The commutation relations in Eq.(11) imply that $\hat{p}_i$ and $\hat{m}_i$ together form an $SO(4)$ algebra. Consider one quasiparticle magnetically polarized in the z-direction, that is, $\hat{m}_z|\psi(q = 0)\rangle = |\psi(q = 0)\rangle$. At $t = 0$,

TABLE I: Classification of hermitian operators, monomials of relative momentum and external electric, magnetic and strain tensor fields into their respective irreducible representations of $O_h \times Z_2^T$, for a minimal effective theory having symmetries given in Eq.(6). The symbols of the irreducible representations follow the conventional definition of Ref.[5], and the $\pm$ in superscript denotes whether this representation changes sign under $\hat{T}$. $\mathbf{B} \star \mathbf{q}$ stands for $(B_y q_z + B_z q_y, B_z q_x + B_x q_z, B_x q_y + B_y q_x)$.

Irreducible representation	A_{2u}^-	A_{2g}^-	A_{1u}^-	T_{2u}^+	T_{2g}^+	T_{1u}^+	T_{1g}^-	A_{1g}^+
bilinear Operators	$\psi^\dagger \tau_x \psi$	$\psi^\dagger \tau_y \psi$	$\psi^\dagger \tau_z \psi$	$\psi^\dagger \tau_x \sigma_i \psi$	$\psi^\dagger \tau_y \sigma_i \psi$	$\psi^\dagger \tau_z \sigma_i \psi$	$\psi^\dagger \sigma_i \psi$	$\psi^\dagger \psi$
Applied fields		$B_x B_y B_z$	$\mathbf{E} \cdot \mathbf{B}$		$(E_y E_z, E_x E_z, E_x E_y)$ $(B_y B_z, B_x B_z, B_x B_y)$ $(\epsilon_{yz}, \epsilon_{xz}, \epsilon_{xy})$	E_i	B_i	E^2 B^2
Monomials of momentum	$q_x q_y q_z$				$(q_y q_z, q_x q_z, q_x q_y)$			q^2
cross coupling	$\epsilon_{yz} q_x + \epsilon_{zx} q_y + \epsilon_{xy} q_z$			$(\mathbf{B} \star \mathbf{q})_i$		$(\mathbf{B} \times \mathbf{q})_i$	$(\mathbf{E} \times \mathbf{q})_i$	$\mathbf{E} \times \mathbf{B} \cdot \mathbf{q}$

an electric field is applied along x-direction. According to Eq.(11), at $t > 0$, we have

$$[\cos(2\lambda_E t)\hat{m}_z + \sin(2\lambda_E t)\hat{p}_y]|\psi(t)\rangle = |\psi(t)\rangle. \quad (12)$$

Specially, at $t = (n - 1/4)\pi/\lambda_E$, the quasiparticle is completely electrically polarized along y-direction, and is spin unpolarized $\langle\psi(t)|\hat{m}_i|\psi(t)\rangle = 0$. Therefore an electric field rotates a magnetic dipole into an electric dipole, hence the name "cross-Larmor precession".

How could cross-Larmor precession be observed in experiments? The original Larmor precession is observed in the absorption in ferrogmagnets[18], where two elements are essential: a polarized spin configuration and an oscillating magnetic field component perpendicular to the magnetization. In our system, we first use a magnetic field $\mathbf{B}_0$ to spin-polarize the electrons at $\mathbf{q} = 0$ along z-direction. Then we use a polarized light propagating along y-direction, the $\mathbf{E}$-vector of which is polarized in the x-direction. With this geometry the Larmor precession is minimized, because the $\mathbf{B}$-vector of the light is parallel to the spin polarization. The cross-Larmor precession, on the other hand, is maximized because the electric field is perpendicular to the spin polarization. We therefore predict a resonant absorption edge at a frequency $|2\lambda_B \mathbf{B}_0|$, assuming that the system be exactly at half-filling. This is what we call a cross-resonant absorption, because the level splitting is obtained using a magnetic field, while the resonance is realized using an electric field. While $SO(4)$ algebra in Eq.(11) is a sufficient, but not necessary, condition for the presence of cross-resonant absorption. An example illustrating the non-necessity is shown in sec.S4 of SM, where the other two representations at $\mathbf{R}$ in 222.103 are analyzed. There we show, though the $SO(4)$ algebra no longer holds, the cross-resonant absorption is still present. We emphasize that neither the $SO(4)$ algebra nor the cross-resonant absorption is restricted to a specific momentum $[\mathbf{R} = (\pi/a, \pi/a, \pi/a)]$ or a specific magnetic space group (222.103). The little group at $\mathbf{R}$ in 222.103 is $G_\mathbf{R} = O_h \times Z_2^T$. As one breaks O_h down to T_h, D_{4h} and D_{2h}, one finds that $R_{1/2}$ remains an irreducible representation. When $G_\mathbf{R} = T_h \times Z_2^T$, both the $SO(4)$ algebra and the cross-resonant absorption hold; and as $G_\mathbf{R}$ is reduced to $D_{4h,2h} \times Z_2^T$, the polarization operators $\hat{p}_{x,y,z}$ and magnetization operators $\hat{m}_{x,y,z}$ no longer form the six generators of $SO(4)$, but the cross-resonant absorption still appears (See sec.S3 of SM for the derivation of the above statements). Due to the preservation of cross-resonant absorption in symmetry reduction, we predict that at least four magnetic space groups (222.103, 223.109, 200.17 and 201.21) in which certain irreducible representations at $\mathbf{R}$ shows $SO(4)$, and 12 groups (222.103, 223.109, 200.17, 201.21, 126.386, 130.432, 131.446, 135.492, 47.256, 48.264, 55.361 and 56.373) that potentially host cross-resonant absorption.

Guidelines for finding materials The four combinations $(\chi_S, \chi_T, \chi_{PT}) = (-1,+1,-1), (+1,-1,+1), (+1,+1,-1), (-1,-1,+1)$ are restricted to magnetic materials, realized as elementary excitations with momentum at corners of the mBZ, and they bring about novel physical effects as are discussed above. Hence it is vital that we provide clues as to where these excitations may be found in real materials. In mathematics, invariants such as χ_T, χ_{PT} and χ_S exactly correspond to the invariants of the second group cohomology[19], $\mathcal{H}^2[G_\mathbf{Q}, U(1)]$, of the little co-group $G_\mathbf{Q}$, which classify the projective representations of $G_\mathbf{Q}$. Here we insert a few technical comments on $G_\mathbf{Q}$. As we focus on the elementary excitations centered at high-symmetry momentum $\mathbf{Q}$, the full magnetic space group M is reduced to the little group $M(\mathbf{Q}) \subset M$ that leaves $\mathbf{Q}$ invariant, up to a reciprocal lattice vector. This little group has lattice translation Tr as its normal subgroup, so that a quotient group can be defined $M(\mathbf{Q})/Tr$, which is always isomorphic to a magnetic point group $G_\mathbf{Q}$, called the little co-group of M at $\mathbf{Q}$. As far as type-IV magnetic space groups are concerned, $G_\mathbf{Q}$ has the simple structure of a point group direct-product time reversal. The invariants of each of the 32 $G_\mathbf{Q}$'s can be calculated, and are listed in Table S1.

However, it is not obvious that all the possible values of these invariants may be taken in elementary excitations of real materials. While we are unable to address this general question, a full answer can be obtained, when the discussion is restricted to excitations that form bands (magnon or electron). Throughout this article, symbols such as C_{2x} or T all refer to elements of some $G_{\mathbf{Q}}$. Yet, one should keep in mind that physically, $g \in G_{\mathbf{Q}}$ represent a coset in $M(\mathbf{Q})/Tr$, out of which a representative element $\tilde{g} \in M(\mathbf{Q})$ may be chosen. A degenerate-multiplet of Bloch eigenstates at $\mathbf{Q}$ can either be considered as a *projective* representation of $G_{\mathbf{Q}}$, or a linear representation of $M(\mathbf{Q})$. Generically, $\tilde{g}$ contains a fractional lattice translation, and the fractional translations and the particle statistics in $\tilde{g}$ uniquely determine the invariants of $G_{\mathbf{Q}}$[20]. In sec.S2 of SM, we calculate the invariants for each high-symmetry momentum in every type-IV magnetic space group. In Table S4, we list all magnetic space groups with respective high-symmetry momenta where magnons and electrons carry $(\chi_S, \chi_T, \chi_{PT}) = (-1,+1,-1),(+1,-1,+1),(+1,+1,-1),(-1,-1,+1)$, values restricted to magnetic systems.

A final technical remark on terminologies. We use “quantum numbers” and “invariants” inter-changeably for readability, as the former concept is familiar to non-experts. Rigorously speaking they are certainly not the same: different quantum numbers correspond to different irreducible representations, while different invariants refer to different classes of representations. The invariants of $G_{\mathbf{Q}}$ solely depends on M and $\mathbf{Q}$, and all the representations at $\mathbf{Q}$ share the same set of invariants.

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Figures

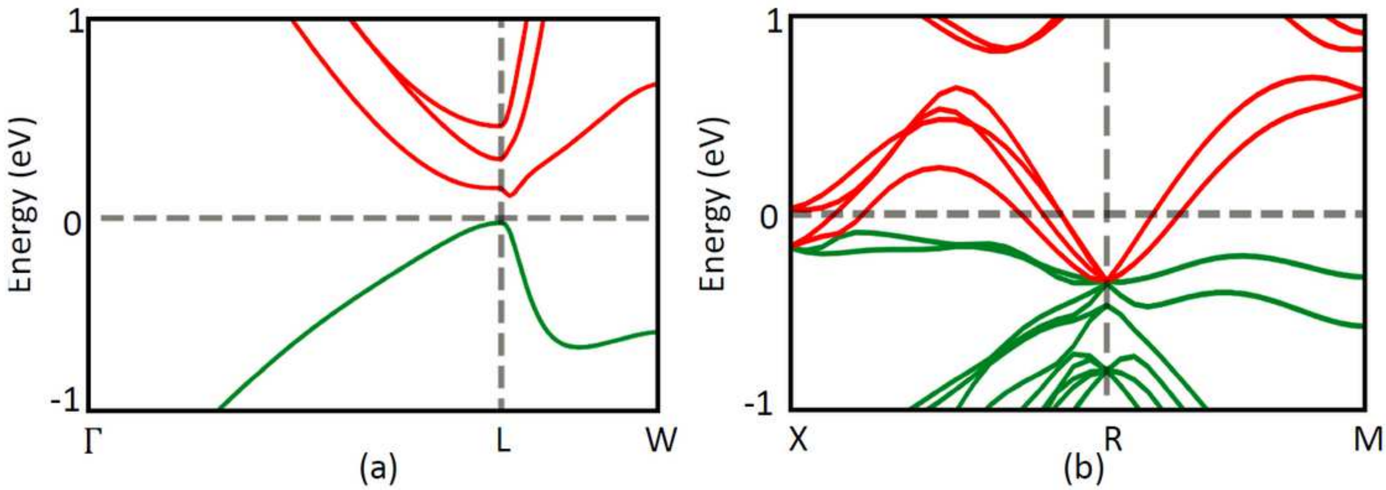

Figure 1

Electron excitations centering at BZ corners. (a) In SnTe, the conduction bottom (and valence top) is located at L instead of Γ. (b) In BaPPt, the conduction and the valence bands touch each other at R. In both cases, there are bands of elementary excitations centering at some nonzero and high-symmetry momentum. These band structures are downloaded from http://materiae.iphy.ac.cn

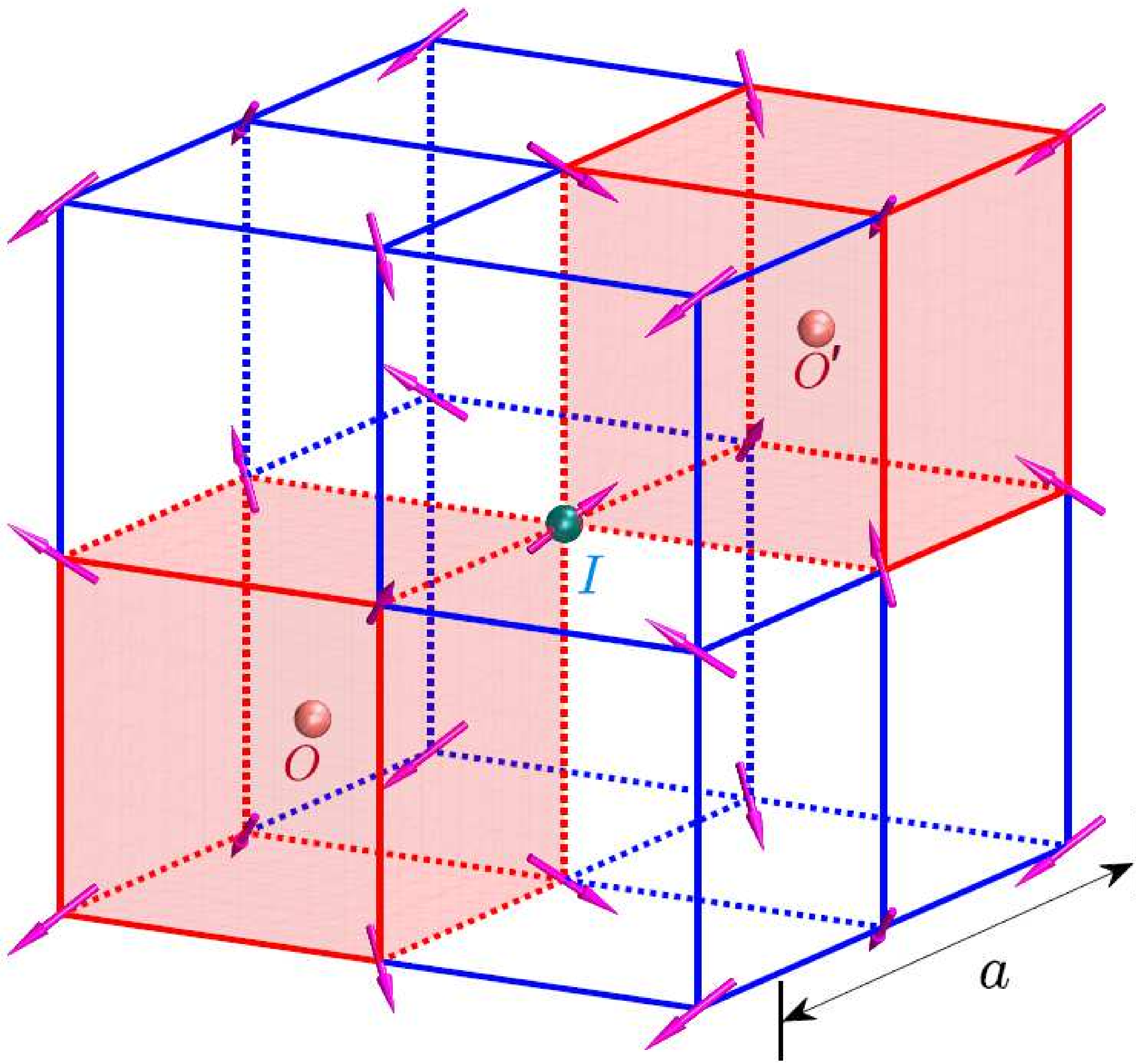

Figure 2

The magnetic unit cell with lattice constant a of a magnetic structure having magnetic space group 222.103, conjectured as the symmetry for the magnetic ground state of NdZn. Yellow circles O;O0 are body centers of point group symmetry O, and orange circle I is an inversion center. T is time reversal combined with a lattice translation that relates the two cubes outlined in red. The local moments are polar- ized so that they are all-out with respect to O and all-in with respect to O0.

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- SupMatver1.pdf