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: \( T^2 = (PT)^2 = -1 \) for half-odd-integer spins and \( T^2 = (PT)^2 = +1 \) for integer spins. Here we show that for elementary excitations in magnetic materials, this “locking” between quantum numbers is lifted: \( T^2 \) and \( (PT)^2 \) 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-Larmor 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 \( \hat{T} = e^{i\hat{S}_y s}K \), where \( \hat{S}_y \) is the y-component of the spin operator. Therefore we have \( T^2 = (-1)^{2s} \), where \( s(s+1)h^2 = \hat{S}^2 \).

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-\( s \), \( \chi_T \) and \( \chi_{PT} \) 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, \( \chi_S \) (the definition of which is modified due to the absence of continuous rotation), \( \chi_T \) and \( \chi_{PT} \), 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 \( \chi_S \) 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 \( \hat{C}_{2x}, \hat{C}_{2y}, \hat{C}_{2z} \), satisfies our constraint, while the group \( C_{2h} \), having only one, does not. The redefined rotation invariant \( \chi_S \) 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
Further unlocking of invariants on a magnetic lattice

Is it possible to further unlock the values of $\chi_T$ and $\chi_{PT}$ 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 $T \rightarrow T_{phy}T_{1/2}$, where $T_{phy}$ is pure time reversal operator acting only on internal degrees of freedom, and $T_{1/2}$ 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 $\chi_T$ as $\chi_T \equiv T^2 = (T_{phy}T_{1/2})^2$. As expected, the translation part in $T$ in general changes the value of $\chi_T$, and could also make $P$ and $T$ not commute[7, 12]. One can use the theory of projective representations to show that $(\chi_T, \chi_{PT})$ can take all possible values of $(+1, +1)$, $(+1, -1)$, $(-1, +1)$ and $(-1, -1)$, irrespective of the rotation invariant $\chi_S$. 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 $T \rightarrow T_{phy}(\pi \times y+z/2)$, where $(x+y+z)/2$ is a lattice vector of the nonmagnetic lattice. It is straightforward to check $T^2 = (-1)^{2\nu_0}t_{x+y+z}$, $P^2 = t_{x+y+z}PT$, and $\chi_S = (-1)^{\nu_0}$. Therefore, at mBZ corner $R = (\pi/a, \pi/b, \pi/c)$, we have

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

(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-
we pick one representation
different irreducible representations,
example, and focus on mBZ corner
with the first effect, so we focus on the second, altogether
nature itself[17]. The invariants,
and thereby modifying the band struc-
ture itself. The invariants,
around 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 $O'$.

\[ \hat{T} = \tau_z \sigma_y K, \]  
\[ \hat{P} = i \tau_y, \]  
\[ \hat{C}_{2x} = i \sigma_x, \]  
\[ \hat{C}_{31} = \hat{C}_{3,111} = -\exp(-i\sigma_{111}\pi/3), \]  
\[ \hat{C}_{4z} = i \tau_z \exp(-i\sigma_2\pi/4), \]

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:
\[ h_0[\psi] = -\frac{1}{2m} \int d^3 \psi i \tau_y (\sigma_x \partial_y^2 + \sigma_y \partial_x^2 + \sigma_z \partial_z^2) \psi. \]  

The minimal coupling terms to the electric field are
\[ h_E[\psi, \mathbf{E}] = -\lambda_E \mathbf{E} \cdot \int d^3 \psi i \tau_y \sigma \psi; \]
the minimal coupling terms to the magnetic field
\[ h_B[\psi, \mathbf{B}] = -\lambda_B \mathbf{B} \cdot \int d^3 \psi i \sigma \psi, \]
where $\lambda_{E,B}$ are coupling constants. From Eq.(8,9),
we have the effective polarization and magnetization operators:
\[ \hat{P}_i = -\frac{\delta (h_0 + h_E + h_B)_{i}}{\delta E_i} = \lambda_E \tau_z \sigma_i, \]  
\[ \hat{M}_i = -\frac{\delta (h_0 + h_E + h_B)_{i}}{\delta B_i} = \lambda_B \sigma_i. \]

We note that Eq. (10) implies the quantum nature of po-
larization $\hat{P}_i$ in this minimal effective theory, as different
components do not commute
\[ [\hat{P}_i, \hat{P}_j] = i \epsilon_{ijk} \hat{m}_k, [\hat{P}_i, \hat{m}_j] = i \epsilon_{ijk} \hat{p}_k, \]
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. Con-
sider one quasiparticle magnetically polarized in the $z$-
direction, that is, $\hat{m}_z |\psi(q = 0)\rangle |\psi(q = 0)\rangle$. At $t = 0,$
an electric field is applied along $x$-direction. According to Eq. (11), at $t > 0$, we have

$$\left[ \cos(2 \lambda_F t) \hat{m}_z + \sin(2 \lambda_F t) \hat{p}_y \right] \psi(t) = \psi(t).$$

(12)

Specially, at $t = (n - 1/4) \pi/\lambda_F$, the quasiparticle is completely electrically polarized along $y$-direction, and is spin unpolarized $\langle \psi(t) | \hat{m}_z | \psi(t) \rangle = 0$. 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 experiments 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 $B_y$ to spin-polarize the electrons at $q = 0$ along $z$-direction. Then we use a polarized light propagating along $y$-direction, the $E$-vector of which is polarized in the $x$-direction. With this geometry the Larmor precession is minimized, because the $B$-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 $2 \lambda_B B_0$, assuming that the system is 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 $G_{\mathbf{R}} = O_h \times Z^2_2$. 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 $G_{\mathbf{R}} = T_h \times Z^2_2$, both the $SO(4)$ algebra and the cross-resonant absorption hold; and as $G_{\mathbf{R}}$ is reduced to $D_{4h,2h} \times Z^2_2$, the polarization operators $p_{x,y,z}$ 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 $\chi_T$ and $\chi_{PT}$ exactly correspond to the invariants of the second group cohomology[19], $H^2[G_{\mathbf{Q}}, U(1)]$, 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 $T\mathbf{R}$ as its normal subgroup, so that a quotient group can be defined $M(\mathbf{Q})/T\mathbf{R}$, 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

| Irreducible representation | $A_{-2u}$ | $A_{2g}$ | $A_{1u}$ | $T_{2u}^+$ | $T_{2g}^+$ | $T_{1u}^+$ | $T_{1g}^-$ | $A_{1g}$ | $B_{1g}$ |
|---------------------------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|----------|
| bilinear Operators | $\psi' \tau_x \psi$ | $\psi' \tau_y \psi$ | $\psi' \tau_z \psi$ | $\psi' \tau_x \sigma_1 \psi$ | $\psi' \tau_y \sigma_1 \psi$ | $\psi' \tau_z \sigma_1 \psi$ | $\psi' \sigma_1 \psi$ | $\psi' \psi$ | $\psi' \psi$ |
| Applied fields | $B_x B_y B_z$ | $E \cdot B$ | $(E_x E_z, E_x E_y, E_y E_z)$ | $(E_x B_z, B_x B_z, B_z B_y)$ | $(\epsilon_{y z}, \epsilon_{x z}, \epsilon_{x y})$ | $E_i$ | $B_i$ | $E^2$ | $B^2$ |
| Monomials of momentum | $q_x q_y q_z$ | $(q_y q_x, q_z, q_y)$ | $(B \times q)_i$ | $(E \times q)_i$ | $(E \times B \cdot q)$ |

TABLE I: Classification of hermitian operators, monomials of relative momentum and external electric, magnetic and strain tensor fields into their respective irreducible representations of $O_h \times Z^2_2$, 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 ± in superscript denotes whether this representation changes sign under $\hat{T}$. $B \cdot q$ stands for $(B_q B_x + B_q B_y + B_q B_z)$.
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 $G_{2x}$ or $T$ all refer to elements of some $G_Q$. Yet, one should keep in mind that physically, $g \in G_Q$ represent a coset in $M(Q)/T$, out of which a representative element $\tilde{g} \in M(Q)$ may be chosen. A degenerate-multiplet of Bloch eigenstates at $Q$ can either be considered as a projective representation of $G_Q$, or a linear representation of $M(Q)$. Generically, $\tilde{g}$ contains a fractional lattice translation, and the fractional translations and the particle statistics in $\tilde{g}$ uniquely determine the invariants of $G_Q$ [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” interchangeably 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 $G_Q$ solely depend on $M$ and $Q$, and all the representations at $Q$ share the same set of invariants.

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[1] T. D. Lee, R. Oehme, and C. N. Yang, Phys. Rev. 106, 340 (1957), URL https://link.aps.org/doi/10.1103/PhysRev.106.340.

[2] R. Streater and A. Wightman, *PCT, spin and statistics, and all that* (Princeton University Press, 1989), ISBN 978-0-691-07062-1.

[3] S. Weinberg, *The Quantum theory of fields. Vol. 1: Foundations* (Cambridge University Press, 2005), ISBN 978-0-521-67053-1, 978-0-511-25204-4.

[4] M. G. Vergniory, L. Elcoro, Z. Wang, J. Cano, C. Felser, M. I. Aroyo, B. A. Bernevig, and B. Bradlyn, Phys. Rev. E 96, 023310 (2017), URL https://link.aps.org/doi/10.1103/PhysRevE.96.023310.

[5] C. Bradley and A. Cracknell, *The Mathematical Theory of Symmetry in Solids: Representation Theory for Point Groups and Space Groups*, EBSCO ebook academic collection (OUP Oxford, 2010), ISBN 9780195828376, URL https://books.google.com/books?id=MQUDDAAQBAJ.

[6] B. Bradlyn, J. Cano, Z. Wang, M. G. Bernevig, C. Felser, R. J. Cava, and B. A. Bernevig, Science 353 (2016), ISSN 0036-8075, URL https://science.sciencemag.org/content/353/6299/aaf537.full.pdf, URL https://science.sciencemag.org/content/353/6299/aaf537.

[7] R. S. K. Mong, A. M. Essin, and J. E. Moore, Phys. Rev. B 81, 245209 (2010), URL https://link.aps.org/doi/10.1103/PhysRevB.81.245209.

[8] C. Fang, M. J. Gilbert, and B. A. Bernevig, Phys. Rev. B 88, 085406 (2013), URL https://link.aps.org/doi/10.1103/PhysRevB.88.085406.

[9] C. Fang, M. J. Gilbert, and B. A. Bernevig, Phys. Rev. Lett. 112, 106401 (2014), URL https://link.aps.org/doi/10.1103/PhysRevLett.112.106401.

[10] H. Watanabe, H. C. Po, and A. Vishwanath, Science Advances 4 (2018), URL https://advances.sciencemag.org/content/4/8/eaat8685.full.pdf, URL https://advances.sciencemag.org/content/4/8/eaat8685.

[11] G. Hua, S. Nie, Z. Song, R. Yu, G. Xu, and K. Yao, Physical Review B 98, 201116 (2018).

[12] J. Cano, B. Bradlyn, and M. G. Bernevig, APL Materials 7, 101125 (2019), https://doi.org/10.1063/1.5124314, URL https://doi.org/10.1063/1.5124314.

[13] Y. Xu, L. Elcoro, Z. Song, B. J. Wieder, M. G. Vergniory, N. Regnault, Y. Chen, C. Felser, and B. A. Bernevig, *High-throughput calculations of antiferromagnetic topological materials from magnetic topological quantum chemistry* (2020), 2003.00112.

[14] J. Zou, Q. Xie, G. Xu, and Z. Song, National Science Review (2020), ISSN 2095-5138, nwwa169, https://academic.oup.com/nsr/article-pdf/doi/10.1093/nsr/nwwa169/33528562/nwwa169.pdf, URL https://doi.org/10.1093/nsr/nwwa169.

[15] C. J. BRADLEY and B. L. DAVIES, Rev. Mod. Phys. 40, 359 (1968), URL https://link.aps.org/doi/10.1103/RevModPhys.40.359.

[16] S. V. Gallego, J. M. Perez-Mato, L. Elcoro, E. S. Tasci, R. M. Hanson, K. Momma, M. I. Aroyo, and G. Madarica, Journal of Applied Crystallography 49, 1750 (2016), URL https://doi.org/10.1107/S1600576716012863.

[17] I. Andoscar, *Concepts in Solids: Lectures on the Theory of Solids*, Advanced book classics series (World Scientific, 1997), ISBN 9789810232313, URL https://books.google.com/books?id=2NEKzzbMBrQG.

[18] J. H. E. Griffiths, Nature 158, 670 (1946), URL https://doi.org/10.1038/158670a0.

[19] A. Hatcher, *Algebraic Topology* (Cambridge University Press, 2005), ISBN 9780521517499, URL https://books.google.com/books?id=cFgAPAAACAAJ.

[20] J.-Q. Chen, M.-J. Gao, and G.-Q. Ma, Rev. Mod. Phys. 57, 211 (1985), URL https://link.aps.org/doi/10.1103/RevModPhys.57.211.